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

Leticia F. Cugliandolo\textsuperscript{a}, Giuseppe Gonnella\textsuperscript{b}, Antonio Suma\textsuperscript{c}

\textsuperscript{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
\textsuperscript{b}Dipartimento di Fisica, Università di Bari and INFN, Sezione di Bari, via Amendola 173, Bari, I-70126, Italy
\textsuperscript{c}SISSA - Scuola Internazionale Superiore di Studi Avanzati, Via Bonomea 265, 34136 Trieste Italy

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.

Keywords: diffusion processes, active matter

1. Introduction

Active matter is characterised 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 \cite{1, 2}. All these systems live, or function, in conditions far from thermodynamic

Email addresses: leticia@lpthe.jussieu.fr (Leticia F. Cugliandolo), gonnella@ba.infn.it (Giuseppe Gonnella), antonio.suma@gmail.com (Antonio Suma)
equilibrium and pose challenging questions to non-equilibrium statistical mechanics. Active matter exhibits non-trivial collective properties that have no analogue 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 \[3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13\].

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 \[15, 16, 17, 18\].

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

\[
F_{\text{fene}} = -\frac{k r}{1 - (r^2/r_0^2)},
\]

with \(k > 0\) and \(r = r_1 - r_2\) the vector linking the centres of the spherical colloids, with diameter \(\sigma_d\) and mass \(m_d\). An additional Weeks-Chandler-Anderson potential,

\[
V_{\text{wca}}(r) = \begin{cases} 
V_{\text{LJ}}(r) - V_{\text{LJ}}(r_c) & r < r_c \\
0 & r > r_c 
\end{cases}
\]
with
\[
V_{\text{LJ}}(r) = 4\epsilon \left[ \left( \frac{\sigma_d}{r} \right)^{12} - \left( \frac{\sigma_d}{r} \right)^6 \right],
\]
(2)

where \(\epsilon\) is an energy scale and \(r_c\) is the minimum of the Lennard-Jones potential, \(r_c = 2^{1/6}\sigma_d\), 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 \(\hat{n}\), are constant in modulus but follow the molecules’ rotations, and are the same for the two spheres belonging to the same molecule,
\[
\mathbf{F}_{\text{act}} = F_{\text{act}} \mathbf{n}.
\]
(3)

\(F_{\text{act}}\) is directed from the \(i\)th colloid (tail) to the \(i+1\)th 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
\[
m_d \ddot{\mathbf{r}}_i(t) = -\gamma \dot{\mathbf{r}}_i(t) + \mathbf{F}_{\text{fene}}(\mathbf{r}_{i,i+1}) + \eta_i - \sum_{j=0}^{2N} \frac{\partial V_{\text{wca}}^{ij}}{\partial \mathbf{r}_{ij}} \frac{\mathbf{r}_{ij}}{r_{ij}} + \mathbf{F}_{\text{act}i},
\]
(4)
\[
m_d \ddot{\mathbf{r}}_{i+1}(t) = -\gamma \dot{\mathbf{r}}_{i+1}(t) - \mathbf{F}_{\text{fene}}(\mathbf{r}_{i,i+1}) + \eta_{i+1} - \sum_{j=0}^{2N} \frac{\partial V_{\text{wca}}^{i+1,j}}{\partial \mathbf{r}_{i+1,j}} \frac{\mathbf{r}_{i+1,j}}{r_{i+1,j}} + \mathbf{F}_{\text{act}i}
\]

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

The coupling to the thermal bath at temperature \(T\) is modeled in the manner of Langevin, with \(\gamma\) the friction coefficient and \(\eta\) a Gaussian random noise with zero mean, \(\langle \eta_a(t) \rangle = 0\), and
\[
\langle \eta_a(t) \eta_{b}(t') \rangle = 2\gamma k_B T \delta_{ab} \delta(t - t'),
\]
(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 white noise acting independently on the two beads.

The surface fraction is
\[
\phi = N \frac{S_d}{S}
\]
(6)
with $S_d = \pi \sigma_d^2/2$ 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, $\text{Pe}$, is a dimensionless ratio between the advective transport rate and the diffusive transport rate. For particle flow one defines it as $\text{Pe} = L v / D$, with $L$ a typical length, $v$ a typical velocity, and $D$ a typical diffusion constant. We choose $L \to \sigma_d$, $v \to F_{\text{act}}/\gamma$ and $D \to D_{\text{cm}} = k_B T/(2\gamma)$ of the passive dumbbell to be derived below; then,

$$\text{Pe} = \frac{2\sigma_d F_{\text{act}}}{k_B T}.$$  \hspace{1cm} (7)

The active Reynolds number $\text{Re}_{\text{act}} = m_d F_{\text{act}}/(\sigma_d \gamma^2)$ 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 $r \approx \sigma_d$. Details on the calculations can be found in [23, 24]. Here, we simply summarise the main results. Within this approximation, at absolute times and time-differences that are longer than the inertial time-scale $t_I = m_d / \gamma$, not taking into account its periodic character, the angle $\theta$ 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

$$\langle \theta^2 \rangle = \theta_0^2 + 2D_R t$$ \hspace{1cm} (8)

with $\theta_0$ the initial angle, $t$ the time-delay, and the angular diffusion constant

$$D_R = \frac{2k_B T}{\gamma \sigma_d^2}.$$ \hspace{1cm} (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, $\langle \theta^2 \rangle \to 2D_R t$. 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 becomes flat.
The translational mean-square displacement is ballistic in the limit $t \ll t_I$, and crosses over to a very rich behaviour beyond this time-scale,

$$\langle \Delta r_{cm}^2(t) \rangle = 4D_{cm}^{pd} t + \left( \frac{F_{act}}{\gamma} \right)^2 \frac{2}{D_R} \left( t - \frac{1 - e^{-D_R t}}{D_R} \right), \quad (10)$$

where

$$D_{cm}^{pd} = \frac{k_B T}{2\gamma} \quad (11)$$

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

$$\langle \Delta r_{cm}^2 \rangle = 4D_{cm}^{pd} t + \left( \frac{F_{act}}{\gamma} \right)^2 t^2, \quad (12)$$

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

$$t^* = \frac{4D_{cm}^{pd}\gamma^2}{F_{act}^2} = \frac{2k_B T \gamma}{F_{act}^2} = \left( \frac{4}{\text{Pe}} \right)^2 \frac{\sigma_d^2}{4D_{cm}^{pd}} = \left( \frac{4}{\text{Pe}} \right)^2 t_a. \quad (13)$$

Note that these two intermediate regimes might be hidden if the system parameters are such that $t^* < t_I$ or $t^* > t_a$. They can also be easily confused with a super-diffusion behavior $\langle \Delta r_{cm}^2 \rangle \sim t^\alpha$ with $1 < \alpha < 2$ if they are not well separated ($t_I \simeq t^* \simeq t_a$). In the large $\text{Pe}$ limit one has $t^* \ll t_a$. In the last time-lag regime $t \gg t_a$, we recover normal diffusion,

$$\langle \Delta r_{cm}^2 \rangle = 4D_A t, \quad (14)$$

with the diffusion coefficient

$$D_A(F_{act}, T, \phi = 0) = \frac{k_B T}{2\gamma} \left[ 1 + \frac{1}{2} \left( \frac{F_{act} \sigma_d}{k_B T} \right)^2 \right] = D_{cm}^{pd} \left( 1 + \frac{\text{Pe}^2}{8} \right). \quad (15)$$

3.1. The distributions for the single dumbbell

The infinitesimal increment of the centre of mass position, $\text{d}r_{cm}$, is a random variable and its distribution is due to the Gaussian random character of the noise $\xi_x$ and the, for the moment unknown, random character of $n_x \equiv$
\[ \cos \theta. \] In order to establish the pdf of the latter, we assume that \( \theta \) is uniformly distributed in the interval \([−\pi, \pi]\), \( p_\theta(\theta) = (2\pi)^{-1} \). Therefore, for \( 0 \leq \theta \leq \pi \)

\[
p_{n_x}(n_x) = \frac{1}{2\pi \sqrt{1 - n_x^2}} \int_0^\pi \frac{d\theta}{2\pi} \delta(n_x - \cos \theta) = \frac{1}{2\pi \sqrt{1 - n_x^2}}
\]  

(16)

This calculation can be repeated for \(-\pi \leq \theta < 0\) with the same result and the overall numerical pre-factor is fixed by normalisation:

\[
p_{n_x}(n_x) = \frac{1}{\pi \sqrt{1 - n_x^2}} \quad \text{for } n_x \in [-1, 1].
\]  

(17)

In order to estimate the pdf of the translational displacement of the centre of mass position, we now use the over-damped equation for a small increment \( \Delta x_{\text{cm}} \), with the notation used in [24]

\[
\Delta x_{\text{cm}} = \frac{\sqrt{4k_BT\gamma}}{2\gamma} \Delta W + v_{\text{act}} \Delta t \cos \theta
\]  

(18)

with \( v_{\text{act}} = F_{\text{act}}/\gamma \) and \( \Delta W \) a gaussian noise, distributed as

\[
p_{\Delta W}(\zeta) = \frac{1}{\sqrt{2\pi \Delta t}} e^{-\zeta^2/(2\Delta t)},
\]  

(19)

with \( \zeta \in [-\infty, \infty] \).

The pdf of \( \Delta x_{\text{cm}} \) is then

\[
p(\Delta x_{\text{cm}}) = \int d\zeta d n_x \delta \left( \Delta x_{\text{cm}} - \frac{\sqrt{4k_BT\gamma}}{2\gamma} \zeta - v_{\text{act}} \Delta t \ n_x \right) p_{n_x}(n_x) p_{\Delta W}(\zeta)
\]

The naive comparison of the order of magnitude of the last two terms inside the delta-function using \( \zeta \sim (\Delta t)^{1/2} \) and \( n_x \simeq 1 \) yields, after multiplying by \( \sigma_d \gamma/(k_B T \Delta t) \),

\[
\left( \frac{\sigma_d^2 \gamma}{k_B T \Delta t} \right)^{1/2} \approx \frac{\sigma_d F_{\text{act}}}{k_B T}.
\]  

(20)

In this way the second member corresponds to Pe. Two limits are clear:

– For \( \text{Pe} \ll \text{left-hand-side in Eq. (20)} \), so that the active-force induced last term in the argument of the Dirac delta can be neglected, the two integrals decouple and \( \Delta x_{\text{cm}} \) is naturally Gaussian distributed.

6
For Pe \gg \text{left-hand-side in Eq. (20)}, so that the noise term in the argument of the Dirac delta can be neglected, the two integrals decouple again and

\[
p(\Delta x_{\text{cm}}) \propto \frac{1}{\sqrt{1 - \left(\frac{\Delta x_{\text{cm}}}{v_{\text{act}} \Delta t}\right)^2}}
\]

with two peaks at \(\Delta x_{\text{cm}} = v_{\text{act}} \Delta t\).

Otherwise, the double integral yields a complex result:

\[
p(\Delta x_{\text{cm}}) \propto \int_{-1}^{1} dn_x \exp \left[ -\frac{(2\gamma)^2}{2\Delta t (4k_B T \gamma)} (\Delta x_{\text{cm}} + v_{\text{act}} \Delta t \ n_x)^2 \right] \frac{1}{\sqrt{1 - n_x^2}}
\]

The displacement between two times, \(\Delta x = x_{\text{cm}}(t + t_0) - x_{\text{cm}}(t_0)\), is the sum of the small increments with each of these independently distributed according to Eq. (22).

4. Translational motion at finite density

The interacting case cannot be solved analytically. We focus here on the numerical determination of the centre of mass and angular displacement statistics. Details on the numerical method used for solving the dynamical equations are given in [23]. We set \(m_d = \sigma_d = k_B = \epsilon = 1\), \(r_0 = 1.5\), \(k = 30\) and \(\gamma = 10\) in proper physical units. These choices assure overdamped motion and negligible dumbbell vibrations. We used between 15000 and 20000 dumbbells in each simulation. We fix the strength of the active force to be \(F_{\text{act}} = 0.1\) and we vary the temperature in order to access different Péclet numbers that we choose to be Pe = 40, 20, 4, 2. The remaining parameter is density and we typically use \(\phi = 0.01, 0.1, 0.3, 0.5, 0.7\), see Fig. 1 that shows two instantaneous snapshots of the dumbbell configurations of systems with \(\phi = 0.5\) (left) and \(\phi = 0.7\) (right). The single-dumbbell characteristic time-scales for these parameters are summarised in Table 1.

Aspects of the phase diagram and the dynamics of this system were already established in [20, 21, 23]. At sufficiently low temperature and large active force the system phase separates into gas-like spatial regions and clusters of agglomerated dumbbells. The dynamic phase transition between homogeneous and aggregated phases was determined by the change in behaviour of
the probability distribution function, $\rho$, of the local density, $\phi_x$. At the critical Pe at which the system starts aggregating the density distribution $\rho$ not only becomes asymmetric but starts developing a second peak at the density of the clusters. Snapshots of typical configurations and their analysis along these lines can be found in [24]. In the rest of the paper we use sufficiently low Péclet numbers so that the system is in the homogenous phase though with important fluctuations, as we will see.

| $T^*$ | Pe | $t_\alpha$ | $t^*$ |
|-------|----|-----------|-------|
| 0.005 | 40 | 1000      | 10    |
| 0.01  | 20 | 500       | 40    |
| 0.05  | 4  | 100       | 1000  |
| 0.1   | 2  | 50        | 4000  |

Table 1: Parameters and characteristic times as defined in Sect. 3

4.1. Center of mass translational mean-square displacement

In Fig. 2 we show the center of mass Mean Square Displacement (MSD) normalised by time-delay in such a way that a plateau signals normal dif-

Figure 1: Typical snapshots of a system with $\phi = 0.5, 0.7$, linear size 70 $\sigma_d$ and Pe = 40. In each dumbbell the green colloid is the head and the red one is the tail, and they are joined by a line.
fusion. The two panels display data at $T = 0.005$ and $T = 0.1$, under the same active force $F_{\text{act}} = 0.1$. Each panel shows data for eight densities given in the key and the case $\phi = 0$ corresponds to the single dumbbell problem. The characteristic times $t_I$, $t^*$, $t_a$ (see Table I) are shown with small vertical arrows. These plots show several interesting features that reproduce, to a certain extent, the single particle motion summarised above:

- In all cases there is a first ballistic regime (the dashed segment close to the data is a guide-to-the-eye) with a pre-factor that is independent of $\phi$ and increases with temperature. (The case $t \ll t_I$ of the single dumbbell.)

![Figure 2: The center of mass MSD normalised by time-delay, for an active system under $F_{\text{act}} = 0.1$ at $T = 0.005, 0.1$ (Pe = 40, 2), with different densities given in the key. The Péclet number induces a strong qualitative change in $\langle \Delta r_{\text{cm}}^2 \rangle$, see the text for a detailed discussion. The two dashes in the first panel represent the ballistic dependence $\sim t^2$. The dashed segment in the last panel is a guide-to-the-eye for the density dependence of the last crossover time-delay that increases weakly with $\phi$. The vertical black arrows indicate the single dumbbell time-scales $t_I$ and $t_a$, while the red arrows indicate the single dumbbell characteristic time $t^*$, for each case.](image)

- The dynamics slow down next and, depending on Pe and $\phi$, the normalised MSD attains a plateau associated to normal diffusion or decreases, suggesting sub-diffusion. (The case $t_I \ll t \ll t^* \ll t_a$ of the single dumbbell.) For instance, there is sub diffusion for Pe = 2 and $\phi \geq 0.4$ and Pe = 40 and $\phi \geq 0.7$.

- Subsequently, the dynamics accelerate with a second super-diffusive regime in which the curves for all $\phi$ look approximately parallel and very close to ballistic at sufficient high Pe. (The case $t_I \ll t^* \ll t \ll t_a$ of the single dumbbell.)
Finally, the late normal diffusive regime is reached with all curves saturating at $D_A$. (The case $t_I \ll t^*$, $t_a \ll t$ of the single dumbbell.) This regime is beyond the time-window explored for $\phi = 0.7$.

It is hard to ensure whether the intermediate regime is super-diffusive or simply ballistic as the time-scales $t^*$ and $t_a$ are not sufficiently well separated at high Pe and not even ordered as $t^* < t_a$ at low Pe, leading to the mixture of the diffusion-ballistic-diffusion regimes.

A rather good fit, not shown here, of the finite density data in the limit $Pe \gg 1$ and for time-delays such that $t \geq t^*$ is achieved by using the single dumbbell expression in Eq. (10)

$$\langle r_{cm}^2 \rangle (t) = 4D^\phi \left( t - \frac{1 - e^{-D^\phi R t}}{D^\phi R} \right), \quad Pe \gg 1, \quad (23)$$

without the first term (negligible if $Pe \gg 1$) and upgrading the remaining parameters, $D^\phi_A$ and $D^\phi_R$, to be density-dependent fitting parameters, as done in [14, 25]. The quality of this fit was discussed in [24].

The crossover time-delay between the last ballistic or super-diffusive, and the diffusive regimes increases, though rather weakly, with $\phi$, at low Pe, see the inclined dashed line in the last panel that is also a guide-to-the-eye.

In [24] we showed that the qualitative dependence of $D_A$ on $k_B T$ for the single dumbbell case ($\phi = 0$), is maintained under interactions ($\phi \neq 0$). For $Pe \ll 1$, $D_A$ is dominated by thermal fluctuations and increases with $k_B T$. Instead, for $Pe \gg 1$, $D_A$ is dominated by the work done by the active forces. $D_A$ saturates at small values of $T$ for $\phi > 0.2$. Instead, at high temperatures $D_A$ seems to retain the linear growth with temperature of the single dumbbell at least for the temperatures used in the simulations.

The $\phi$ dependence of $D_A$ at fixed $T$ and for different active forces was discussed in [23, 24] where it was shown how the Tokuyama-Oppenheimer [26] law of the passive system was simplified under activation. On the one hand, we showed that the ratio of diffusion coefficients of the active system at finite density and single passive dumbbell $D_A(F_{act}, T, \phi)/D_{cm}^{pd}$ depends on $F_{act}$ and $T$ only through $Pe$, as it does for the single dumbbell. The numerical data suggested [23, 24]

$$D_A(F_{act}, T, \phi) \simeq D_{cm}^{pd} \left( 1 + \frac{Pe^2}{8} \right) e^{-b(Pe)\phi} \quad (24)$$

with $b$ a non-monotonic function of $Pe$ [23] for $Pe = 40$ and $Pe = 66$, and

$$D_A(F_{act}, T, \phi) \simeq D_A(F_{act}, T, 0) \left[ 1 + a_1(Pe) \phi + a_2(Pe) \phi^2 \right] \quad (25)$$
for Pe = 4 and Pe = 20, with $a_1$ negative in all cases while $a_2$ changing sign from negative at Pe $< 20$ to positive at Pe $> 20$ (leading to a growing behaviour at large $\phi$ that is not physical). At Pe = 20 the density dependence is almost linear as $a_2$ is very close to zero.

Figure 3: Normalized distribution of the centre of mass horizontal displacements, $\Delta x$, in a system with density $\phi = 0.1$. Four Péclet numbers are used in each panel, Pe = 40, 20, 4, 2 or, equivalently, $T = 0.005$, 0.01, 0.05, 0.1, as indicated in the keys. The time-delay in each of the four panels is $t = t_I$, 10 $t_I$, $t_a/2$, 10 $t_a$ (from left to right and from top to bottom). $t_I = 0.1$ and the values of $t_a$ depend on Pe as given in Table 1. The probability distribution functions are scaled with $\sigma_x = \langle \Delta x^2 \rangle^{1/2}$. The solid curves are Gaussian pdfs in normal form (with zero mean and unit variance) and represent the data in the first two panels ($t = t_I$, 10 $t_I$) rather accurately. Instead, the data for high Pe in the last two panels ($t = t_a/2$, 10 $t_a$) are not Gaussian. See the main text for a discussion.
4.2. The fluctuations of the centre of mass displacements

We study the distribution of centre of mass displacements

\[ P(\Delta x) = \frac{1}{N} \sum_{i=1}^{N} \langle \delta (\Delta x - (x_{cm}(t + t_0) - x_{cm}(t_0))) \rangle \] (26)

or the self-part of the van Hove correlation function.

In the zero density limit and under no active force the distribution of \( \Delta x \) is Gaussian. We will now determine how this limiting form is modified by the active force and the interactions in the various time-delay regimes.

In Fig. 3 we display the statistics of the horizontal center of mass displacements in a system with a relatively low density, \( \phi = 0.1 \). Data for Pe = 40, 20, 4, 2 are gathered in each of the panels that correspond to different time-delays, \( t = t_I, 10 t_I, t_a/2 \) and \( 10 t_a \). The data are scaled by the horizontal contribution to the mean-square displacement, \( \sigma_x = (\Delta x^2)^{1/2} \). The solid lines are Gaussian pdfs in their normal form and describe the data for short time-delays and all Pe in the first two panels very accurately. Instead, the data in the last two panels are close to the Gaussian form only for the low Pe’s while for high Pe’s the shape of the pdfs is different. In the third panel in Fig. 3 the time-delay, \( t = t_a/2 \), is such that the mean-square displacements are in the second ballistic regime, that in the single dumbbell case corresponds to \( \sigma^2 = \langle \Delta r_{cm}^2 \rangle \simeq (F_{act}/\gamma)^2 t^2 \). The distribution of \( \Delta r \) is peaked around a constant value of \( F_{act}t_a/(2\gamma) \) which projected on one axis gives this double shape. The down-pointing arrows inside the plot indicate these instants for \( Pe = 40 \) and are close to the location of the peaks in the finite density case.

From the Gaussian fit of the bare data for \( P(\Delta x) \) in the last diffusive regime (\( t = 10 t_a \), fourth panel in Fig. 3) we extracted \( D_A \) and we found good agreement with the values of \( D_A \) obtained in the analysis of the mean-square displacement \[ 24 \] (not shown).

In the following two figures, Figs. 4 and 5 we checked the density dependence of the centre of mass displacement distribution. From the first to the fourth panels \( t = t_I, 10 t_I, t_a/2, 10 t_a \), respectively. In each panel data for \( \phi = 0.01, 0.1, 0.3, 0.5, 0.7 \) are shown.

In the cases in which activation is strong, Fig. 4 at short time delays (first two panels) all systems have Gaussian fluctuations. At long-time delays (last two panels) the distributions depend on \( \phi \). In the regime III there is a two peak structure at low density, while the central part becomes close to
Figure 4: Distribution of center of mass translation displacement in the horizontal direction, $\Delta x$, for $\text{Pe} = 40$ (or $T = 0.005$), and various densities $\phi = 0.01, 0.1, 0.3, 0.5, 0.7$. The four panels correspond to time-delays in the four regimes labelled I, II, III and IV ($t_f, 10 t_f, t_a/2$ and $10 t_a$, respectively). For I and II the Gaussian in normal form describes the data very well. In the last two panels the statistics are not Gaussian and there is a non-trivial density and time-delay dependence that we discuss in the main text. The straight lines in the third panel ($t = t_a/2$) are exponential fits to the tails of the $\phi = 0.7$ data.

flat at higher densities, due to stronger interactions, and then develops two exponential wings at larger absolute displacements. In the regime IV the distributions do not have the double peak structure and are Gaussian close to $\Delta x \simeq 0$ for all densities. Looking carefully at the MSD for $\text{Pe} = 40$ in the left panel in Fig. 2, one notices that the curves in this regime are less flat at low density while they are closer to being flat at $\phi = 0.5$. The crossover to normal diffusion is, therefore, slower for lower density. The long-lasting super-diffusive behaviour seems to be related to the non-Gaussianity of the pdfs. The MSD for $\text{Pe} = 2$ in the right panel in Fig. 2 are flatter earlier for
φ ≤ 0.5 and, consistently, the pdfs are Gaussian for all these densities (see Fig. 5). The case φ = 0.7 is different since the system is far from the last diffusive regime for the time-delays used.

In the cases in which activation is weak, Fig. 5, once again at short time delays (first two panels) all systems have Gaussian fluctuations. At the intermediate time delays (third panel) the distributions depend on φ and, for high densities, see φ = 0.5, 0.7 in the plot, there is an excess weight on large deviations with respect to the Gaussian, that is close to exponential. The effect becomes more evident when the sub-diffusive behavior is more pronounced, see Fig. 2. At still longer time-delays (fourth panel) the statistics becomes Gaussian again for all densities, except for the case at φ = 0.7 since in this case the time-delay is still too short to reach the final diffusive regime.

5. Rotational motion at finite density

We turn now to the rotational dynamics. In Fig. 6 we display the angular MSD normalized by time-delay. The two panels show data for $F_{\text{act}} = 0.1$ and $Pe = 40$ and $Pe = 2$, and the same densities as in Fig. 2. These plots also show interesting features:

– In all cases there is a first ballistic regime with a pre-factor that is independent of φ and increases with temperature (The case $t \ll t_I = m_d/\gamma$ of the single dumbbell.)

– Next, the dynamics slow down and, depending on $T$ and φ, the normalised MSD may attain an ever-lasting plateau associated to normal diffusion for low φ at any temperature, or even decrease, suggesting sub-diffusion, at high enough φ.

– At high Pe and sufficiently high density the dynamics accelerate next, with a second super-diffusive regime that crosses over to a final diffusive regime.

– In the late normal diffusive regime all curves saturate and the height of the plateau yields the different $D_R$ coefficients that we discuss below.

In the phase separated regime the dumbbell clusters rotate [20, 21]. It is possible that strong fluctuations not far from the critical point have an important rotational component than enhances/advects rotational diffusion giving rise to an observable contribution to displacement.

The diffusion constant decreases with temperature below a crossover beyond which it increases approximately linearly with temperature [24]. The $F_{\text{act}}$-independence of $D_R$ is lost as soon as the interaction between dumbbells
is switched on. The density dependence is also quite complex and was discussed in [24]. Finally, we showed that $D_R/(k_B T)$ depends on $F_{\text{act}}$ and $k_B T$ only through $Pe$,

$$D_R(F_{\text{act}}, T, \phi) = k_B T \ f_R(Pe, \phi)$$

(27)

with $f_R(Pe, 0) = f_R(0, 0) = 2/(\gamma \sigma_d^2)$. At low densities, while the master curve decreases with $\phi$ in the whole range considered for $Pe < 20$, it becomes flat at $Pe = 20$ and it increases with $\phi$ for $Pe > 20$, for $\phi \leq 0.5$. This would suggest:

$$f_R(Pe, \phi) \simeq \frac{2}{\gamma \sigma_d^2} + a(Pe, \phi)$$

(28)
with \( \phi(\text{Pe}, \phi) \) almost linear in \( \phi \) and the slope changing sign at \( \text{Pe} \approx 20 \) for small \( \phi \). At all \( \text{Pe} \) there is a cross-over at high enough densities after which the rotational diffusion constant decreases with increasing density. One can associate this feature to the fact that for sufficiently dense systems rotations are inhibited and \( D_R \) decreases.

### 5.1. The angular displacement distribution

Figure 6 demonstrates that for low enough density, \( \phi = 0.1 \) in this figure, the angular displacement distribution function at all time delays and for all Péclet numbers can be put into a normal Gaussian form after normalisation by \( \sigma_{\theta} = \langle \Delta \theta^2 \rangle^{1/2} \).

In Figs. 8 and 9 we analyse the density dependence of the normalised probability distribution of angular displacements. In Fig. 8 a high Péclet number is used, \( \text{Pe} = 40 \), while in Fig. 9 the Péclet number is low, \( \text{Pe} = 2 \). In the first case, the four time-regimes I, II, III, IV, in the behaviour of the center of mass translational mean-square displacement, are well separated. In the second case, they are not. We see that for \( \phi = 0.01, 0.1, 0.3 \) the data in both figures collapse onto the normal Gaussian. The higher density data, \( \phi = 0.5 \), deviate from this master curve when the time delay is chosen to be \( t = 10 t_I \) for \( \text{Pe} = 40 \), and \( t = t_a/2 = 25 \) for \( \text{Pe} = 2 \). The data points for \( \phi = 0.7 \) in the last two panels in the two figures have a peak at \( \Delta \theta = 0 \) corresponding to dumbbells that do not rotate between the two times and...
two exponential wings typical of heterogeneous systems. Note that these pdfs resemble the ones in [27] though for translational displacements in this case.

6. Conclusions

We considered the diffusion properties of a system of active dumbbells with repulsive interaction. We focused on the Péclet number and density regime in which the global system is homogeneous and we studied the fluctuations of the centre of mass translation and angular displacements.

We first summarised the translational and rotational MSD of the system.
In the single particle limit, the translational MSD has a very rich time-delay dependence, with four distinct time regimes (ballistic, diffusive, ballistic and diffusive) separated by three characteristic times (the shortest inertial, $t_I$, the diffusive, $t_a$, and an additional one, $t^* \propto t_a/Pe^2$, that lies in between the other two for large Pe). This rich structure survives under finite densities with modified parameters. The diffusion constant in the last diffusive regime has a non-monotonic dependence on temperature, as for the single dumbbell case, and it decreases with increasing self-propelled particle density at all temperatures. Moreover, it depends on temperature and active force only through the Péclet number at all densities explored. In general, the Pe
Figure 9: Normalized distribution of angular displacements $\Delta \theta$ for $\text{Pe} = 2$. Data for various densities $\phi = 0.01, 0.1, 0.3, 0.5, 0.7$ are collected in each panel. The time-delay in the first ($t = t_I$) and last ($t = 10 t_a$) panels lie in the inertial ballistic and last diffusive regimes I and IV, respectively, for $\phi \leq 0.5$. The time-delays in the second and third panels ($t = 10 t_I$ and $t = t_a/2$, respectively) are in the intermediate crossover between these two. $t^* = 4000 \gg t_a = 50$, see the Table 1 for this low Pe number. The solid curves are Gaussians in normal form. The deviations from the Gaussian in the intermediate regime are pronounced for lower densities than for $\text{Pe} = 40$. The solid straight lines are exponential fits to the tails in the $\phi = 0.7$ data.

dependence is non-monotonic.

The behavior of the rotational MSD, that is rather simple for a single dumbbell with just one crossover between ballistic and diffusive behaviour, reflects the behavior of the translational MSD at finite densities, where intermediate regimes also appear. The late epochs rotational diffusion constant increases with temperature (though not linearly) at all densities and active forces simulated and depends on temperature and activity only through $\text{Pe}$. At low densities, its dependence on density changes from decreasing at low
We have then evaluated the distribution functions for the centre of mass and angular displacements for time-delays corresponding to the various dynamical regimes. For time-delays shorter or of the order of the inertial time $t_I$, the distributions were always found to be very close to a Gaussian, for all the $\phi$ and $Pe$ considered. At large $Pe$, always in the homogeneous phase but not far from the critical value ($Pe/Pe_c \approx 0.62$) \cite{24}, for time-delays corresponding to the super-diffusive or second ballistic regime of the single particle, while the angular distributions remain Gaussian except at the highest density considered $\phi = 0.7$, the translational displacement distributions show a two-peak character at low density becoming more rounded when the density increases. The position of the peaks corresponds to the analytic estimate given in Sec. 3.1. The distributions get closer to a Gaussian in the last regime. The effects on the final diffusive regime due to the cross-over with the preceding super-diffusive regime are more pronounced than at small $Pe$ even at times of the order of $10 t_a$. Accordingly, non-Gaussian effects can be seen in the translational distributions at these times. The case at $\phi = 0.7$ is different since, for the time-delay considered, the system is still far from the final diffusive regime. At small $Pe$, when the effects of interactions are less relevant ($Pe/Pe_c \approx 0.03$), the second regime becomes sub-diffusive when the density increases. In correspondence with this, deviations from the Gaussian are found in both translational and angular displacement distributions. Finally, both distributions have a Gaussian character in correspondence with the last diffusive regime, except at $\phi = 0.7$. In this very high density limit we find exponential tails in the translational and rotational distributions, and a central peak at vanishing angular displacement.

After this work we plan to analyse the motion of tracers in contact with this active sample and, especially, to analyse the existence of a parameter to be interpreted as an effective temperature \cite{22} from the mobility and diffusive properties of the sample and the tracers, as done in \cite{28,29,30} for another active matter model and in \cite{31} for a sample of active Janus particles.

Acknowledgments: LFC is a member of Institut Universitaire de France. G.G. acknowledges the support of MIUR (project PRIN 2012NNRKAF).
References

[1] R. Golestanian, T. B. Liverpool, A. Ajdari, Propulsion of a molecular machine by asymmetric distribution of reaction products, Phys. Rev. Lett. 94 (2005) 220801.

[2] R. Howse, R. A. L. Jones, A. J. Ryan, T. Gough, R. Vafabakhsh, R. Golestanian, Self-motile colloidal particles: from directed propulsion to random walk, Phys. Rev. Lett. 99 (2007) 048102.

[3] J. Toner, Y. Tu, S. Ramaswamy, Hydrodynamics and phases of flocks, Ann. of Phys. 318 (2005) 170.

[4] D. A. Fletcher, P. L. Geissler, Active biological materials, Ann. Rev. Phys. Chem. 60 (2009) 469.

[5] G. Menon, Active matter, in: J. Krishnan, A. Deshpande, P. Kumar (Eds.), Rheology of Complex Fluids, Springer, 2010.

[6] S. Ramaswamy, The mechanics and statistics of active matter, Ann. Rev. Cond. Matt. Phys. 1 (2010) 323.

[7] M. E. Cates, Diffusive transport without detailed balance in motile bacteria, Rep. Prog. Phys. 75 (2012) 042601.

[8] P. Romanczuk, M. Bär, W. Ebeling, B. Lindner, L. Schimansky-Geier, Active brownian particles, Eur. Phys. J. Special topics 202 (2012) 1.

[9] T. Vicsek, A. Zafeiris, Collective motion, Phys. Rep. 517 (2012) 71.

[10] M. C. Marchetti, J. F. Joanny, S. Ramaswamy, T. B. Liverpool, J. Prost, M. Rao, R. A. Simha, Hydrodynamics of soft active matter, Rev. Mod. Phys. 85 (2013) 1143.

[11] G. de Magistris, D. Marenduzzo, An introduction to the physics of active matter, Physica A 418 (2015) 65.

[12] J. Elgeti, R. Winkler, G. Gompper, Physics of microswimmers - single particle motion and collective behavior, Rep. Prog. Phys. (to appear) arXiv:1412.2692
[13] G. Gonnella, D. Marenduzzo, A. Suma, A. Tiribocchi, Phase separation and coarsening in active matter, arXiv:1502.02229.

[14] X.-L. Wu, A. Libchaber, Particle diffusion in a quasi-two-dimensional bacterial bath, Phys. Rev. Lett. 84 (2000) 3017.

[15] J. P. Hernández-Ortíz, C. G. Stoltz, M. D. Graham, Transport and collective dynamics in suspensions of confined swimming particles, Phys. Rev. Lett. 95 (2005) 204501.

[16] G. Miño, T. E. Mallouk, T. Darnige, M. Hoyos, J. Dauchet, J. Dunstan, R. Soto, Y. Wang, A. Rousselet, E. Clement, Enhanced diffusion due to active swimmers at a solid surface, Phys. Rev. Lett. 106 (2011) 048102.

[17] G. Grégoire, Y. Chaté, H. Tu, Active and passive particles: Modeling beads in a bacterial bath, Phys. Rev. E 64 (2001) 011902.

[18] I. Llopis, I. Pagonabarraga, Dynamic regimes of hydrodynamically coupled self-propelling particles, EPL 999 (2006) 75.

[19] C. Valeriani, M. Li, J. Novosel, J. Arlt, D. Marenduzzo, Colloids in a bacterial bath: simulations and experiments, Soft Matter 7 (11) (2011) 5228–5238.

[20] G. Gonnella, A. Lamura, A. Suma, Phase segregation in a system of active dumbbells, Int. J. Mod. Phys. C 25 (2014) 1441004.

[21] A. Suma, D. Marenduzzo, G. Gonnella, E. Orlandini, Motility-induced phase separation in an active dumbbell fluid, EPL 108 (2014) 56004.

[22] L. F. Cugliandolo, The effective temperature, Journal of Physics A: Mathematical and Theoretical 44 (48) (2011) 483001.

[23] A. Suma, G. Gonnella, G. Laghezza, A. Lamura, A. Mossa, L. F. Cugliandolo, Dynamics of a homogeneous active dumbbell system, Phys. Rev. E 90 (2014) 052130.

[24] L. F. Cugliandolo, G. Gonnella, A. Suma, Rotational and translational diffusion in an interacting active dumbbell system. arXiv:1501.04054.

[25] Y. Fily, M. C. Marchetti, Athermal phase separation of self-propelled particles with no alignment, Phys. Rev. Lett. 108 (2012) 235702.
[26] M. Tokuyama, I. Oppenheim, Dynamics of hard-sphere suspensions, Phys. Rev. E 50 (1994) 16.

[27] D. Levis, L. Berthier, Clustering and heterogeneous dynamics in a kinetic monte carlo model of self-propelled hard disks, Phys. Rev. E 89 (2014) 062301.

[28] D. Loi, S. Mossa, L. F. Cugliandolo, Effective temperature of active matter, Phys. Rev. E 77 (2008) 051111.

[29] D. Loi, S. Mossa, L. F. Cugliandolo, Effective temperature of active complex matter, Soft Matter 7 (2011) 3726–3729.

[30] D. Loi, S. Mossa, L. F. Cugliandolo, Non-conservative forces and effective temperatures in active polymers, Soft Matter 7 (2011) 10193–10209.

[31] J. Palacci, C. Cottin-Bizonne, C. Ybert, L. Bocquet, Sedimentation and effective temperature of active colloidal suspensions, Phys. Rev. Lett. 105 (2010) 088304.