Rotational and translational diffusion in an interacting active dumbbell system

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We study the dynamical properties of a two-dimensional ensemble of self–propelled dumbbells with only repulsive interactions. This model undergoes a phase transition between a homogeneous and a segregated phase and we focus on the former. We analyse the translational and rotational mean square displacements in terms of the Péclet number, describing the relative role of active forces and thermal fluctuations, and of particle density. We find that the four distinct regimes of the translational mean square displacement of the single active dumbbell survive at finite density for parameters that lead to a separation of time-scales. We establish the Pe and density dependence of the diffusion constant in the last diffusive regime. We prove that the ratio between the diffusion constant and its value for the single dumbbell depends on temperature and active force only through the Péclet number at all densities explored. We also study the rotational mean square displacement proving the existence of a rich behavior with intermediate regimes only appearing at finite density. The ratio of the rotational late-time diffusion constant and its vanishing density limit depends on Pe and density only. At low Péclet number it is a monotonically decreasing function of density. At high Péclet number it first increases to reach a maximum and next decreases as a function of density.

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I. INTRODUCTION

Active matter is made of self-propelled particles immersed in a thermal bath and in interaction. These systems are characterised by the continuous partial conversion of internal energy into work \[1,2\]. Nature offers many examples, at very different scales: the cytoskeleton, bacterial colonies and algae suspensions, bird flocks and schools of fish among others \[3\]-[11]. Self-propelled units can also be artificially realized in the laboratory in many different ways, for example, by surface treatment of colloidal particles \[12\].

Active matter is inherently out of equilibrium and exhibits non-trivial properties that have no analogue in passive, equilibrium materials. For example, large scale coherent motion and self-organised dynamic structures have been observed in colonies of bacteria in the absence of any attractive interaction \[13\]-[19], and a phase separation into an aggregate and a gas-like phase has been found in theoretical models \[20\]-[23] and, recently, also in experiments \[20\] for suspensions of self-motile particles only subject to steric interactions.

The dynamical properties of a suspension are significantly affected by self-propulsion. For instance, the comparison of the diffusion constant \(D\) of a dilute solution of passive spherical colloids with the one of run-and-tumble bacteria shows that the Stokes-Einstein formula and the fluctuation-dissipation theorem do not hold for the active system \[14\]-[30]. Indeed, assuming the Stokes-Einstein relation, \(D\) is given by \(D = k_B T / (3 \pi \eta a)\) where \(T\) is the temperature, \(\eta\) the fluid viscosity, and \(a\) the diameter of the colloids. The diffusion coefficient in a three-dimensional system of run-and-tumble bacteria \[14\] is evaluated as \(D_A \approx \tau^2_{\text{run}} / (6 \tau)\) where \(\tau\) is the duration of each run and \(l_{\text{run}}\) its length. Using \(\tau \approx 1\ s\), \(l_{\text{run}} \approx 10 - 30\ \mu m\), water viscosity \(\eta \approx 10^{-3}\ \text{Pa s}\), and \(a \approx 1\ \mu m\), one finds \(D_A / D \approx 10^3\).

This argument suggests to analyse how the diffusive behaviour is affected by self-propulsion more carefully. Actually, several experimental studies addressed this question. Wu and Libchaber considered the mean-square displacement of passive tracers coupled to a dilute suspension of Escherichia coli and found that an initial super-diffusive behaviour crosses over to normal diffusion at late times \[14\]. The super-diffusive behaviour was interpreted as being due to the presence of coherent structures in the bacterial bath. A similar study was carried on by Leptos \textit{et al.} on a suspension of algae. These authors found a linear time-dependence of the passive tracer’s mean-square displacement at all measured times \[31\]. The tracer’s diffusive constant was found to depend linearly on the density of the swimmers \[31\] while, reducing the dimensionality, the density-dependence was enhanced to the power \(3/2\) \[32\]. Results on the diffusion coefficient of tracers in contact with bacterial suspensions with hydrodynamics playing a relevant role were given in \[33\]-[35].

Other studies focused on the mean-square displacement of the active particles themselves. A linear dependence of the diffusion constant of the active swimmers on the so-called active flux (active swimmers density times their mean velocity) was found for different kinds of swimmers in contact with a solid wall \[30\]. The simulation of Hernández-Ortiz \textit{et al.} show ballistic behaviour crossing over to normal diffusion for the swimmer and passive tracer particles though with different density-dependence of the diffusion constant in the latter regime. The swimmer’ diffusion constant decreases with density at low swimmer density while it increases at large values; the diffusion constant of the passive tracer has, instead, a monotonic dependence with density and it consistently increases with it \[16\]. The Lattice Boltzmann study in \[37\] also shows a crossover between ballistic and diffusive behaviour at relative high self-propelled particle density and a super-diffusive regime associated to the formation of large scale clusters at low densities.

A detailed study of diffusion properties in models for self-propelled particles at different densities for the interesting cases where self-propulsion has been recognised to be an interaction capable of producing a phase transition is lacking in the literature. Results for the case of self-propelled polar disks have been presented in \[21\]. Moreover, we can mention the paper by Grégoire \textit{et al.} \[38\], who considered a model with explicit alignment particle interaction \emph{à la Vicsek} and they interpreted the super-diffusive behaviour of \[14\] in terms of the crossover found in their model close to the critical point.

Swimmers typically have elongated shape. We have therefore decided to study the diffusive properties of rotational and translational degrees of freedom in a system of active dumbbells. This model was introduced in \[39\] to describe the experimental behaviour of a bacterial bath coupled to colloidal tracers. A first study of its phase diagram appeared in \[23\]-[26] where it was shown that for certain (relatively high) densities and active forces the system phase separates into dense and loose spatial regions. A later study of this model \[40\] focused on the dumbbell effective temperature defined in terms of a fluctuation-dissipation relation \[41\]. However, a detailed analysis of the translational and rotational mean-square displacement in the full range of time-delays and varying the three more relevant parameters (temperature, activity and density) simultaneously, was not performed yet. We present this analysis here.

The paper is organised as follows. In Section 2 the dumbbell model is reviewed. In Section 3 the numerical results for the interacting active system are presented. The phase diagram of the system is analysed in terms of the Péclet number. This is a preliminary step needed to fix the region of the parameter space to be considered for the measurements of the diffusive properties. Then the translational and rotational mean-square displacement are analysed in all their dynamic regimes. Special emphasis is put on the analysis of the parameter dependence of the diffusion coefficient in the asymptotic limit. A discussion will complete the paper in Section 4.
II. THE MODEL

A dumbbell is a diatomic molecule formed by two spherical colloids with diameter \( \sigma_d \) and mass \( m_d \) linked together. The atomic positions are noted \( \mathbf{r}_1 \) and \( \mathbf{r}_2 \) in a Cartesian system of coordinates fixed to the laboratory. The colloids are subject to internal and external forces.

Typically, one assumes that there is an elastic link between the colloids modelled by the finite extensible non-linear elastic form

\[
\mathbf{F}_{\text{fene}} = -\frac{k \mathbf{r}}{1 - (r^2/r_0^2)}
\]

with \( k > 0 \). The denominator ensures that the spheres cannot go beyond the distance \( r_0 \) with \( r \) the distance between their centres of mass. An additional repulsive force is added to ensure that the two colloids do not overlap. This is the Weeks-Chandler-Anderson (WCA) 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

\[
V_{\text{LJ}}(r) = 4\epsilon \left[ \left( \frac{\sigma_d}{r} \right)^{12} - \left( \frac{\sigma_d}{r} \right)^{6} \right],
\]

where \( \epsilon \) is an energy scale and \( r_c \) is the minimum of the Lennard-Jones potential, \( r_c = 2^{1/6}\sigma_d \).

The dynamic equations for one dumbbell are

\[
m_d \ddot{\mathbf{r}}_i(t) = -\gamma \dot{\mathbf{r}}_i(t) + \mathbf{F}_{\text{fene}}(\mathbf{r}_{i,i+1}) + \eta_i - \sum_{j=0}^{2N} \frac{\partial V_{\text{wca}}^{ij}}{\partial \mathbf{r}_{ij}} \frac{\mathbf{r}_{ij}}{r_{ij}} + \mathbf{F}_{\text{act}i},
\]

\[
m_d \ddot{\mathbf{r}}_{i+1}(t) = -\gamma \dot{\mathbf{r}}_{i+1}(t) - \mathbf{F}_{\text{fene}}(\mathbf{r}_{i,i+1}) + \eta_{i+1} - \sum_{j=0}^{2N} \frac{\partial V_{\text{wca}}^{i+1,j}}{\partial \mathbf{r}_{i+1,j}} \frac{\mathbf{r}_{i+1,j}}{r_{i+1,j}} + \mathbf{F}_{\text{act}i},
\]

with \( i = 1, 3, ... 2N - 1, \) \( \mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j, \) \( r_{ij} = |\mathbf{r}_{ij}| \) and \( V_{\text{wca}}^{ij} \equiv V_{\text{wca}}(\mathbf{r}_{ij}) \) with \( V_{\text{wca}} \) defined in Eq. (2). Once the active force is attached to a molecule a sense of back and forth atoms is attributed to them; \( \mathbf{F}_{\text{act}} \) 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. \( \mathbf{F}_{\text{act}} \) changes direction together with the molecule’s rotation.

The coupling to the thermal bath is modelled as usual, with a friction and a noise term added to the equation of motion. \( \gamma \) is the friction coefficient. The noise \( \mathbf{\eta} \) is a Gaussian random variable with

\[
\langle \eta_{ia}(t) \rangle = 0,
\]

\[
\langle \eta_{ia}(t)\eta_{ib}(t') \rangle = 2\gamma k_B T \delta_{ij} \delta_{ab} \delta(t - t'),
\]

with \( k_B \) the Boltzmann constant and \( T \) the temperature of the equilibrium environment in which the dumbbells move. \( a \) 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

\[
\phi = N \frac{S_d}{S}
\]

with \( S_d \) the area occupied by an individual dumbbell, \( S \) the total area of the box where the dumbbells move and \( N \) their total number. The spring is supposed to be massless and void of surface. Therefore, in \( d = 2, \) \( S_d = \pi \sigma_d^2/2. \) 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 $Pe = L/v/D$, with $L$ a typical length, $v$ a typical velocity, and $D$ a typical diffusion constant. We choose $L \to \sigma_d$, $v \to F_{act}/\gamma$ and $D \to D_{cm}^{\text{ind}} = k_B T/(2\gamma)$ of the passive dumbbell to be derived below; then,

$$Pe = \frac{2\sigma_d F_{act}}{k_B T}. \quad (8)$$

Another important parameter is the active Reynolds number

$$Re_{act} = \frac{m_d F_{act}}{\sigma_d \gamma^2}, \quad (9)$$

defined in analogy with the usual hydrodynamic Reynolds number $Re = L v/\nu$, where $\nu$ is the kinematic viscosity of a given fluid, representing the ratio between inertial and viscous forces. Here we set $L \to \sigma_d$, $v \to F_{act}/\gamma$ and $\nu \to \gamma \sigma_d^2/m_d$.

A. A single dumbbell

The equation of motion for the position of the centre of mass, $r_{cm} = (r_1 + r_2)/2$, of a single dumbbell is

$$2m_d \ddot{r}_{cm}(t) = -2\gamma \dot{r}_{cm}(t) + 2F_{act}(t) + \xi(t) \quad (10)$$

with the new noise $\xi(t) = \eta_1(t) + \eta_2(t)$ with vanishing average, $\langle \xi_a(t) \rangle = 0$, and correlation

$$\langle \xi_a(t)\xi_b(t') \rangle = 4\gamma k_B T \delta_{ab} \delta(t - t'). \quad (11)$$

This is the Langevin equation of a point-like particle with mass $2m_d$, under a force $2F_{act}$, and in contact with a bath with friction coefficient $2\gamma$ at temperature $T$.

The equation of motion for the relative position of the two monomers, $r = r_1 - r_2$, is

$$m_d \ddot{r}(t) = \gamma \dot{r}(t) + 2F_{\text{int}}(t) + \zeta(t) \quad (12)$$

with the new noise $\zeta(t) = \eta_1(t) - \eta_2(t)$ having zero average, $\langle \zeta_a(t) \rangle = 0$, and correlation

$$\langle \zeta_a(t)\zeta_b(t') \rangle = 4\gamma k_B T \delta_{ab} \delta(t - t'). \quad (13)$$

Note that the noises $\xi$ and $\zeta$ are independent, $\langle \xi_a(t)\zeta_b(t') \rangle = 0$, for all $a, b$ at all times. $F_{\text{int}}$ includes the elastic and repulsive forces internal to the single dumbbell.

Equations (10) and (12) are coupled by the fact that $F_{act}$ acts along the axis of the molecule, the orientation of which changes in time. Equation (12) controls the molecule’s elongation and its rotational motion while Eq. (10) determines the translational properties of the dumbbell.

1. Elongation and rotation

Let us call $\hat{u}_||$ the instantaneous unit vector pointing from monomer 1 to monomer 2 along the axis of the molecule, $\theta$ the angle between $\hat{u}_||$ and an axis fixed to the laboratory, and $\hat{u}_\perp$ a unit vector that is perpendicular to $\hat{u}_||$ at all times. Using $\dot{r} = \dot{r}_|| + r \dot{u}_||$, with $r$ the modulus of $r$ and $\hat{u}_|| = \theta \hat{u}_\perp$ (note that we use here the Stratonovich discretisation scheme of stochastic differential equations [43] and we are thus entitled to apply the usual rules of calculus), one has

$$m_d (\ddot{r} - r \ddot{\theta}^2) = -\gamma \dot{r} + 2F_{\text{int}} + \zeta_||, \quad (14)$$
$$m_d (2r \ddot{\theta} + r \ddot{\theta}) = -\gamma r \dot{\theta} + \zeta_\perp, \quad (15)$$

where we decomposed the noise into the parallel and perpendicular directions, $\zeta = \zeta_|| \hat{u}_|| + \zeta_\perp \hat{u}_\perp$. The relations between the unit vectors in the fixed laboratory and the co-moving frame are given by

$$\hat{u}_x = \cos \theta \hat{u}_|| - \sin \theta \hat{u}_\perp, \quad \hat{u}_y = \sin \theta \hat{u}_|| + \cos \theta \hat{u}_\perp. \quad (16)$$
With this, for any noise we write
\[
\zeta = (\zeta_x \cos \theta + \zeta_y \sin \theta) \mathbf{u}_|| + (-\zeta_x \sin \theta + \zeta_y \cos \theta) \mathbf{u}_\perp,
\]
and
\[
\zeta_|| = \xi_x \cos \theta + \xi_y \sin \theta, \quad \zeta_\perp = -\xi_x \sin \theta + \xi_y \cos \theta.
\]
The system of equations (14)-16 for \( r \) and \( \theta \) cannot be solved exactly. We will assume that the internal and viscous forces are such that the inertial contributions (all terms proportional to \( m_d \)) can be neglected. We then have
\[
\gamma \dot{r} = 2F_{\text{int}} + \xi_x \cos \theta + \xi_y \sin \theta,
\]
\[
\gamma \dot{\theta} = -\xi_x \sin \theta + \xi_y \cos \theta.
\]
Putting together \( r \) and \( \theta \) into a vector \( \mathbf{y} = (r \ \theta) \), this set of equations reads
\[
\dot{y}_\alpha = h_{\alpha}[\mathbf{y}] + g_{\alpha \beta}[\mathbf{y}] \zeta_\beta,
\]
where the \( \beta \) index is a Cartesian one, \( \zeta_1 = \xi_x \) and \( \zeta_2 = \xi_y \), and the index \( \alpha \) yields \( y_1 = r \) and \( y_2 = \theta \). The components of the vector \( \mathbf{h} \) and the matrix \( g \) can be easily read from Eqs. (19) and (20). In the last term the noise appears multiplying a function of the stochastic variable \( \mathbf{y} \).

One can now average Eqs. (19) and (20) over the Cartesian white noise by using the rules of Stratonovich stochastic calculus described in [43-45]:
\[
\langle g_{\alpha \beta} \zeta_\delta \rangle = D \langle g_{\nu \beta} \frac{\partial}{\partial y_\nu} g_{\alpha \beta} \rangle
\]
where all factors are evaluated at the same time and \( D = 2\gamma k_BT \). The explicit calculation yields
\[
\gamma \frac{d\langle r \rangle}{dt} = 2\langle F_{\text{int}} \rangle + D\gamma^{-1}\langle r^{-1} \rangle,
\]
\[
\gamma \frac{d\langle \theta \rangle}{dt} = 0.
\]
The first equation is independent of \( \theta \) but it involves the average of different functions of \( r \). The second equation implies \( \langle \theta \rangle = \theta_0 = \theta(0) \) and, as we will take random initial conditions with average \( \langle \theta_0 \rangle_{ic} = 0 \), then \( \langle \theta \rangle \rangle_{ic} = 0 \). The statistics of \( \theta \) can be further analysed from the equation for the angular variance
\[
\gamma \frac{d}{dt}\langle \theta^2 \rangle = 2D\gamma^{-1}\langle r^{-2} \rangle.
\]
If we assume that \( r \) does not fluctuate around \( \sigma_d \), otherwise stated, that the molecule is approximately rigid,
\[
r \approx \sigma_d,
\]
this equation implies angular diffusion
\[
\langle \theta^2 \rangle = \theta_0^2 + 2Dt
\]
with the angular diffusion constant
\[
D_R = \frac{D}{\gamma^2 \sigma_d^2} = \frac{2k_BT}{\gamma \sigma_d^2}.
\]
The same technique can be used to compute all moments of the angular variable and thus show that it is Gaussian distributed within the rigid molecule approximation.

2. The center of mass

We now focus on the statistical properties of the centre of mass position and velocity that depend upon the active force. One readily solves Eq. (10)
\[
\mathbf{r}_{cm}(t) = \left( \mathbf{r}_0 + \mathbf{v}_0 m_d \frac{t}{\gamma} \right) - \frac{\mathbf{v}_0 m_d}{\gamma} \ e^{-\frac{\mathbf{v}_0}{m_d} t} + \frac{1}{2\gamma} \int_0^t dt' \left[ 1 - e^{-\frac{\mathbf{v}_0}{m_d} (t-t')} \right] \left[ 2\mathbf{F}_{\text{act}}(t') + \mathbf{\xi}(t') \right],
\]
\[
\mathbf{v}_{cm}(t) = \mathbf{v}_0 e^{-\frac{\mathbf{v}_0}{m_d} t} + \frac{1}{2m_d} \int_0^t dt' \ e^{-\frac{\mathbf{v}_0}{m_d} (t-t')} \left[ 2\mathbf{F}_{\text{act}}(t') + \mathbf{\xi}(t') \right],
\]
with \( \mathbf{r}_0 = \mathbf{r}_{cm}(0) \) and \( \mathbf{v}_0 = \mathbf{v}_{cm}(0) \).

From Eq. (30) and thanks to \(((\cos \theta))_{ic} = ((\sin \theta))_{ic} = 0 \) one finds \(((\mathbf{v}_{cm}))_{ic} = 0 \) and, after some long but straightforward integrations,

\[
2m_d[(v_{cmx})^2]_{ic} = k_B T + \frac{F_{act}^2}{\gamma (t_I^{-1} + t_a^{-1})}
\]

with

\[
t_I = \frac{m_d}{\gamma} \quad \text{and} \quad t_a = D_R^{-1} = \frac{\gamma \sigma_d^2}{2k_B T} = \frac{\sigma^2}{4D^2_{cm}}
\]

in the long time limit, beyond \( t_I \). As, typically, \( t_a \gg t_I \), one has

\[
2m_d[(v_{cmx})^2]_{ic} \simeq k_B T + \frac{m_dF_{act}^2}{\gamma^2}.
\]

With a similar calculation, starting now from Eq. (29), we calculate the mean-square displacement (MSD)

\[
\langle \Delta \mathbf{r}_{cm}^2 \rangle(t) = \langle (\mathbf{r}_{cm}(t + t_0) - \mathbf{r}_{cm}(t_0))^2 \rangle_{ic}
\]

in the limit \( t_0 \gg t_I \), where \( t \) denotes time-delay henceforth.

In the limit \( t \ll t_I \),

\[
\langle \Delta \mathbf{r}_{cm}^2 \rangle(t) = 2(v_{cmx})^2 t^2
\]

where \( \langle v_{cmx}^2 \rangle = [(v_{cmx})^2]_{ic} \) is the velocity given in Eq. (31). The factor two is due to the sum over the two Cartesian directions.

In the limit \( t \gg t_I \)

\[
\langle \Delta \mathbf{r}_{cm}^2 \rangle(t) = 4D_{cm}^p t + \left( \frac{F_{act}}{\gamma} \right)^2 \frac{2}{D_R} \left[ t - \frac{1 - e^{-D_R t}}{D_R} \right],
\]

where

\[
D_{cm}^p = \frac{k_B T}{2\gamma}
\]

is the diffusion constant in the passive limit, \( F_{act} = 0 \), see [40]. This equation presents several time scales and limits. (Similar calculations for an active ellipsoid were presented in [46].) For \( t_I \ll t \ll t_a \) one finds

\[
\langle \Delta \mathbf{r}_{cm}^2 \rangle = 4D_{cm}^p t + \left( \frac{F_{act}}{\gamma} \right)^2 t^2,
\]

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

\[
t^* = \frac{4D_{cm}^p}{F_{act}^2} = \frac{2k_B T \gamma}{F_{act}^2} = \left( \frac{4}{P_e} \right)^{\gamma} \frac{\sigma_a^2}{4D_{cm}^p} = \left( \frac{4}{P_e} \right)^{\gamma} t_a.
\]

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 super-diffusion \( t^* \) with \( 1 < \alpha < 2 \) if they are not well separated \((t_I \simeq t^* \simeq t_a)\). See [40] and Fig. 4 below for more details. In the large Pe limit one has \( t^* \ll t_a \). In the last time-lag regime \( t \gg t_a \), we recover normal diffusion,

\[
\langle \Delta \mathbf{r}_{cm}^2 \rangle = 4D_A t,
\]

with the diffusion coefficient

\[
D_A(F_{act}, T, \phi = 0) = \frac{k_B T}{2\gamma} \left[ 1 + \frac{1}{2} \left( \frac{F_{act} \sigma_d}{k_B T} \right)^2 \right].
\]

In terms of the diffusion constant of the center of mass of the passive dumbbell and the Péclet number the above equation reads \( D_A(P_e, \phi = 0) = D_{cm}^p (1 + Pe^2/8) \).
III. NUMERICAL

In this Section we present results from numerical simulations and we focus on three issues: the phase diagram, the translational diffusion properties and the rotational diffusion properties. Details on the numerical method used for solving the dynamical equations \((4)\) are given in \([40]\). We set \(m_d = \sigma_d = k_B = \epsilon = 1\) in proper physical units, \(r_0 = 1.5\), \(k = 30\), \(\gamma = 10\), assuring over-damped motion and negligible dumbbell vibrations. Depending on the plots we used between 15000 and 20000 dumbbells in the simulations.

A. The phase diagram

Aspects of the phase diagram and the dynamics of this system were already established in \([25, 26]\). It was shown in these papers that at sufficient low temperature and large active force the system phase separates into gas-like spatial regions and clusters of agglomerated dumbbells.

The model has three important energy scales, \(\epsilon\), \(k_B T\) and \(F_{\text{act}} \sigma_d\). Keeping \(\epsilon\) and all other parameters fixed, we will try to determine whether the phase diagram depends upon \(k_B T\) and \(F_{\text{act}} \sigma_d\) separately or only through their ratio, \(i.e.\) through the Péclet number \(Pe\), as usually assumed \([23]\). The other free parameter to be varied is the global density of the sample, \(\phi\).

In the four panels in Fig. 1 we show the probability distribution function, \(\rho\), of the local density, \(\phi_x\), for four values of the active force, \(F_{\text{act}} = 0.05, 0.1, 0.5, 1\) in the different panels. The global density of the system is \(\phi = 0.5\).

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In the four panels in Fig. 1 we show the probability distribution function, \(\rho\), of the local density, \(\phi_x\), for four values of the active force, \(F_{\text{act}} = 0.05, 0.1, 0.5, 1\). Each panel contains results for the same set of Péclet numbers \(Pe(T, F_{\text{act}})\) obtained by different combinations of temperature and active force. The system has global packing fraction \(\phi = 0.5\). We used the same operative definition of the local density as in \([25, 26]\). We divided the full system in square plaquettes with linear size \(10\sigma_d\) that is much smaller than the linear size of the full sample and big enough to sample \(\phi_x\) correctly. We improved the statistics by sampling over many different runs of the same kind of system.

At low \(Pe\) the system is homogeneous and \(\rho\) is peaked around \(\phi_x = \phi = 0.5\). The critical \(Pe\) at which the system starts aggregating is approximately the same in all panels, \(Pe \approx 65\). Around this value the density distribution \(\rho\) not only becomes asymmetric but starts developing a second peak at \(\phi_x > 0.5\) that characterises the dense phase in the
Snapshots of the system for $F_{\text{act}} = 0.1$ (cfr. the upper right panel in Fig. 1), and $T = 0.001, 0.002, 0.003, 0.01$ corresponding to $Pe = 200, 100$, both phase separated, $Pe = 66$, close to critical, and $Pe = 20$, homogeneous (from left to right and from top to bottom). The global density is $\phi = 0.5$.

system. Snapshots of typical configurations of the system at $F_{\text{act}} = 0.1$ and four values of $Pe$ are shown in Fig. 2. The location of the central peak at $Pe$ less than the critical value is independent of all parameters (apart from $\phi$) while the location of the peak at $\phi_x > 0.5$ is situated at different values of $\phi_x$ for different $F_{\text{act}}$ and the same $Pe$ (compare the different panels in Fig. 1). The reason for this is that the strength of the interactions between the dumbbells under different $F_{\text{act}}$ is different as $F_{\text{act}}/\epsilon$ varies with $F_{\text{act}}$. A larger active force permits the dumbbells to compact, while a lower one allows for looser clusters.

We repeated the analysis above for the case with total packing fraction $\phi = 0.6$ and we found the same values for the critical Péclet number and for the densities of the separated phases. In Table I we report these density values for the cases with $F_{\text{act}} = 1, 0.5, 0.1, 0.05$ and $Pe = 100, 200$. As observed, the coexistence values get closer for smaller active forces even though the Péclet number remains the same.

| $Pe$ | $F_{\text{act}} = 0.05$ | $F_{\text{act}} = 0.1$ | $F_{\text{act}} = 0.5$ | $F_{\text{act}} = 1$ |
|------|------------------|------------------|------------------|------------------|
| 200  | 0.37             | 0.34             | 0.21             | 0.049            |
|      | 0.70             | 0.71             | 0.80             | 0.89             |
| 100  | 0.44             | 0.41             | 0.37             | 0.096            |
|      | 0.66             | 0.68             | 0.77             | 0.87             |

TABLE I. Density values of the two coexisting phases related to the histograms in Fig. 1.
B. Translational diffusion properties

In [14] the diffusion properties of a tracer immersed in a bacteria bath were monitored. A crossover between a super-diffusive regime at short time-delays and a diffusive regime at long time-delays was reported. The crossover time, $t_c$, was found to increase linearly with the density of the active medium, showing that the crossover is not due to the tracer’s inertia but to the dynamic properties of the bacteria bath. We explore here the same issues by focusing on the MSD of the center of mass of the dumbbells, defined in Eq. (34). We will consider, for the rest of the paper, sufficiently low Péclet numbers such that the system will always be in the homogenous phase even though fluctuation effects can be relevant, as we will see.

Several single dumbbell trajectories are shown in Fig. 3 for different values of the temperature and global density, under the same active force $F_{\text{act}} = 0.1$. The trajectories correspond to a total time interval that includes the late diffusive regime (see below). At low temperature and global density ($T = 0.005$ and $\phi = 0.1$, upper left panel) we see periods of long directional motion. These are reduced at higher global density ($\phi = 0.4$ upper right panel). Increasing temperature ($T = 0.05$ and $T = 0.5$ lower left and right panels, respectively) the trajectories become more similar to the ones of passive diffusion. The single dumbbell diffusion coefficient, as calculated from Eq. (41), would be $D_A = 0.050$, $0.0075$, $0.025$ for the cases at $T = 0.005$, $0.05$, $0.5$, respectively. Note the non-monotonic dependence on temperature, also visible from the figures.

![Figure 3](image_url)

FIG. 3. Several trajectories of one bead in different dumbbells. The active force is $F_{\text{act}} = 0.1$ and the evolution time interval is $t = 10000$ in all panels. The other parameters are $T = 0.005$ and $\phi = 0.1$, $0.4$ (upper panels, left and right), and $T = 0.05$, $0.5$ and $\phi = 0.1$ (lower panels, left and right).

In Fig. 4 we show the center of mass MSD normalised by time-delay in such a way that normal diffusion appears as a plateau. The four panels display data at four temperatures, $T = 0.005$, $0.01$, $0.05$, $0.1$, all under the same active force $F_{\text{act}} = 0.1$. Each panel has five curves in it, corresponding to five different densities given in the key. In all cases $m_d = 1$ and $\gamma = 10$ implying $t_f = 0.1$. The characteristic times $t_I$, $t^*$, $t_a$ are shown with small vertical arrows in each panel. These plots show several interesting features:

- 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 as given by Eq. (41) (The case $t \ll t_f$ of the single dumbbell.)
- Next, the dynamics slow down and, depending on $T$ and $\phi$, the normalised mean-square displacement may attain a
plateau associated to normal diffusion (low $T$) or even decrease, suggesting sub-diffusion. (The case $t_I \ll t \ll t^* \ll t_a$ of the single dumbbell.)

- The dynamics accelerate next, with a second super-diffusive regime in which the curves for all $\phi$ in each panel look approximately parallel and very close to ballistic at $T = 0.005$, 0.01, 0.05. (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 a plateau that yields the different $D_A$ coefficients. (The case $t_I \ll t^*, t_a \ll t$ of the single dumbbell.)

It is hard to assert whether the intermediate regime is super-diffusive or simply ballistic as the time-scales $t^*$ and $t_a$ are not sufficiently well separated (and not even ordered as $t^* < t_a$ in the last panel). Moreover, in the last two panels (high $T$ or low $Pe$) the diffusion-ballistic-diffusion regimes are mixed, due to the fact that the condition $t^* \ll t_a$ is no longer satisfied. The effective slope in the intermediate super-diffusive regime decreases when the density increases.

A rather good fit 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. (30)

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

without the first term (negligible if $Pe \gg 1$) and upgrading the remaining parameters, $D_A^\phi$ and $D_R^\phi$, to be density-dependent fitting parameters, as done in [14, 21]. This is shown in Fig. 4 (left panel). For not that large values of $Pe$ one could recover the remaining parameter and use instead $\langle \Delta r_{cm}^2(t) \rangle = 4D_{cm}^{\phi, pd} t + 4D_A^\phi \left( t - \frac{1 - e^{-D_R^\phi t}}{D_R^\phi} \right)$ with an additional fitting parameter. Figure 4 (right panel) also shows a good agreement between the values of $D_R^\phi$ found in these fits and the values of the rotation diffusion coefficient $D_R(F_{act}, T, \phi)$ coming from the late time-delay diffusive regime in the rotational MSD discussed in Sec. III D.

The crossover time-delay between the last ballistic or super-diffusive, and the diffusive regimes seems quite $\phi$-independent in the first two panels $T = 0.005$, 0.01 and it increases, though rather weakly, with $\phi$, in the last two
panels, $T = 0.05$, 0.1, see the inclined dashed line in the last panel that is also a guide-to-the-eye. This crossover time-delay is the one that we could associate to the $t_C$ in [14]. The strongest effect of density is though on the first diffusive or sub-diffusive regime.

Let us now discuss the normal diffusive regime at longest time-lags. In [40] we presented plots for the translational diffusion and we studied $D_A$ as a function of $F_{\text{act}}$ and $\phi$ at fixed temperature. In particular, we compared the $\phi$ dependence to the Tokuyama-Oppenheimer law for colloids [47]. Here we examine, instead, the $T$ and $\phi$ dependence of $D_A$ for fixed active force, $F_{\text{act}}$.

The first question we want to answer is whether $D_A$ depends on $k_B T$ as for the single dumbbell case ($\phi = 0$), the functional form recalled in Eq. (11). For $F_{\text{act}}\sigma_d/k_B T \ll 1$ such that the quadratic term can be neglected this equation implies the linear growth of $D_A$ with $k_B T$. Instead, when the second term dominates, i.e. for very small thermal energy with respect to the work performed by the active force, $D_A$ should decay as $1/(k_B T)$ with a slope that is quadratic in $F_{\text{act}}\sigma_d$. In Fig. 6 we display $D_A$ as a function of $T$ for various values of $\phi$ given in the key and $F_{\text{act}} = 0.1$. The theoretical values for $\phi = 0$ are included in the figure (with open triangles joined by a dotted curve). Here, we used the measured value for the distance between the centres of the two colloids, that is $\sigma_d = 0.96$.

The error-bars are smaller than the symbol size and we do not display them. The curves show a minimum located at $k_B T_{\text{min}} = F_{\text{act}}\sigma_d/\sqrt{2}$ for $\phi = 0$, that weakly increases with $\phi$. The two regimes, $Pe \ll 1$ and $Pe \gg 1$, still exist and $D_A$ is dominated by thermal fluctuations in the former and by the work done by the active force in the latter as in the single dumbbell limit. We see a saturation of $D_A$ at small values of $T$ for $\phi > 0.2$ and therefore the breakdown of the single dumbbell $1/(k_B T)$ behaviour at low temperatures. 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.

Figure 5 also shows that for the Pe that we used $D_A$ is a decreasing function of $\phi$ at all fixed temperatures. This fact can be better appreciated in the left panel in Fig. 7 where $D_A$ is plotted as a function of $\phi$ for various temperatures given in the key. (Recall that the $\phi$ dependence of $D_A$ at fixed $T$ and for different active forces was discussed in [40] where it was shown how the Tokuyama-Oppenheimer [47] law of the passive system was simplified under activation to a decay that is close to a simple exponential. We will come back to this issue below.)

The non-monotonicity of $D_A$ as a function of $T$ already discussed in Fig. 6 is confirmed by the data presentation in Fig. 7 with the minimum situated around $T \approx 0.07$. In the right panel we observe the opposite behaviour in the ratio $D_A(F_{\text{act}} = 0.1, T, \phi)/D_A(F_{\text{act}} = 0.1, T, 0)$, first growing for increasing $T$ to reverse its trend at around $T \approx 0.05 - 0.07$. Consistently with the behaviour found in [40], there are temperatures such that the data for the above ratio cross each other when the density is increased, see for example $T = 0.01$, 0.1 (or $Pe = 2$, 20).

We have repeated this analysis for a stronger active force and we found that the results are consistent, with a crossover temperature that grows with $F_{\text{act}}\sigma_d$, as predicted by the single dumbbell equation, though we cannot assert that the dependence be linear.

FIG. 5. (Left panel) Fit of the center of mass MSD normalised by time-delay with the expression in Eq. (42). $Pe = 40$ and the different data sets correspond to the global densities given in the key. (Right panel) The rotation diffusion coefficient as extracted from the fit of the center–of–mass MSD ($D_R^0$) in the left panel and from the late-time diffusive rotational MSD, see Sec. III C, labeled “measured” in the plot.

1. The late-epochs translation diffusion coefficient

Let us now discuss the normal diffusive regime at longest time-lags. In [40] we presented plots for the translational diffusion and we studied $D_A$ as a function of $F_{\text{act}}$ and $\phi$ at fixed temperature. In particular, we compared the $\phi$ dependence to the Tokuyama-Oppenheimer law for colloids [47]. Here we examine, instead, the $T$ and $\phi$ dependence of $D_A$ for fixed active force, $F_{\text{act}}$.

The first question we want to answer is whether $D_A$ depends on $k_B T$ as for the single dumbbell case ($\phi = 0$), the functional form recalled in Eq. (11). For $F_{\text{act}}\sigma_d/k_B T \ll 1$ such that the quadratic term can be neglected this equation implies the linear growth of $D_A$ with $k_B T$. Instead, when the second term dominates, i.e. for very small thermal energy with respect to the work performed by the active force, $D_A$ should decay as $1/(k_B T)$ with a slope that is quadratic in $F_{\text{act}}\sigma_d$. In Fig. 6 we display $D_A$ as a function of $T$ for various values of $\phi$ given in the key and $F_{\text{act}} = 0.1$. The theoretical values for $\phi = 0$ are included in the figure (with open triangles joined by a dotted curve). Here, we used the measured value for the distance between the centres of the two colloids, that is $\sigma_d = 0.96$.

The error-bars are smaller than the symbol size and we do not display them. The curves show a minimum located at $k_B T_{\text{min}} = F_{\text{act}}\sigma_d/\sqrt{2}$ for $\phi = 0$, that weakly increases with $\phi$. The two regimes, $Pe \ll 1$ and $Pe \gg 1$, still exist and $D_A$ is dominated by thermal fluctuations in the former and by the work done by the active force in the latter as in the single dumbbell limit. We see a saturation of $D_A$ at small values of $T$ for $\phi > 0.2$ and therefore the breakdown of the single dumbbell $1/(k_B T)$ behaviour at low temperatures. 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.

Figure 5 also shows that for the Pe that we used $D_A$ is a decreasing function of $\phi$ at all fixed temperatures. This fact can be better appreciated in the left panel in Fig. 7 where $D_A$ is plotted as a function of $\phi$ for various temperatures given in the key. (Recall that the $\phi$ dependence of $D_A$ at fixed $T$ and for different active forces was discussed in [40] where it was shown how the Tokuyama-Oppenheimer [47] law of the passive system was simplified under activation to a decay that is close to a simple exponential. We will come back to this issue below.)

The non-monotonicity of $D_A$ as a function of $T$ already discussed in Fig. 6 is confirmed by the data presentation in Fig. 7 with the minimum situated around $T \approx 0.07$. In the right panel we observe the opposite behaviour in the ratio $D_A(F_{\text{act}} = 0.1, T, \phi)/D_A(F_{\text{act}} = 0.1, T, 0)$, first growing for increasing $T$ to reverse its trend at around $T \approx 0.05 - 0.07$. Consistently with the behaviour found in [40], there are temperatures such that the data for the above ratio cross each other when the density is increased, see for example $T = 0.01$, 0.1 (or $Pe = 2$, 20).

We have repeated this analysis for a stronger active force and we found that the results are consistent, with a crossover temperature that grows with $F_{\text{act}}\sigma_d$, as predicted by the single dumbbell equation, though we cannot assert that the dependence be linear.
Next, we analyse in Fig. 8 whether the ratio of diffusion coefficients of the active system at finite density and single passive dumbbell $D_A(F_{act}, T, \phi)/D_{cm}$ depends only on the Peclét number, as it does for the single dumbbell problem. With this aim, we fix $F_{act}$ and we vary $T$, and the values $Pe = 4, 20, 40, 66$ in each panel are obtained from three different combinations of $F_{act}$ and $T$. In all panels the collapse of data is very good. Note the change in concavity of the collapsed data that occurs at $Pe = 20$. This value is relatively far from the transition between homogeneous and segregated phases estimated in [26, 40], and the system configurations are still homogeneous, see the last panel in Fig. 2 though with a distribution of local densities, $\phi_x$, with a certain width, see Fig. 1.

These results suggest

$$D_A(F_{act}, T, \phi) = k_B T f_A(Pe, \phi)$$

with $f_A(Pe, 0) = (2\gamma)^{-1}(1 + Pe^2/8) = D_A(F_{act}, T, 0)/(k_B T)$ and $f_A$ a decreasing non-linear function of $\phi$ at fixed $Pe$, in the homogeneous phase. This relation is equivalent to

$$\frac{D_A(F_{act}, T, \phi)}{D_A(F_{act}, T, 0)} = \frac{f_A(\text{Pe}, \phi)}{f_A(\text{Pe}, 0)}$$

The l.h.s. is what we studied in [40] as a function of $F_{act}$ and $\phi$, keeping $T$ fixed, and we proposed

$$\frac{D_A(F_{act}, T, \phi)}{D_A(F_{act}, T, 0)} = e^{-b(F_{act}) \phi}$$
with $b$ a non-monotonic function of $F_{\text{act}}$. Knowing now that $D_A/(k_B T)$ depends on $F_{\text{act}}$ and $T$ only through $P$\`{e}clet, we deduce

$$D_A(F_{\text{act}}, T, \phi) = D_{\text{cm}}^p (1 + P \phi^2) e^{-b(P)\phi}.$$  \hspace{1cm} (46)

Note that in [40] the maximum in $b$ appeared at $F_{\text{act}} \simeq 0.1$ that, for the temperature used, $T = 0.05$, corresponds to $P \simeq 4$. Thus, $f_A(P, \phi)$ should be monotonically increasing with $P$, at all fixed $\phi$, for $P \geq 4$ as occurs when comparing the data on the different panels in Fig. 8. In Fig. 8 we included, with dotted black lines, the exponential fits in Eq. (46) where the only free parameter is $b(P)$. The values of $b(P)$ are $1.1, 1.6, 2.8, 4.1$ for $P = 4, 20, 40, 66$, in agreement with what we reported in [40].

However, while we see that the exponential fit is very good at all $\phi$ for $P = 40$ and $P = 66$, it is not as good for the smaller $P$ data. The red line-points in Fig. 8 represent, instead, the result of the fit

$$D_A(F_{\text{act}}, T, \phi) = D_A(F_{\text{act}}, T, 0) [1 + a_1(P)e^2 P \phi + a_2(P)e^2 \phi^2].$$  \hspace{1cm} (47)

This functional form gives a better representation of the data for $P = 4$ and $P = 20$, and an equivalent one for $P = 40$, while it is clearly worse than the exponential one for $P = 66$. The fitting parameters are given in the keys. One notices that $a_1$ is negative in all cases while $a_2$ changes sign from negative at $P < 20$ to positive at $P > 20$ (leading to a growing behaviour at large $\phi$ that is not physical). At $P = 20$ the density dependence is almost linear as $a_2$ is very close to zero.

C. Rotational diffusion properties

Having discussed in detail the translational diffusion properties we turn now to the rotational ones.

In Fig. 9 we display the angular MSD normalized by time-delay. The four panels show data obtained for the same parameters as the ones used in Fig. 4 with $F_{\text{act}} = 0.1$. Each panel, corresponding to the cases with $T = 0.005, 0.01, 0.05, 1$ and P\`{e}clet number shown in the internal label, includes curves for five different densities,
\[ \langle \Delta \theta^2 \rangle / 2t \]

**FIG. 9.** The angular MSD for the Pe numbers in the labels and, with different lines, various densities given in the keys to each panel. The dash in the first panel highlights the initial ballistic behavior. The vertical arrows indicate the characteristic times \( t_I, t^*, t_a \). Note that the vertical scale is different in the two panels above and in the two panels below.

\( \phi = 0.1, 0.2, 0.3, 0.4, 0.5 \), given in the key. These plots also show several interesting features:

- In all cases there is a first ballistic regime with a pre-factor that is independent of \( \phi \) 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 \( \phi \), the normalised MSD may attain an ever-lasting plateau associated to normal diffusion for low \( \phi \) at any temperature, or even decrease, suggesting sub-diffusion, at enough high \( \phi \).
- At low temperature \( T = 0.005, 0.01 \) (Pe=40, 20) 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 \[ 25, 26 \]. 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.

### 1. The late-epochs rotation diffusion coefficient

We now study whether the linear temperature dependence of the single dumbbell angular diffusion constant, Eq. (28), survives the interactions between dumbbells in the finite density problem, see Fig. 10. The data points are compatible with a linear behaviour at sufficiently high temperature, with a slope that depends upon \( \phi \). The trend in the curves reverses below the crossover at \( T \approx 0.01 \) with larger values of \( D_R \) for larger values of \( \phi \) (see the right panel in the same figure).

From Fig. 11 one easily concludes that the \( F_{act} \)-independence of \( D_R \) is lost as soon as the interaction between dumbbells is switched on at finite density. This fact can be seen, for instance, by comparing the \( T = 0.1 \) data, one of the two temperatures included in both panels, sharing the same value, slightly larger than \( 10^{-2} \), at \( \phi = 0 \). While in the case \( F_{act} = 0.1 \) (left panel) \( D_R \) clearly decreases with \( \phi \), in the case \( F_{act} = 1 \) (right panel) \( D_R \) is almost constant.
These figures also show the change in trend operated at an $F_{\text{act}}$-dependent $T$: at high temperature $D_R$ decreases with $\phi$ while at low temperature $D_R$ increases with $\phi$. The change occurs at $T \simeq 0.01$ for $F_{\text{act}} = 0.1$ and at $T \simeq 0.1$ for $F_{\text{act}} = 1$ suggesting that the change is controlled by $\text{Pe}$.

Finally, we analyse whether $D_R/(k_B T)$ depends on $F_{\text{act}}$ only via $\text{Pe}$. To this end, in Fig. 12 we repeat the analysis shown in Fig. 8 for $D_A$. The four panels show $D_R/(k_B T)$ against $\phi$ for $\text{Pe} = 4$, 20, 40, 66. In each panel we include data for three pairs of $F_{\text{act}}$ and $T$ leading to the same $\text{Pe}$. We see that the data points collapse on different master curves in each panel. This suggests

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

(48)

with $f_R(\text{Pe}, 0) = f_R(0, 0) = 2/(\gamma \sigma_d^2)$. The data also show a change in trend of the function $f_R$ at around $\text{Pe} = 20$. At low densities, while the master curve decreases with $\phi$ for $\text{Pe} < 20$, it becomes flat at $\text{Pe} = 20$ and it increases with $\phi$ for $\text{Pe} > 20$. This would suggest:

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

(49)

with $a(\text{Pe}, \phi)$ almost linear in $\phi$ and the slope changing sign at $\text{Pe} \simeq 20$ for small $\phi$. All panels, e.g. at all $\text{Pe}$, show 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. Note that a crossover around $\text{Pe} = 20$ was also found in the dependence of the translational diffusion coefficient on density.
IV. CONCLUSIONS

We have presented a thorough study of the translational and rotational MSD of a system of interacting active dumbbells. We focused on the low density regime in which the global system is homogeneous. We reach higher densities than the ones used in [14, 31]. We restrain the Pe to be small enough (and possibly much smaller than in the experiments) to keep the system in its homogeneous phase.

We showed that, in the single passive 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, $t_d$, and an additional one, $t^* \propto t_d/\text{Pe}^2$, that lies in between the other two for large Pe). This rich structure survives under finite densities with modified parameters. The super-diffusive behaviour shown in [14] could be associated to the second ballistic regime we find at finite densities. We found that 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, we proved that it depends on temperature and active force only through the Péclet number at all densities explored. In general, though the Pe dependence is non-monotonic, for the temperatures and active forces used, in agreement with [40], we found that the diffusion constant is a decreasing function of Pe.

Next we moved to the analysis of the rotational MSD. While in the single dumbbell case its time-delay dependence is rather simple, with a single crossover between ballistic and diffusive behaviour, intermediate regimes appear at finite densities. The late epochs diffusion constant increases with temperature (though not linearly) at all densities and active forces simulated. The independence on active force is lost at finite densities. We proved that the angular diffusion constant depends on temperature and activity only through the Péclet number and that, at low densities, its dependence on density changes from decreasing at low Pe to increasing at high Pe. We can ascribe the change in behaviour to the large scale density fluctuations that appear close to the transition from homogeneous to phase separated phases at a critical Pe. The large and rather compact clusters in this region of parameters rotate coherently [25, 26] and may be the cause for the increase of $D_R$ with $\phi$. On the other hand, at large enough densities rotations are strongly inhibited and the value of $D_R$ decreases for all Pe.

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 from the mobility and diffusive properties of the sample and the tracers, in the manner done in [30, 48–56] for different active systems.

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