Fluctuations and effective temperature in an active dumbbell system

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I. INTRODUCTION

Active matter refers to systems driven out of equilibrium by internal or external energy sources. They are characterized by many peculiar properties not present in their passive counterparts, like clustering, anomalous diffusion, giant fluctuations, unexpected rheological properties[1–3]. An open question for these systems is a coherent definition of an effective temperature[4].

We consider here a two-dimensional system of active dumbbells[5]. Each dumbbell is composed by two colloids kept together by an elastic potential, with an excluded volume interaction modeled through a Weeks-Chandler-Anderson (WCA) potential. They are immersed in an implicit solvent modeled by the Langevin equation. The activity is modeled by a constant force acting along the main axis of the dumbbell. The model can be intended as a coarse-grained description of the behavior of simple bacteria. Hydrodynamic interactions are ignored, being much more demanding computationally.

The two goals of this work are the following. First we want to analyze the diffusion and fluctuation properties of the dumbbell system. At strong enough activity, or small enough temperature, and at sufficient high density, dumbbells segregate into a concentrated and a dilute phase. We focus on the regime without clustering, when the system is globally homogeneous. We find four different regimes for the translational and angular mean square displacement, and show the dependence of the diffusion coefficient of the late-epoch diffusion regime from the temperature, activity and density. We find for example, that for sufficiently high activity, the rotation diffusion is enhanced from increasing density which is different from what usually happens in passive colloidal systems[6]. For what concerns the behavior of the distribution functions of the displacements, at strong activity, we find significant deviations from the gaussian behavior in the superdiffusive regime found before the last usual diffusive regime. At small activity, the initial inertial regime is followed by a subdiffusive regime and also in this case we find slowly decaying codes of the distributions not corresponding to gaussian behavior.

Second, we want to investigate about the definition of the effective temperature in this system, usually defined by a dynamic fluctuatuon-dissipation relation. For this purpose, we introduce spherical tracers, kinetically coupled with the dumbbells, in order to test the notion of effective temperature. The effective temperature of the tracers will be compared with that obtained by studying the active dumbbell system by alone. In general, the study of the dynamics of tracers, more accessible experimentally than that of the non-equilibrium system itself, is a convenient way to analyze non-equilibrium systems.

For a single active dumbbell we analytically calculate the diffusion coefficient for its center of mass together with the displacement induced by a pulling force, arriving to a definition of an effective temperature through a fluctuation-dissipation relation. Then we numerically evaluate the above quantities for systems with different densities, temperature and activity. We show how the non trivial non monotonic behavior of diffusion and mobility, at varying activity, is reflected in the behavior of the effective temperature.

On the other hand, we calculate the effective temperature of the active system by analysing the velocity distribution function and a fluctuation dissipation relation for the tracers. The tracer velocity distributions is gaussian and a temperature can be evaluated by the variance of the distribution. We find that the tracer effective temperature, calculated by both methods, for high values of the mass of the tracers, converge to the value of the effective temperature found in the system without tracer.

In the next sections we show selected results for the translation and rotational mean square displacements and for the effective temperature in the system without tracers.

II. MEAN SQUARE DISPLACEMENT

Fig.1 shows the mean square displacement of the center of mass (upper panel) and rotational angle (lower panel) of dumbbells for a high Péclet number and different densities. The Péclet number represents the ratio between active advective contribution to transport rate and diffusive contribution. Different regimes can be observed, depending on the combination of the random noise, the activity and the density of the system.

These regimes correspond to those found analytically in the case of a single dumbbell, where a first ballistic inertial regime is followed by a diffusive regime, then by another ballistic regime due to activity and at the end by the late epoch final diffusive regime. It is interesting to observe that, while the single dumbbell mean square rotational displacement only exhibits an initial inertial regime followed by the diffusive final regime, at final densities four regime can be observed also for this quantity.

Fig.2 shows the dependence on the density of the rotational diffusion constant, at a fixed value of the Péclet number, varying the temperature T and the active force F_{act} simultaneously[5]. The behavior is independent on the value of T, F_{act} chosen. Clustering effects induce unusual higher rotational diffusion when the density increases, for $\phi < 0.5$.

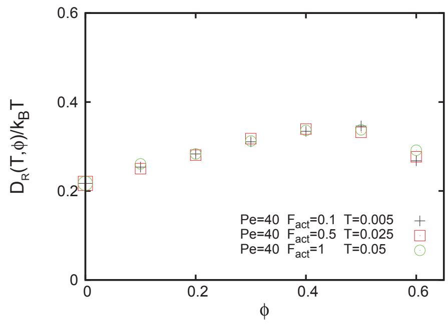

FIG. 2. Rotational diffusion coefficient at same Peclet number and different set of active force and temperature.

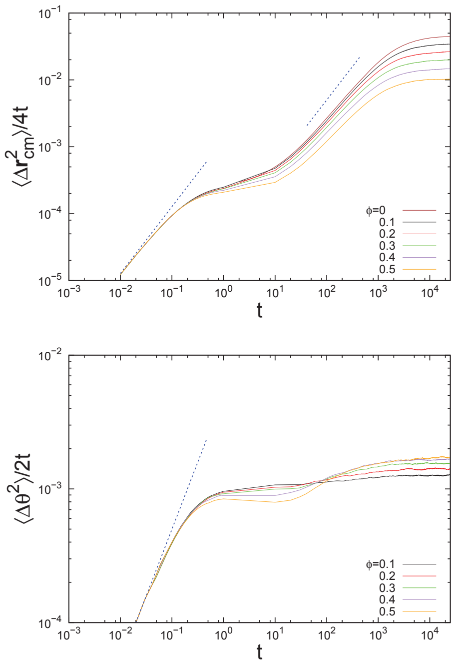

FIG. 1. Translational and rotational mean square displacement of active dumbbells at different densities.

III. EFFECTIVE TEMPERATURE

Fig.3 suggests the dependence of the effective temperature on the square of the Péclet number. The theoretical line and tha data at different densities are shown. Further analysis would show a non-monotonic behavior as a function of the density. T_{Jeff} is calculated by a fluctuation-dissipation relation involving the mean square displacement in the last diffusive regime and the integrated linear response. At the value $F_a = 0.1$ we compared the value of the effective temperature shown above with that coming from the velocity distribution of tracers at different increasing masses. We found that the temperature of the tracer reached the one calculated from the system itself when the ratio between the mass of the tracer and that of the dumbbells is of the order of 10^4.

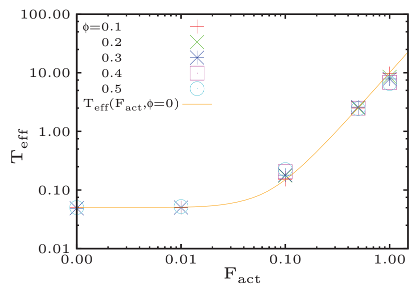

FIG. 3. Effective temperature as a function of the active force.

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