Supplementary Information: Collective dynamics of active dumbbells near circular obstacle

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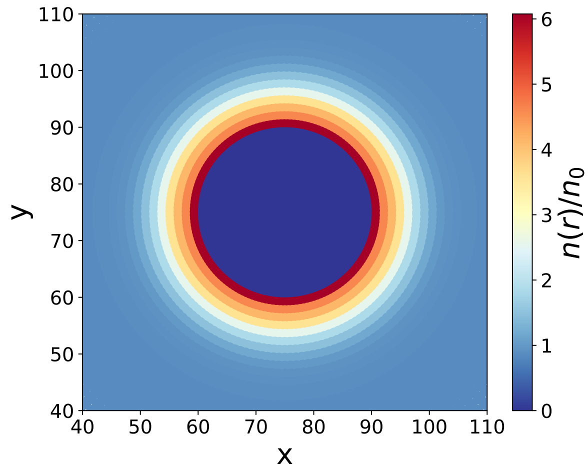

FIG. 1. The color map reflects the average density of active dumbbells around the obstacle of radius $R_o = 15$ at a given $Pe = 40$. The central dark blue patch depicts the circular obstacle with zero density of the active dumbbells. The color bar shows the variation of the normalized density around the obstacle's surface. Only a portion of the simulation box is displayed to clarify the density profile.

I. NORMALISED DENSITY MAP

The normalized average density profile of active dumbbells, represented by $n(r)/n_0$ shown in Figure 1, exhibits a distinctive pattern. Near the obstacle's surface, $n(r)/n_0$ has a maximum value, signifying the highest concentration of active dumbbells. As one moves away from the surface, $n(r)/n_0$ gradually decreases, and far from the surface, the density of the active dumbbells approaches unity, i.e., the bulk value. This indicates that near the surface, the density profile is significantly higher than the bulk, displaying an aggregation of active dumbbells on the obstacle's surface.

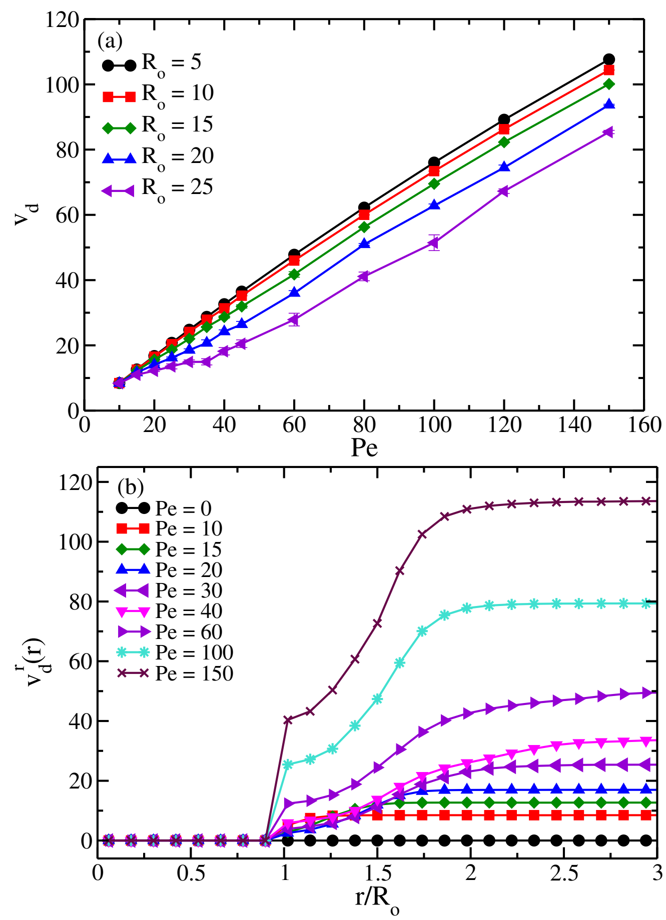

FIG. 2. (a) The variation of average directed speed, as a function of Pe for different radii (R_o). (b) The distribution of average directed speed $v_d^r(r)$ from the center of obstacle for various Pe at a given $R_o = 15$.

II. DIRECTED SPEED

To provide detailed insights into the dynamics of a single active dumbbell, we analyze the average directed speed of a dumbbell in the presence of a static obstacle. The average directed speed (v_d) is defined as the average projection of the velocities of active dumbbells along their axes of orientations, i.e., $v_d = < \mathbf{v} \cdot \hat{\mathbf{n}} >$. Figure 2-a displays the average directed speed of a dumbbell as a function of Péclet number (Pe) for various obstacle radii. Directed speed also grows linearly with Pe at a fixed obstacle radius R_o; however, as R_o increases, the

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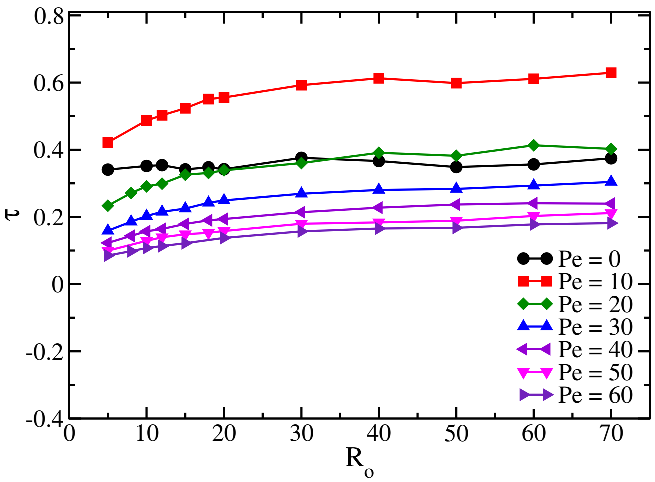

FIG. 3. Variation of the residence time τ as a function of R_o for various Pe.

$\mathrm{v_d} - Pe$ curve shifts downwards, reflecting the decrease in the directed speed. This is because aggregation size becomes more prominent for higher R_o, as discussed in the manuscript. Consequently, within these aggregates, the active dumbbells slow down considerably. The increased aggregation size contributes to a reduction in speeds; as a result, it leads to decay in the directed speed for larger R_o.

Nevertheless, despite this slowdown, active dumbbells form ordered jammed structures around the circumference of the surface that generate torque on the cluster, therefore having the significant tangential speed to make them rotate around the obstacle.

Furthermore, we probe the average directed speed $\mathrm{v_d^r}(r)$ as a function of radial distance r from the center of an obstacle for various Pe at fixed obstacle radius $R_o = 15$. As expected, for the passive system $Pe = 0$, the average directed speed is zero; therefore, $\mathrm{v_d^r}(r)$ remains zero at all distances, see Fig. 2-b. While for low activity ($Pe < 10$), the directed speed $\mathrm{v_d^r}(r)$ near the obstacle's surface and far from them is nearly the same due to lack of dense aggregation on the surface, in this limits the density of active dumbbells is everywhere roughly same as in bulk phase. However, for $Pe \geq 15$ aggregation of the dumbbell sets on the surface, the speed of dumbbells is significantly reduced near the surface, as illustrated in Fig. 2-b. The directed speed monotonically grows as we go far from the surface until it reaches a plateau corresponding to the speed of active dumbbells in the homogeneous bulk phase.

III. RESIDENCE TIME

Now, we present the residence time of an active dumbbell on the obstacle's surface in the dilute concentration as a function of radius R_o and active speed Pe. We place a randomly oriented active dumbbell on the obstacle's surface to compute this time. Then, we measure the average duration a dumbbell spends within a cutoff radius of 1.5 from the surface of a circular obstacle, called here residence time τ. This calculation is averaged over 2500 randomly oriented particles on the obstacle's surface.

Figure 3 illustrates the variation of the residence time τ as a function of obstacle radius R_o for different Péclet numbers Pe. For a passive system, i.e., $Pe = 0$, the residence time τ remains constant across all R_o values. However, for active systems, the residence time weakly increases with R_o for all Pe. As Pe increases, the curve shifts downward, indicating that the residence time decreases for larger Pe. This reduction in residence time at higher Pe values is attributed to active particles exiting in the cutoff region at higher speeds, primarily when oriented away from the surface. In summary, our finding indicates that, in the dilute limit, the residence time of active dumbbells demonstrates only a weak dependence on both curvature radius (R_o) and Péclet number (Pe). Further, the effect of the concentration of the active dumbbells leads to dramatic increases of τ, as discussed in the main manuscript.

IV. SUPPLEMENTARY MOVIES

Here, we provide various supporting movies to illustrate the collective dynamics of active dumbbells around the static obstacle and the dynamic behavior of a tracer particle in the medium of active dumbbells.

Movie S1: The movie shows the dynamics of the active dumbbells at Péclet number $Pe = 10$ at a given obstacle radius $R_o = 15$. Only the central portion of the simulation box is presented for clarity.

Movie S2: The movie shows the dynamics, aggregation, and rotation of the active dumbbells on the surface of an obstacle at Péclet number $Pe = 20$ at a given radius $R_o = 15$. Only the central portion of the simulation box is presented for clarity.

Movie S3: The movie shows the dynamics, aggregation, and rotation of the active dumbbells on the surface of an obstacle at Péclet number $Pe = 40$ at a given radius $R_o = 15$. Only the central portion of the simulation box is presented for clarity.

Movie S4: The movie shows the dynamics of the active dumbbells at Péclet number $Pe = 40$ at a given obstacle radius $R_o = 5$. Only the central portion of the simulation box is presented for clarity..

Movie S5: The movie shows the dynamics, aggregation, and rotation of the active dumbbells on the surface of an obstacle of radius $R_o = 10$ at Péclet number $Pe = 40$. Only the central portion of the simulation box is presented for clarity.

Movie S6: The movie illustrates the dynamic behavior of a tracer particle of radius $R_o = 15$ at $Pe = 10$ in the solution of the active dumbbells.

Movie S7: The movie illustrates the dynamic behavior of a tracer particle of radius $R_o = 15$ at $Pe = 40$ in the solution of the active dumbbells.