Supplementary material for "Phototaxis of active colloid by self-thermophoresis"

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I. ANGULAR VELOCITY AND SELF-PROPELLED VELOCITY

In the main text, the phototaxis of the active Janus particle is quantified by the stationary positional and orientational probability distributions. In order to look in more detail into this phototactic behaviors, we also measure the orientation- and position-dependent angular velocities and self-propelled velocities of the Janus particle for both nonuniform and uniform beams, as plotted in Figs. S1 and S2.

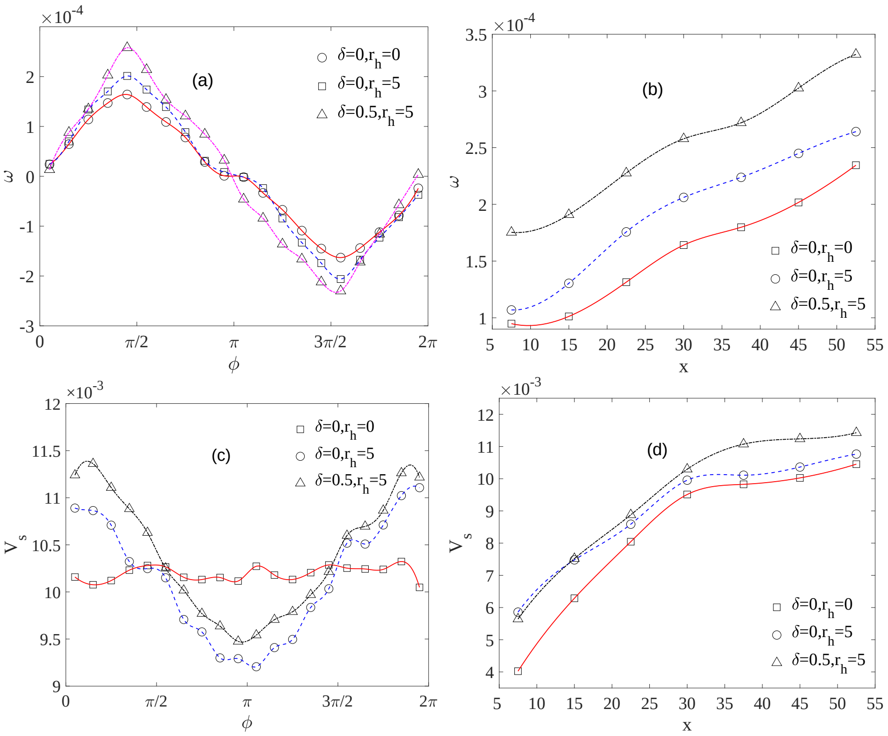

FIG. S1: (a-b) The angular velocities of the Janus particle in the inhomogeneous beam as a function of (a) the particle orientation with the particle position $x = 30$ (middle beam intensity), and (b) the particle position with the particle orientation $\phi = \pi/2$ (the maximum ω). Here, the positive ω corresponds to a counter-clockwise rotation. (c-d) The self-propelled velocities of the Janus particle in the inhomogeneous beam as a function of (c) the particle orientation with $x = 30$, and (d) the particle position with $\phi = 0$. Different symbols refer to different particle parameters. The dimension of the simulation box is 120×60, except that in (c) the simulation box of 60×60 is used to avoid possible extra finite-size effect on v_s induced due to the difference in the system size between in the x and y directions.

In the nonuniform beam, the angular velocity ω of the Janus particle depends on the

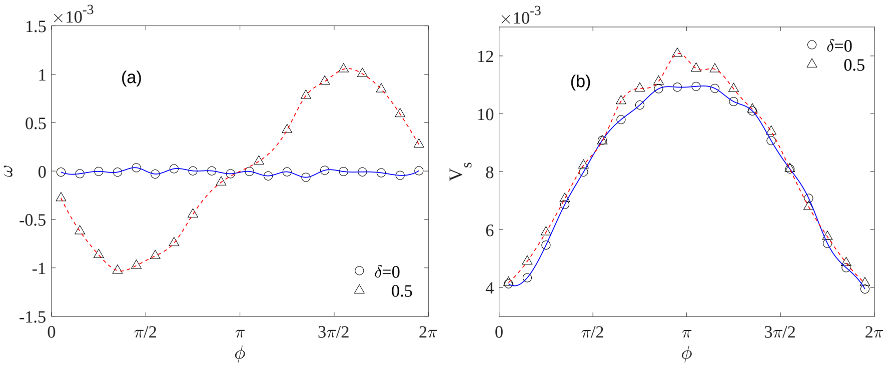

FIG. S2: The angular velocities (a) and the self-propelled velocities (b) of the Janus particle in the uniform beam as a function of the particle orientation. Owing to the uniform beam, the angular velocity and the self-propelled velocity are independent of the particle position.

particle orientation and behaves like a sinusoidal function (Fig. S1(a)), so $\phi = \pi$ is the stable equilibrium point of the particle orientation. The maximum ω (at $\phi = \pi/2$) increases with the light intensity (hence x) and also increases with δ and r_h, as plotted in Fig. S1(b). As displayed in Fig. S1(c), the self-propelled velocity v_s (motility) of the Janus particle of $r_h \neq 0$ is orientation-dependent. The motility at $\phi = 0$ is larger than that at $\phi = \pi$, since the particle at $\phi = 0$ receives stronger light. While, for $r_h = 0$ the motility is independent of the orientation. Figure S1(d) indicates that v_s clearly increases with the light intensity, resulting in a spatially varying motility. For the uniform beam, ω and v_s both depend on the particle orientation, as plotted in Fig. S2. The ω behaves like an inverse sinusoidal function (Fig. S2(a)), such that $\phi = 0$ is the stable equilibrium point of the particle orientation. The v_s has a maximum at $\phi = \pi$ (Fig. S2(b)), since which corresponds to the configuration that the light-absorbing hemisphere of the Janus particle is completely irradiated. All these results are consistent with the stationary orientational and positional distributions of the Janus particle in the main text.

II. FINITE-SIZE EFFECT

In the 2D simulation systems, hydrodynamics and gradient fields are long-ranged, although the 2D properties cannot affect the existence of the alignment effect, the orientation-dependent motility and the spatially inhomogeneous motility. Thus, the underlying mechanism of the phototaxis of the self-thermophoretic Janus particle is qualitatively unchanged.

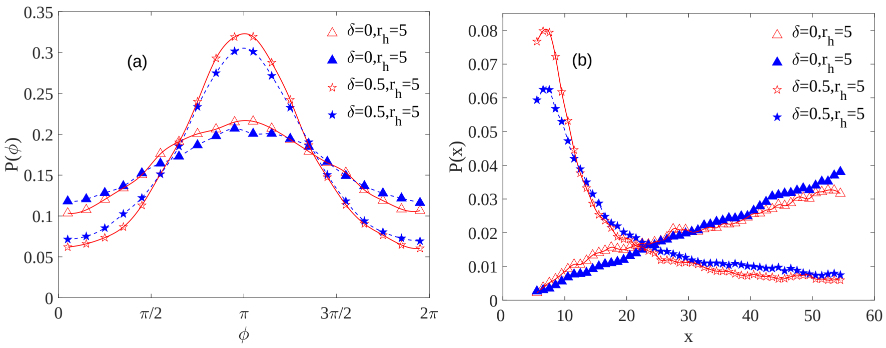

FIG. S3: Finite-size effect for the orientation (a) and position (b) distributions of the active Janus particle in the inhomogeneous beam. The red open symbols correspond to the original system in the main text, and the blue solid symbols to the larger system with twice box size, where other system parameters are the same as those of the original system.

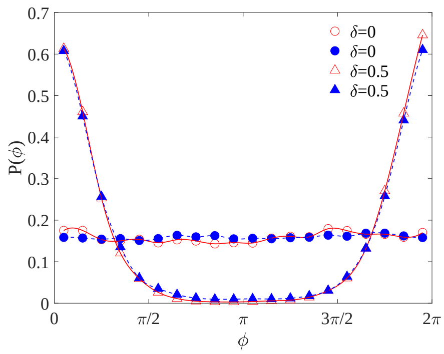

FIG. S4: Finite-size effect for for the orientation distribution of the Janus particle in the uniform beam. The red open and blue solid symbols correspond to the original system and the larger system (twice box size), respectively.

To evaluate finite-size effect due to particle self-interactions via periodic boundary conditions, we perform simulations with twice box size for several typical system parameters. The results indicate that the finite-size effect only slightly influences the observed dynamics, as shown in Figs. S3 and S4.

III. ALIGNMENT OF ACTIVE BROWNIAN PARTICLE

For the active Brownian particle with a spatially varying motility, the theoretical calculation (Eqs.(2)-(5) in the main text) and the Brownian dynamics simulation both show that

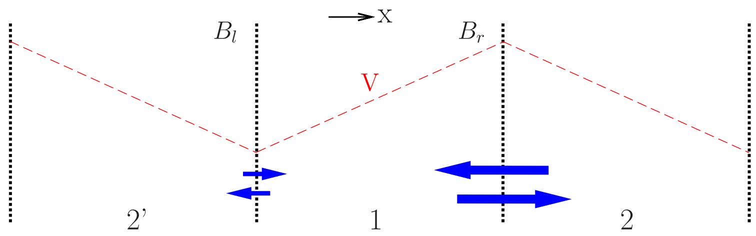

FIG. S5: Active Brownian particle self-propelling with a spatially inhomogeneous motility. The system consists of the left-half box (1) and the right-half box (2). Box (2') is the periodic image of box (2) due to the periodic boundary condition. The red dashed lines represent the inhomogeneous self-propelled velocity, the blue arrows represent the particle fluxes, and the vertical dotted lines (B_l and B_r) separate the left and right boxes.

the orientation probability distribution has a maximum value rather than being flat. The active Janus particle of $r_h = 0$ has a similar result. This seems counter-intuitive, since the equation of motion for the orientation just describes a plain random diffusion. We point out that this result actually arises from the spatially inhomogeneous motility.

To understand this intuitively, we consider the stochastic model sketched in Fig. S5. Due to symmetry, we only discuss the angle distribution in box (1). Image the initial position and orientation distributions are uniform everywhere. Because the motility (self-propelled velocity) varies with the particle position and the rotational diffusion (D_r) is homogeneous, the persistent length (v/D_r) is also position-dependent. Because the particle motility is smaller near border B_l than near B_r, within the same time interval there are more particles moving (self-propelling) into box (1) from box (2) through border B_r than through border B_l (see the blue arrows). This leads to an increase of the probability of the particle with its orientation against the x-axis. Similarly, the difference in the particle fluxes from box (1) to box (2) across border B_l and across B_r results in a decrease of the probability of the particle with its orientation along the x-axis. Consequently, the particle in box (1) more possibly orients against the x-axis (namely $\phi = \pi$). Reversely, due to symmetry the particle in box (2) more possibly orients along the x-axis (namely $\phi = 0$). The argument intuitively explains the result of Fig.4 (and those for $r_h = 0$ and $\delta = 0$) in the main text.

Note that the non-flat orientational distribution is not a boundary effect. For a region far away from the boundary, according to the above discussion one can easily find that an initial flat distribution is not stable once the particle motility is position-dependent.