

Experimental realization of the “lock-and-key” mechanism in liquid crystals

Supplemental Information

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1 Drag coefficient analysis

The average velocity v throughout the trajectory is $1 \mu\text{m/s}$ and the radius of the colloid $a = 8 \mu\text{m}$. Using typical material constants density $\rho = 1.38 \text{ g/cm}^3$, viscosity $\eta = 14.31 \text{ mPa} \cdot \text{s}$, elastic constant $K = 10^{-12} \text{ g/cm}^3$, we can find $Re = \frac{\rho va}{\eta} = 3 \times 10^{-6} \ll 1$ and $Er = \frac{\rho va}{K} = 0.1 \ll 1$. Therefore the viscous force balances the elastic force and elastic forces will exceed the viscous forces and so the director field will not be strongly affected by the flow field.

Since the particle moves near the wall is in close proximity to three surfaces (those that form the top and bottom of the cell, and the wavy wall), corrections to the viscous drag on the sphere must be addressed to account for interactions with these boundaries. Since there are no exact analyses or simulations that address this geometry, we approximate the drag coefficient as the sum of two contributions, C_{gap} accounting for the sphere in a thin gap, using the analysis of Ganatos [1], the other, C_{\parallel} accounting for the motion of a sphere parallel to a bounding wall, adopting the results of O’Neill [2]. In addition, the particle moves toward the wavy wall, which could require an additional contribution to the drag coefficient, C_{\perp} . We estimate the magnitude of this contribution using the analysis of Brenner [3], and find that the changes in the drag coefficient for the wall distances explored by our particles is sufficiently weak that this contribution can be ignored.

The motion with respect to the wavy wall can be decomposed into v_{\perp} and v_{\parallel} :

$$\begin{cases} v = \sqrt{v_{\perp}^2 - v_{\parallel}^2} \\ v_{\perp} = v \cos(\theta - \psi) \\ v_{\parallel} = v \sin(\theta + \psi) \end{cases} \quad (1)$$

where $\theta = \tan^{-1}\left(\frac{v_y}{v_x}\right)$ and $\psi = \tan^{-1}\left(\frac{dy}{dx}\right) = \tan^{-1}(h'(x))$, assuming the wavy surface is located at $y = h(x)$.

Brenner [3] studies the interaction of a spherical moving perpendicular to a surface, where the Stokes' drag is corrected by a factor of C_{\perp} as a function of normalized distance to the wall $\alpha = \frac{d}{a}$:

$$\frac{F_{\perp}}{6\pi\eta a v_{\perp}} = C_{\perp}(\alpha) \quad (2)$$

C_{\perp} is calculated via Equation (2.19) in Brenner's paper, the drag correction values are tabulated in Table 1 in the above reference. At $\alpha = 1$, $C_{\perp} \rightarrow \infty$, but for the course of our trajectory, C_{\perp} varies from 1.6 to 1.9.

The parallel motion of a sphere near the wall is studied by O'Neill [2], the correction to Stokes' equation owing to the presence of the wall is:

$$\frac{F_{\parallel}}{6\pi\eta a v_{\parallel}} = C_{\parallel}(\alpha) \quad (3)$$

where C_{\parallel} is also a function of α . It is determined by Equation (26) and tabulated in [2].

Based on the α from our trajectory, C_{\perp} and C_{\parallel} both vary from 1.3-1.9 (as shown in Fig. 1).

The movement is also constrained in \hat{z} . Given the symmetries of the experimental configuration and the elastic repulsion from the gap walls, it is reasonable to assume that the particle is centered in the gap. The drag coefficient is given graphically in Fig. 3(a) in terms of $\beta = \frac{l}{a}$ for a gap of half-width l comparable to the sphere radius a in the analysis of Ganatos, Pfeffer and Weinbaum [1]. From that graph, for spheres and gaps of size that correspond to our experiment, the combined effect of two surfaces yields $C_{gap} = 3$.

Furthermore, the anisotropy of viscosities must be accounted for in LC. For micron-sized particle moving in 5CB, typical values of viscosities are $\eta_{\perp} = 14.3 \text{ mPa} \cdot \text{s}$ and $\eta_{\parallel} = 7.83 \text{ mPa} \cdot \text{s}$. Our trajectories consist of prolonged motion parallel to the wall (transverse to the director field), followed by a reversal and

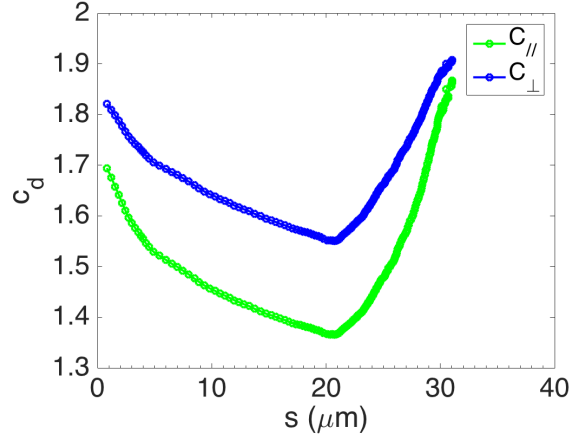


Figure 1: Drag coefficients at each arclength s from Brenner (C_{\perp}) and O'Neill (C_{\parallel}) calculated from the distance of the colloid from the wall at each point along the trajectory

docking event (parallel to the director field, with significant near field splay-matching interactions. For this docking segment, the more relevant viscosity may be η_{\parallel} .

Our aim is to extract an order of magnitude estimate for the interaction energy. We do this in two ways. In one, we use the transverse viscosity η_{\perp} for the entire trajectory, and estimate the net drag coefficient from the gap and interactions with the wavy wall to be about $C_D \approx 4$. Based on this correction factor, the energy U can be found by integrating the velocity over the entire trajectory:

$$U = C_D \delta \pi \eta a \int_0^{s_f} v ds \quad (4)$$

By this method, we find $U \approx 10^5 k_B T$.

In a more careful treatment, we decompose the motion into v_{\perp} and v_{\parallel} . We assume the colloid is close enough to the surface that the relevant viscosity for v_{\perp} is η_{\parallel} , and that for v_{\parallel} is η_{\perp} . We let $C_{gap} \approx 3$. The drag force can be decomposed as follows:

$$\begin{cases} F_{\parallel, gap} = C_{gap} \delta \pi \eta_{\perp} a v_{\parallel} \\ F_{\parallel, wall} = C_{\parallel}(\alpha) \delta \pi \eta_{\perp} a v_{\parallel} \\ F_{\perp, wall} = C_{\perp}(\alpha) \delta \pi \eta_{\parallel} a v_{\perp} \end{cases} \quad (5)$$

The energy dissipation throughout the trajectory, summing up all contributions:

$$U = 6\pi a \left(\eta_{\parallel} \int_0^{s_f} C_{gap} v ds + \eta_{\parallel} \int_0^{s_f} C_{\parallel} v_{\parallel} ds_{\parallel} + \eta_{\perp} \int_0^{s_f} C_{\perp} v_{\perp} ds_{\perp} \right) \quad (6)$$

where s_{\parallel} and s_{\perp} are the parallel and perpendicular components of the arc length s . $s_{\parallel} = s \cdot \sin(\theta - \psi)$ and $s_{\perp} = s \cdot \cos(\theta - \psi)$.

By this method, we find U to differ by 2 percent from the one viscosity and one drag coefficient approximation. This small difference is owing to the fact that the rate of migration for the last stage of docking after the reversal is extremely slow. For the purposes of an order of magnitude estimate, we give the simpler discussion in the main text.

2 Videos

2.1 Video 1

A spherical particle ($2a = 15 \mu\text{m}$) with a ‘‘Saturn ring’’ defect migrates near a wavy wall. The particle migrates at $8 \mu\text{m/s}$, due to external flow, and its center of mass is $14 \mu\text{m}$ away from the surface. The viscous force distorts the director field. The distortion of the wall decays farther away from the wall. As a result, the particle cannot dock. The video is real time.

2.2 Video 2

A spherical particle ($2a = 15 \mu\text{m}$) with a ‘‘Saturn ring’’ defect migrates near a wavy wall. The particle is under the influence of homeotropic boundary condition of the wall, consists of ‘‘hills’’ and ‘‘dales’’, which distorts the director field. The particle traces out a curved trajectory: first it is ‘‘kicked’’ up, then it reverses its direction and finally it docks into its final position, matching its splay distortion with that of the ‘‘dale’’. The video is real time.

2.3 Video 3

A spherical particle ($2a = 5 \mu\text{m}$) with downward-orienting dipolar defect finds its equilibrium position on top of a ‘‘hill’’ which best matches its director field. The video is real time.

2.4 Video 4

A spherical particle ($2a = 5 \mu\text{m}$) with upward-orienting dipolar defect finds its equilibrium position on the bottom of a “dale” which best matches its director field. The video is real time.

References

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