Active depletion torque between two passive rods

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The active depletion torque experienced by two anisotropic objects in an active bath is a conceptional generalization of the equilibrium entropic torque. Using Brownian dynamics simulations, we compute the active depletion torque suffered by two passive rods immersed in an ensemble of active Brownian particles. Our results demonstrate that the active depletion torque is qualitatively different from its passive counterpart. Interestingly, we find that the active depletion torque can be greatly affected by the external constraint applied on the rotational degree of freedom of the rods, and even the direction may be changed with the orientational constraint, which is in contrast to the equilibrium depletion torque. The main reason for the remarkable features of the active depletion torque is that the active particles can significantly accumulate in the vicinity of the rods due to persistent self-propulsion, which is sensitively dependent on the constraint strength and the rod configurations. Our findings could be relevant for understanding the self-assembly and dynamics of anisotropic macromolecules in living environments.

1 Introduction

Active matter, ranging from cell cytoskeleton filaments1 and bacteria colonies2–5 to artificial microswimmers6–12 and shaken non-symmetric granular particles,13,14 are composed of active units that individually convert the stored or environmental energy into autonomous motion.15–18 Due to being inherently out-of-equilibrium, active matter can exhibit striking phenomena, such as motility-induced phase separation,19–23 novel self-organization24–27 and spontaneous collective motion,5,28–31 which is absent in passive systems.

Because of the irreversibility of persistent self-propulsion, which is fundamentally different from irregular thermal motions, active-matter systems often have abnormal mechanical and thermodynamical properties. For example, pressure in active matter is generally not a state function, except for some specific models, i.e., spherical active Brownian particles without orientational coupling with the boundary walls.32 The active noise experienced by a passive intruder in a fluid of self-propelled particles is not the intrinsic attribute of the active bath, but depends on the external potentials applied to the intruder.33 Moreover, the active bath is able to exert a net torque on chiral passive intruders and thus drive their unidirectional rotation,34–37 which only suffer from stochastic rotation in a thermal bath.

In addition to producing direct forces or torques, the active bath can mediate effective interactions between immersed passive objects. A particularly important example is the active depletion force that is a conceptual extension of the equilibrium depletion force. Interestingly, the active depletion force substantially changes with the external constraint suffered by the passive objects,38 in contrast to its equilibrium counterpart that is of entropic origin and independent of the dynamics of suspended objects.39 In other words, the active effective interaction between the free passive objects is not equivalent to that between the fixed objects, although this equivalence has been widely employed to determine the equilibrium entropic force. Given that activity-mediated self-assembly has recently stirred up considerable interest,40–44 and as biological self-assemblies (such as the biological “key–lock” mechanism forming a bond between non-spherical macromolecules45) usually occur in living environments,46,47 it is thus necessary and important to understand deeply the characteristics of the active effective interactions.

Nevertheless, relative to the active depletion force that has been extensively studied,38,48–51 investigation of the active depletion torque between non-spherical passive objects is rare.52,53 In equilibrium, the depletion torque arises from the entropic effect44–49 and plays a vital role for the self-assembly of anisotropic objects.50–63 The equilibrium depletion torque can
be either characterized by the orientational distribution function of two freely rotating non-spherical objects, or equivalently determined by measuring the torques on two fixed objects exerted by the depolarizers. However, in the context of an active bath that is far from equilibrium, it is unfeasible to obtain the active depletion torque from the orientational distribution function. On the other hand, the active depletion torque perhaps is constraint-dependent, similar to the case of the active depletion force, which may disable the measurement of the active depletion torque on free objects with the strategy of fixing objects. The observations thus raise a natural question: how does the external constraint influence the active effective torque?

In this paper, we numerically investigate the active depletion torque experienced by two passive colloidal rods in a two-dimensional fluid of active particles. In particular, we study the effect of the external conditions on the active depletion torque using an angle potential to confine the rod orientation, which roughly mimics external environments that influence the rotational dynamics of the rods, like diverse viscoelastic or crowded media. Compared with the equilibrium case that is independent of the external conditions, the active depletion torque not only has a much larger magnitude but also significantly hinges on the constraint potential. Moreover, both the direction and magnitude of the active depletion torque change sensitively as the rod configurations and orientations vary. The complex behavior of the active depletion torque can be explained based on the joint effects of the entropy-like torque and the motility-induced accumulation of active particles in the concave region formed by the two rods. The constraint dependence of the active depletion torque could open up new possibilities to manipulate non-symmetric objects and direct activity-induced self-assembly.

II Simulation systems

The two-dimensional active bath is composed of 1000 active Brownian particles of diameter \( \sigma_a \), with a packing fraction \( \rho = 0.2 \) to avoid motility-induced clustering. The colloidal rod is simulated as a spherocylinder with a width \( \sigma_r = 1.5\sigma_a \) and cylindrical length \( l = 4.5\sigma_a \), as sketched in Fig. 1(a). Throughout the simulations, the rod centers are fixed with a distance \( d \) between the two rod centers, and the orientation of the rod is described by the included angle between the long axis of the rod and the line connecting the two rod centers, \( \theta_{le} \) and \( \theta_{re} \), which respectively correspond to the left and right rods. According to the system symmetry, we focus on three types of rod configuration [see Fig. 1(b–d)]: symmetric configuration I \( (\theta_{le} = 180^\circ - \theta_{re}) \), parallel configuration II \( (\theta_{le} = \theta_{re}) \) and asymmetric configuration III \( (\theta_{le} = 90^\circ) \). The three configurations are the most representative and cover most of the typical configurations of two rods. Choosing the three configurations thus facilitates a comprehensive exploration of the possible constraint dependence of the active depletion torque, with a relatively low computational cost. For convenience, we also identify the shortest surface separation between the two rods as \( b \). All the inter-particle, particle–rod and rod–rod interactions \( (U_{pp}, U_{pr}, U_{rr}) \) are modelled using a Weeks–Chandler–Andersen potential, \( U(r) = 4[(\sigma/r)^{12} - (\sigma/r)^{6}] + 1 \) if \( r < 2^{1/6}\sigma \) and \( U(r) = 0 \) otherwise, separately with the interaction diameter \( \sigma = \sigma_a \) for \( U_{pp} \), \( \sigma = [\sigma_a + \sigma_r]/2 \) for \( U_{pr} \), and \( \sigma = \sigma_r \) for \( U_{rr} \). In order to investigate the influence of the external constraint environment on the effective torque, the rotational degree of freedom of each rod is independently coupled to an external torsion spring, \( k_0/2(\theta - \theta_o)^2 \), with \( \theta_o \) being the equilibrium orientation and \( k_0 \) the spring stiffness.

The position \( \mathbf{r}_i \) and orientation \( \mathbf{n}_i = (\cos \phi_i, \sin \phi_i) \) of active particle \( i \) are updated via overdamped Langevin equations

\[
\gamma_r \mathbf{f}_i = F_d \mathbf{n}_i - \nabla_r U_i + \sqrt{2k_B T \gamma_r} \xi_r, \\
\gamma \phi_i = \sqrt{2k_B T \gamma_r} \xi_r
\]

with \( \gamma_r(\theta_i = \sigma_a^2\gamma_i/3) \) being the translational (rotational) friction coefficient, \( k_0T = 1 \) being the thermal energy, \( F_d \) being the self-propelling force taken as \( F_d\sigma_a/k_0T = 20 \) in simulations, and \( U_i(r) \) being the steric interactions. Here, \( \xi_r \) and \( \xi_r \) are the Gaussian-distributed white noise of the zero mean and the unit variance.

We take the left rod as an example to describe the evolution of the rod orientation in the simulations. Similarly, the rod orientation evolves via the overdamped Langevin equation

\[
\gamma_w \bar{\theta}_{le} = M - \partial_{\theta_{le}} \left[ k_0/2(\theta_{le} - \theta_{re})^2 \right] + \sqrt{2k_B T \gamma_w} \bar{\xi}_{le},
\]

where \( \bar{\xi}_{le} \) refers to the derivative with respect to the rotational degree of freedom, and \( \gamma_w = \gamma_r(\text{ln} \rho - 0.662 + 0.917/p - 0.050/p^2)^{-1} \).
refers to the rotational friction coefficient of the rod, with 

\[ p = \frac{1}{2} \langle r \rangle + 1 \] 

and \[ 2 \gamma_0 = \tau_1 (1 + \tau_1)^2 / 2 \gamma_2 \]. Here, \( M \) contains the active depletion torque \( M_e \) (only a conceptual extension of the equilibrium depletion torque) arising from the active particle–rod collisions and the torque contributed by the rod–rod interactions. The last term of eqn (2) is the stochastic torque on the rod. In the simulations, the rod orientation fluctuates around its equilibrium position determined by the external angle potential, and the active depletion torque is measured and averaged when the deviation of the rod orientation from its equilibrium angle is lower than 0.5°, i.e., \[ |\theta - \theta_{0}\text{e}| < 0.5° \] and \[ |\theta_{0}\text{e} - \theta_{0}\text{a}| < 0.5° \]. By tuning the spring stiffness, we can achieve different strategies to measure the depletion interactions. For instance, \( k_0 = \infty \) and \( k_0 = 0 \), respectively, correspond to the frozen and free schemes, both of which are equivalent in the equilibrium state.

**III Results and discussions**

### 3.1 Active depletion torque for configuration I

We first compute the active depletion torque \( M_e \) on the two rods for configuration I. We choose a moderate center-to-center distance \( d = 4.0 \sigma_x \). Due to the symmetry, the orientation angle \( \theta_{0}\text{e} \) of the left rod is varied from 59.0° to 90.0° (\( \theta_{0}\text{a} = 180° - \theta_{0}\text{e} \)), where the minimum \( \theta_{0}\text{e} \) is determined when the two rods touch. Fig. 2(a) shows \( M_e \) as a function of \( \theta_{0}\text{e} \) for various reduced constraint strength values \( k = k_0 / k_{0}\text{T} \) ranging from 0 (freely rotating rods) to infinity (fixed rods). For comparison, Fig. 2(a) also plots the corresponding equilibrium depletion torque (namely \( F_{\text{de}} = 0 \)), which is computed only for infinite \( k_0 \) because of its independence of the external constraint. As the two rods in configuration I experience opposite torques, we only consider the torque on the left rod.

Remarkably, \( M_e \) with infinite \( k_0 \) is generally orders of magnitude larger than the passive value, and even the direction of \( M_e \) is opposite to its passive counterpart for most orientations. More interestingly, the whole profile of \( M_e \) rises with increasing constraint strength \( k \) (namely \( M_e \) becomes more positive) [Fig. 2(a)], accompanied by a reversal of the torque direction at small orientational angles. This constraint dependence is similar to the case of the active depletion force\(^{38} \) but is fundamentally distinct from the passive depletion torque that is independent of the constraint. In order to understand the unusual behavior, we qualitatively analyze the origin of the active depletion torque in the following.

Compared with the equilibrium depletion torque (also called the entropic torque owing to its entropic origin), there basically exist two different contributions to the active depletion torque. On the one hand, the rods experience strong collisions with the active particles due to their self-propulsion. Using the idea of the effective temperature, the strong collisions can be roughly approximated as those from the passive particles with an enhanced effective temperature \( T_e \) related to the motility of active particles through \( k_0 T_e = k_0 T + F_{\text{de}} / \tau_e / 2 \gamma_2 \) (with \( \tau_e = \gamma_2 / k_0 T \) the reorientation time of the active particle). Thus, the effective torque on the rods arising from the strong collisions can be approximately regarded as that in an equilibrium system with the effective temperature \( T_e \), which is referred to as the entropy-like torque \( M_{\text{de}} \). The entropy-like torques are usually inclined to rotate the rods to bring them into contact (clockwise or negative \( M_{\text{de}} \)), similar to (but much larger than) the equilibrium entropic torque. On the other hand, the concave region formed by the two rods can trap the active particles due to their persistent motions, leading to an accumulation of active particles, which strengthens with the Peclet number of the active particle.\(^{51,67} \) This accumulation effect can also contribute to an effective torque on the rods, called the accumulation torque \( M_{\text{ac}} \). So, the active depletion torque \( M_e \) is approximately a superposition of the above two contributions, i.e., \( M_e \approx M_{\text{de}} + M_{\text{ac}} \). Although the analysis above is very rough, it can provide an intuitive picture for the main dependence of \( M_e \) on the system parameters, as will be shown below.

For most orientations under study, it is difficult for the active particles to swim through the narrow gap between the fixed rods, which leads to a strong accumulation of active particles between the rods. The accumulation-induced torque generally tends to rotate the rods to separate them, namely an...
For a reversal [Fig. 2(b)]. This difference originates from the following statement: the equilibrium depletion torque, as plotted in Fig. 2(a). Furthermore, the $k_0$ dependence of $M_e$ results from the fact that a stronger constraint produces a more significant accumulation torque $M_a$ (since the active particles can easily pass through the gap between the weakly constrained rods), while $M_e$ is hardly influenced by the constraint. To intuitively show the $k_0$ dependence of the accumulation effect, we separately compute the density maps of active particles for the cases of fixed and free rods, as shown in Fig. 2(c and d), and also give the density difference map between them in Fig. 2(e) to clearly highlight the impact of the constraint on particle accumulation. Although the density map of the active particles for the fixed case is similar in form to that of the free case, the density difference map indicates that the external constraint can significantly enhance the particle accumulation between two rods. As a result, a stronger constraint causes a larger $M_e$.

For all $k_0$, $M_e$ shows a non-monotonic dependence on the rod orientation, with double peaks. Analogous to the non-monotonic behavior of the active depletion force, the peaks of $M_e$ occur at the local maximum accumulation of the active particles ($M_a$ reaches the local maximum), where the narrowest gap of the two rods is close to the thickness of one- or two-layer particles, i.e., $0.9\sigma_a$ or $2 \times 0.9\sigma_a$, with the prefactor 0.9 accounting for the soft potential. Thus, the orientational angles corresponding to the peaks of $M_e$ are separately around $\theta_e = 69.5^\circ$ or $\theta_e = 81.0^\circ$, which is consistent with the results in Fig. 2(a).

To further study the accumulation effect, Fig. 2(b) plots the active depletion torque for a small separation between the rod centers $d = 2.5\sigma_a$. In this case, $M_e$ exhibits a similar $k_0$ dependence to the case of $d = 4\sigma_a$, except for small $\theta_e$ values, where $M_e$ is insensitive to the change in $k_0$ and lacks the direction reversal [Fig. 2(b)]. This difference originates from the following observation: For $d = 4\sigma_a$, active particles accumulate in the upper concave area between the two rods [gray region in Fig. 1(b)], as shown in Fig. 2(c), producing a positive $M_e$. However, for $d = 2.5\sigma_a$ and small $\theta_e$ values, the upper concave space between the rods is so narrow that the active particles only reside in the lower concave area between the two rods [light-green region in Fig. 2(f)], thus generating a negative (clockwise) $M_e$. Independent of $k_0$, this negative accumulation torque always tends to push the top ends of the two rods to touch together, inducing a ‘self-locking’ effect. Thus, the accumulation effect does not depend on the constraint any more as well as $M_e$, such that $M_e$ is not sensitive to $k_0$. Note that for the small separation ($d = 2.5\sigma_a$) the equilibrium depletion torque is always negative [inset of Fig. 2(b)].

To check the finite size effect, we also compute $M_e$ for some typical orientations in a larger system (4000 particles). The obtained results (not shown) are almost the same as those of the present system (1000 particles), indicating that the present system size is suitable for achieving correct simulation results.

### Active depletion torque for configuration II

We next analyze the active depletion torque $M_e$ for the parallel configuration II. Fig. 3(a) shows $M_e$ as a function of the left rod orientation with $d = 4\sigma_a$ for various constraint strength values $k$ ranging from 0 (free) to infinite (fixed). Thanks to the symmetry of the configuration, we only consider $M_e$ on the left rod (identical to that of the right rod). Note that the minimum $\theta_e$ occurs when the two rods touch together. The non-monotonic orientation dependence of $M_e$ is very similar to the case of configuration I [Fig. 2(a)] due to the same reason. Likewise, the reason for the $k_0$ dependence of $M_e$ is also the same as that of configuration I, namely, that the external constraint enhances the particle accumulation, as demonstrated by the density difference of active particles between the fixed and free cases in Fig. 3(c). However, there is only a weak constraint dependence of $M_e$ at small $\theta_e$, relative to the case of Fig. 2(a). This is since, for small $\theta_e$ values, such as $\theta_e = 24.9^\circ$, the accumulation position of the active particles is close to the rod center [see Fig. 3(d)], i.e., the accumulation torque $M_e$ is small because of the short arm of force. In this way, even if the particle accumulation increases with $k_0$, the change in $M_e$ is not prominent (the entropy-like torque $M_e$ is almost independent of the constraint strength $k_0$).

We also compute $M_e$ for a small separation between two rod centers $d = 2.5\sigma_a$, as shown in Fig. 3(b). The $M_e$ value also possesses a significant dependence on the constraint, particularly at small $\theta_e$, unlike the situation of $d = 4\sigma_a$ in Fig. 3(a). In Fig. 3(b), the combination of the small separation $d$ and the small $\theta_e$ shifts the accumulation location of the active particles to the rod ends, i.e., $M_e^a$ with a long arm of force. As a result,
$M_e$ strengthens markedly with the increase of the particle accumulation and hence $k_y$. The corresponding passive depletion torques [the insets of Fig. 3(a and b)] can be understood similarly in terms of those for configuration I.

**Active depletion torque for configuration III**

We now compute the active depletion torque $M_e$ for the asymmetric configuration III. We choose $d = 4.0s_a$ and calculate $M_e$ on the left and right rods as a function of $\theta_{re}$ for various $k_y$, as plotted in Fig. 4(a) and (b), respectively. Here, the magnitude of $M_e$ on the two rods is slightly different, as the two rods with configuration III are neither symmetric nor equivalent in their configurations [Fig. 1(d)]. Again, the constraint strength $k_y$ can impact $M_e$ due to the correlation between $k_y$ and particle accumulation (i.e., $M_e^a$), which is supported by the density difference of the active particles between the fixed and free cases [Fig. 4(e)]. For comparison, we plot the equilibrium depletion torque in the insets of Fig. 4(a and b). The direction discrepancy between the active and passive depletion torques at their maximum magnitudes arises for the same reason as in Fig. 2(a). In addition, we also compute $M_e$ on the left and right rods for $d = 2.5s_a$, as shown respectively in Fig. 4(c and d), as well as their equilibrium counterparts. The dependence of $M_e$ on the constraints and orientation angle can be similarly understood based on the above analysis.

**Separation dependence of active depletion torque**

Finally, in order to investigate the separation dependence of the active depletion torque $M_e$, we choose two typical rod orientations for each configuration and compute $M_e$ as a function of the minimum surface separation $b$ between the two rods (see Fig. 1) for both free and fixed situations. The $M_e$ data on the left rod for configurations I and II are shown in Fig. 5(a) and (b), respectively, and the $M_e$ values experienced by the left and right rods for configuration III are displayed in Fig. 5(c) and (d), respectively. Moreover, the corresponding equilibrium depletion torques are provided in the insets of Fig. 5. It can be seen that $M_e$ exhibits a non-monotonic behavior as the surface distance $b$ is varied. The reason for this non-monotonicity is the same as for the non-monotonic variation of $M_e$ with the rod orientation in Fig. 2–4, since the change in rod orientation amounts to tuning the surface separation between the two rods, which simultaneously influences the entropy-like torque $M_e^e$ and the accumulation torque $M_e^a$. Again, the magnitude of $M_e$ on the fixed rod is much higher than that of the free case, except at large surface separations, where $M_e$ basically vanishes. On the other hand, for the same surface separation $b$, the change in the rod orientation angle can also affect $M_e^a$ and $M_e^e$, and thus has an impact on the magnitude of $M_e$, as shown in Fig. 5.

**IV Conclusion**

Through computer simulations, we systematically study the active depletion torque on two passive rods immersed in an active bath consisting of active Brownian particles. Our results...
show that the active depletion torque differs markedly from its passive counterpart in both magnitude and direction. Strikingly, we find that the active depletion torque depends significantly on the external orientational constraint suffered by the rods and may even reverse the direction with the constraint, in stark contrast to the equilibrium depletion torque. The constraint dependence originates mainly from the strong accumulation effect that results from the persistent self-propulsion of the active particles and sensitively hinges on the external constraint. Nevertheless, the active depletion torque hardly changes with the constraint under some special conditions, due to the ‘self-locking’ effect [Fig. 2(b)] or the vanishing arm of force [Fig. 3(a)]. Our findings provide a deeper insight into understanding biologically-related self-assembly, and could be verified via optically trapping non-spherical particles in a bacterial solution, where angular harmonic potentials are created to confine the particles and determine their active effective torques.

Conflicts of interest

There are no conflicts to declare.

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