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## Effect of reorientation statistics on torque response of selfpropelled particles

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### Effect of reorientation statistics on torque response of self propelled particles

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We consider the dynamics of self-propelled particles subject to external torques. Two models for the reorientation of self-propulsion are considered, run-and-tumble particles, and active Brownian particles. Using the standard tools of non-equilibrium statistical mechanics we show that the run and tumble particles have a more robust response to torques. This macroscopic signature of the underlying reorientation statistics can be used to differentiate between the two types of self propelled particles.

#### I. INTRODUCTION

Self-propelled particles are inherently out of equilibrium objects that consume energy at the scale of individual entities to produce persistent self generated motion. Models of self propelled particles have become the prototype theoretical system used to understand the physics of active materials. These models are directly applicable to micron sized objects such as motile bacteria and self-phoretic colloids [1–9].

There have been numerous theoretical investigations of the collective behavior of active particles in the recent years. Phenomenology uncovered includes cluster formation, phase separation, motility induced segregation [9–16], anomalous behavior of mechanical properties such as pressure [17–20] and rheology [21, 22]. Further, it has been established that the presence of external forces [23–25] or confinement [26, 27] dramatically alters the observed phenomenology in these systems. One striking example has been rectification [25, 28–32], in which asymmetric barriers induce directed transport of self-propelled particles.

Generally, self-propelled particles travel along a body axis  $\hat{\mathbf{u}}$  that has an intrinsic reorientation process. Two model classes of self-propelled particles that have been used extensively are Run-and-Tumble particles (RTPs) and Active Brownian particles (ABPs). The only difference in the dynamics of the two classes is the nature of their reorientation process. The dynamics of an RTP consists of periods of straight line motion followed by a sudden tumble event occurring at some mean tumble rate  $\alpha$ . The tumble event completely decorrelates the orientation and a new orientation is selected at random. There are several examples of motile bacteria that follow run-and-tumble dynamics [33], the most famous example being *Escherichia coli*.[34]. The second class, ABPs, reorient their body axis through gradual rotational diffusion and this diffusion is Brownian with rotational diffusion coefficient  $D_r$ . These dynamics have been observed in experiments of synthetic self-phoretic colloids [5–9].

For times much longer than the angular reorientation time, that is,  $t \gg \frac{1}{\alpha}$  for RTPs and  $t \gg \frac{1}{D_r}$  for ABPs, both

classes of particles exhibit diffusive behavior. Equating the diffusivities at this stage would yield identical phenomenology for both models. This idea has been explored extensively in [1, 13, 23, 25, 35, 36] where the authors find equivalence between the two models at the level of a drift diffusion equation when  $\alpha = (d-1)D_r$ , where d is the spatial dimension.

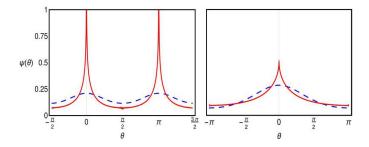


FIG. 1. (color online) Orientation probability distribution functions for RTPs (red/solid) and ABPs (blue/dashed) in the case of both a nematic aligning (left) field and a polar aligning field (right). RTP distributions are sharply peaked about the optimal direction while the ABP distribution is the smooth equilibrium result.

In this work we seek to identify signatures of the reorientation statistics on the long time behavior of selfpropelled particles. In particular we ask the following question : If the swimming parameters are equivalent, how does the long time behavior of ABPs and RTPs differ when subject to external torques? External torques model gradient seeking behavior exhibited by microorganisms such as chemotaxis [33, 34], and aerotaxis [37] in the following sense. A torque effectively makes the tumble rate or the rotational diffusion rate anisotropic, with a lower rate of reorientation in favorable directions. In this sense it has the same effect as a gradient in a chemoattractant or nutrient [38]. Further, such phenomena need not be restricted to biological systems, as micron sized platinum-gold rods have been shown to exhibit directed movement towards regions of higher hydrogenperoxide concentrations [39]. By using the framework of non-equilibrium statistical mechanics we show that runand-tumble particles align with external torques (or gradients) much more robustly than active Brownian particles, indicating that the reorientation behavior of bacteria is ideal for successful gradient seeking.

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#### II. THEORY

Let us consider non-interacting self propelled particles moving in unconstrained 2D space. The statistical mechanics of this system is given in terms of  $\psi(\mathbf{r}, \hat{\mathbf{u}}, t)$ , the probability of finding a particle at a point  $\mathbf{r}$  at a time t oriented in a direction  $\hat{\mathbf{u}} = \cos\theta\hat{x} + \sin\theta\hat{y}$  in space. When the particle reorients its direction through rotational diffusion, the dynamics of this probability distribution obeys a diffusion equation of the form

$$\partial_t \psi(\mathbf{r}, \hat{\mathbf{u}}, t) = -\nabla \cdot [v \hat{\mathbf{u}} \psi(\mathbf{r}, \hat{\mathbf{u}}, t)] + \nabla \cdot [D_t \nabla \psi(\mathbf{r}, \hat{\mathbf{u}}, t)] + \partial_\theta [D_r \partial_\theta \psi(\mathbf{r}, \hat{\mathbf{u}}, t)]$$
(1)

where v is the self propulsion speed of the particle,  $D_t$  is a translational diffusion constant and  $D_r$  is a rotational diffusion constant. When the particle undergoes run and tumble dynamics, the probability distribution obeys a master equation of the form

$$\partial_t \psi(\mathbf{r}, \hat{\mathbf{u}}, t) = -\nabla \cdot [v \hat{\mathbf{u}} \psi(\mathbf{r}, \hat{\mathbf{u}}, t)] + \nabla \cdot [D_t \nabla \psi(\mathbf{r}, \hat{\mathbf{u}}, t)] - \alpha \psi(\mathbf{r}, \hat{\mathbf{u}}, t) + \frac{\alpha}{2\pi} \int d\hat{\mathbf{u}}' \psi(\mathbf{r}, \hat{\mathbf{u}}', t)$$
(2)

where  $\alpha$  is the tumble frequency. This description is valid when the duration of a tumble is short compared to the time scales set by the self propulsion and the tumble frequency of the particle. We are interested in the dynamics of this system in the presence of uniform external torques. So, in the following, we consider the homogeneous limit of Eqs. (1-2) in the presence of a  $\theta$  dependent potential. The dynamical equations of interest then are of the form

$$\partial_t \psi(\theta, t) = \partial_\theta [D_r \partial_\theta \psi(\theta, t)] + \frac{1}{\xi^r} \partial_\theta [\partial_\theta V(\theta) \psi(\theta, t)]] \quad (3)$$

for active Brownian particles and

$$\partial_t \psi(\theta, t) = -\alpha \psi(\theta, t) + \frac{\alpha}{2\pi} \int d\theta' \psi(\theta', t) + \frac{1}{\xi^r} \partial_\theta [\partial_\theta V(\theta) \psi(\theta, t)]]$$
(4)

for run and tumble particles. In the above  $\xi^r$  is a rotational friction constant characteristic of the medium in which the particles move.

We will now consider different choices for the external potential and construct series solutions to Eqs. (3-4) of the form  $\psi(\theta) = a_0 + \sum_{n=1}^{\infty} a_n \cos(n\theta) + b_n \sin(n\theta)$  for different choices of external potential  $V(\theta)$ . Other useful measures to characterize the response of the system are the first two moments of the orientation distribution, namely, the polarization **P** defined as

$$P_{\alpha} = \int d\theta \hat{u}_{\alpha} \psi(\theta)$$

and the nematic order parameter tensor  $\overline{\mathbf{Q}}$ 

$$Q_{\alpha\beta} = \int d\theta (\hat{u}_{\alpha}\hat{u}_{\beta} - \frac{1}{2}\delta_{\alpha\beta})\psi(\theta)$$

These will be calculated as well.

#### III. NEMATIC TORQUE

First we consider an external potential of the form  $V(\theta) = -\gamma \cos(2\theta)$ . Such a field will induce a nematic aligning torque on the particles because of the two minima located at 0 and  $\pi$ . In this case a good characterization of the degree of order will be given by the component of the nematic order parameter tensor describing alignment in the  $\hat{x}$  direction, namely  $Q_{xx}$ .

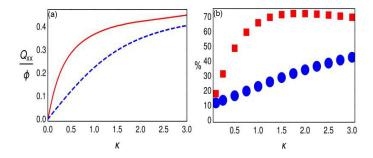


FIG. 2. (color online)(a): RTPs exhibit higher nematic order than ABPs as shown by the nematic order parameter being higher for RTPs (red) than for ABPs (blue/dashed). (b): The percentage of particles oriented within some range  $[\pi/18, \pi/18]$  of the two minima as a function of the parameter  $\kappa$ 

In the following, the parameter  $\kappa$  is the ratio of the field strength of the external potential to the friction coefficient in units of the angular reorientation time and is given by  $\kappa = \frac{\gamma}{\xi^r D_r}$  for active Brownian particles and  $\kappa = \frac{\gamma}{\xi^r \alpha}$  for run and tumble particles. Computing  $Q_{xx}$  from (3), one can show (see Appendix A for details) that for active Brownian particles, we obtain

$$Q_{xx} = \frac{\phi}{2} \frac{I_1(\kappa)}{I_0(\kappa)} \tag{5}$$

which is the equilibrium result for a thermal nematogen [40] at temperature  $\xi^r D_r$  in the presence of an external field. Here  $\phi = \int \psi(\theta) d\theta$  and the  $I_i$ 's are modified Bessel functions of the second kind [41]. For run and tumble particles, the exact value of the order parameter turns out to be a continued fraction of the form

$$Q_{xx} = \frac{\phi}{2} \frac{\kappa}{\frac{1}{2} + \frac{\kappa^2}{\frac{1}{4} + \frac{\kappa^2}{\frac{1}{6} + \frac{\kappa^2}{\frac{1}{8} + \dots}}}}$$
(6)

As seen in Fig.2, when the strength of the torque is small or comparable to the noise strength, the magnitude of nematic ordering is much larger for run-and-tumble particles. This trend persists for quite large values of the torque. But, for asymptotically large values, i.e.,  $\kappa \to \infty$ , the order parameter for RTPs and ABPs aproaches 1/2 as can be seen from eqn. 5-6

Further, We can also exactly compute the orientation distribution functions in the presence of this external torque. For active Brownian particles the distribution is of the form (Appendix A)

$$\psi(\theta) = \frac{e^{\kappa \cos(2\theta)}}{2\pi I_0(\kappa)} \tag{7}$$

which is precisely the equilibrium result and is usually called a Von Mises distribution [42, 43], the analog of the Gaussian distribution on a unit sphere. For run and tumble particles we obtain the following formally exact series solution

$$\psi(\theta) = a_0 + \sum_{n=1}^{\infty} a_{2n}(\kappa) \cos(2n\theta)$$
(8)

where the coefficients are given by

$$a_2 = \frac{2}{\pi} Q_{xx}$$
 and  $a_{2n} = a_{2n-4} - \frac{a_{2n-2}}{(2n-2)\kappa}$  :  $n \ge 2$ 

The orientation distribution is much more peaked around the minima of the external potential for run and tumble particles than for active Brownian particles (see Fig.1). An alternate view of this would be to consider the percentage of particles that align within some neighborhood of the optimal direction (Fig. 2b), which is another manifestation of the stronger torque response of RTPs. This more robust response to external torques is a consequence of the run-and-tumble search strategy being able to sample the optimal directions more efficiently than its Brownian counterpart, as the tumble directions are entirely random and unbiased by the initial orientation.

#### IV. POLAR TORQUE

In this section we consider particles subject to an external potential of the form  $V(\theta) = -\gamma \cos(\theta)$ , i.e., a torque that tends to align their direction of motion along one direction in space. In this case, the relevant measure of the response of the system is the polarization.

For active Brownian particles the polarization is found to be (Appendix A)

$$P_x = \phi \frac{I_1(\kappa)}{I_0(\kappa)} \tag{9}$$

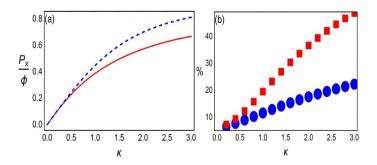


FIG. 3. (color online) (a): The polarization as a function of the parameter  $\kappa$ . The polarization for RTPs (red/solid) is less than for ABPs (blue/dashed) (b):The percentage of particles oriented within some range  $[\pi/18, \pi/18]$  as a function of the parameter  $\kappa$ . It is clear that the percentage of RTPs (red/square) oriented in that range is higher than ABPs (blue/circle).

while for run and tumble particles we have

$$P_{x} = \phi \frac{\kappa}{2 + \frac{\kappa^{2}}{1 + \frac{\kappa^{2}}{\frac{2}{3} + \frac{\kappa^{2}}{\frac{2}{4} + \dots}}}}$$
(10)

where  $\kappa$  is as defined earlier. As in the nematic case in section 3, the result for the active Brownian particle is the same as that of equilibrium. The orientation distribution functions for the two classes are found to be

$$\psi(\theta) = \frac{e^{\kappa \cos(\theta)}}{2\pi I_0(\kappa)} \tag{11}$$

for ABPs, while for RTPs

$$\psi(\theta) = a_0 + \sum_{n=1}^{\infty} a_n(\kappa) \cos(n\theta)$$
(12)

where the coefficients are given by

$$a_1 = \frac{1}{\pi} P_x$$
 and  $a_n = a_{n-2} - \frac{2a_{n-1}}{(n-1)\kappa}$  :  $n \ge 2$ 

These results are plotted as a function of the dimensionless field strength  $\kappa$  in Fig 3a and Fig 1. Unlike in the nematic case, at the level of the moments of the distribution, the ABPs exhibit higher average polar ordering than the RTPs. A better measure of the response in this case is the percentage of particles that find the optimal direction. We find that in terms of this measure the response of the run-and-tumble particle is indeed much more robust for the polar case (see Fig. 3b) and the nematic case (see Fig. 2b). We also see that for both cases the orientation distribution function is much more peaked around the optimal directions.

#### V. DISCUSSION

We have shown that the response of self-propelled particles to external torques is sensitive to the nature of the reorientation statistics of the propulsion direction. We find that run and tumble particles exhibit a more robust response to applied torques in the following sense. When there is one optimal direction for the particle's orientation, such as in the polar case, the fraction of particles that find the optimal direction is greater for those particles using a run-and-tumble search strategy, even though the average polarization is higher for particles undergoing Brownian rotational diffusion. For cases when there is more than one optimal direction for the particles to move in (such as the nematic case, where there exists 2 optimal directions) the run-and-tumble strategy always leads to better alignment as the particles are able to sample the different optimal directions better than through Brownian diffusion.

Even though the torque response is dramatically different based on the reorientation statistics, a number of bulk phenomena such as phase separation and clustering are identical in the two classes of particles. This dichotomy can be understood by noting that the two models of self propulsion considered here have identical correlations but their response is very different. Within the subspace of orientation dynamics, (i.e., integrating out spatial degrees of freedom) the response of the Brownian particle has the conventional fluctuation-dissipation relationship to the correlation, the run-and-tumble particles do not have this property (see Appendix C). Therefore the nature of the reorientation statistics becomes important when considering external perturbations such as confining forces or aligning torques.

Finally we note that the exact expressions obtained in this work for run-and-tumble particles are given in terms of formal infinite series. These series solutions converge very slowly (see Appendix B) and any truncation at low orders drastically fails to capture the true nature of the solution. Therefore, low moment closure estimates, conventionally used in the literature of active particles, is unreliable for the case of run-and-tumble particles though they work very well for the case of active Brownian particles.

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#### Appendix A: Derivation of order parameters and distribution functions

In this appendix, the details of the derivation of steady state solutions to equations (3-4) for different external torques are given. Let us begin by considering the nematic torque. The statistical mechanics in this case is given by a Fokker-Planck equation for active Brownian particles

$$\partial_t \psi(\theta, t) = \partial_\theta [D_r \partial_\theta \psi(\theta, t)] + \frac{2\gamma}{\xi^r} \partial_\theta [\sin(2\theta)\psi(\theta, t)]]$$
(A1)

and the following master equation for run and tumble particles

$$\partial_t \psi(\theta, t) = -\alpha \psi(\theta, t) + \frac{\alpha}{2\pi} \int d\theta' \psi(\theta', t) + \frac{2\gamma}{\xi r} \partial_\theta [\sin(2\theta) \psi(\theta, t)]]$$
(A2)

As described earlier we search for series solutions  $\psi(\theta) = a_0 + \sum_{n=1}^{\infty} a_n \cos(n\theta) + b_n \sin(n\theta)$ . This Fourier decomposition is equivalent to the following moment expansion

$$\psi(\theta) = \frac{1}{2\pi} (\phi + 2P_a \hat{u}_a + 4Q_{\alpha\beta} (\hat{u}_\alpha \hat{u}_\beta - \frac{1}{2} \delta_{\alpha\beta}) + \dots)$$

In this form it is apparent that  $Q_{xx} = \frac{\pi}{2}a_2$ . Using this with Eq.(A1) we arrive at the following hierarchy of equations for active Brownian particles

$$\partial_t a_0 = 0 \tag{A3}$$

$$\partial_t a_n \delta_{n,m} = \frac{\gamma}{\xi^r} m a_n (\delta_{2,n+m} + sgn(m-n)\delta_{2,|m-n|}) -n^2 D_r a_n \delta_{n,m} + \frac{2\gamma}{\xi^r} m a_0 \delta_{2,m}$$
(A4)

$$\partial_t b_n \delta_{n,m} = -\frac{\gamma}{\xi^r} m b_n (\delta_{2,n+m} + sgn(n-m)\delta_{2,|m-n|}) -n^2 D_r b_n \delta_{n,m}$$
(A5)

And similarly we find the corresponding hierarchy for run and tumble particles,

$$\partial_t a_0 = 0 \tag{A6}$$

$$\partial_t a_n \delta_{n,m} = \frac{\gamma}{\xi^r} m a_n (\delta_{2,n+m} + sgn(m-n)\delta_{2,|m-n|}) -\alpha a_n \delta_{n,m} + \frac{2\gamma}{\xi^r} m a_0 \delta_{2,m}$$
(A7)

$$\partial_t b_n \delta_{n,m} = -\frac{\gamma}{\xi^r} m b_n (\delta_{2,n+m} + sgn(n-m)\delta_{2,|m-n|}) -\alpha b_n \delta_{n,m}$$
(A8)

First note that all odd coefficients are zero by the requirement the  $\psi(\theta) = \psi(\theta + \pi)$ . By truncating at arbitrary  $a_{2n+2}$  or  $b_{2n+2}$  and taking the steady state solution, one finds that all  $a_{2n}$  or  $b_{2n}$  couple to the zeroth coefficient  $a_0$  or  $b_0$ . Since  $b_0$  does not exist, the  $b_{2n}$  vanish and by using an iterative procedure, we solve for  $a_2$  and find for active Brownian particles

$$a_{2} = 2a_{0} \frac{\kappa}{2 + \frac{\kappa^{2}}{4 + \frac{\kappa^{2}}{6 + \frac{\kappa^{2}}{8 + \dots}}}}$$
(A9)

while for run and tumble particles we have

- / \

$$a_{2} = 2a_{0} \frac{\kappa}{\frac{1}{2} + \frac{\kappa^{2}}{\frac{1}{4} + \frac{\kappa^{2}}{\frac{1}{6} + \frac{\kappa^{2}}{\frac{1}{8} + \dots}}}$$
(A10)

Beyond Eq.(8) no further analytic treatment for run and tumble particles is available. For active Brownian particles the continued fraction Eq.(A9) is of the form of a Gauss continued fraction. In general we have the following identity for the ratio of modified Bessel functions

$$\frac{I_{\nu}(z)}{I_{\nu-1}(z)} = \frac{z}{2\nu + \frac{z^2}{2(\nu+1) + \frac{z^2}{2(\nu+2) + \frac{z^2}{2(\nu+3) + \dots}}}$$
(A11)

One can find continued fraction representations for all the coefficients in our series solution and by using Eq.(A11) one finds that

$$a_{2n} = \frac{I_n(\kappa)}{I_0(\kappa)} \tag{A12}$$

thus the orientation distribution function is given by the exact form

$$\psi(\theta) = \frac{1}{2\pi} + \frac{1}{\pi I_0(\kappa)} \sum_{n=1}^{\infty} I_n(\kappa) \cos(2n\theta)$$
(A13)

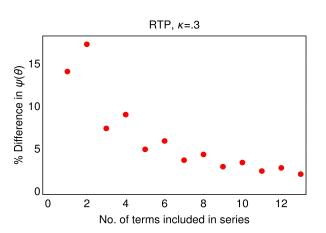
With the help of the following identity, an example of a Jacobi-Anger expansion

$$e^{z\cos(2\theta)} = I_0(z) + 2\sum_{n=1}^{\infty} I_n(z)\cos(2n\theta)$$

Eq.(A13) is able to be summed exactly to the form of Eq.(7). The same process holds for the polar aligning torque and repeating the calculation in that case yields Eq.(9)-(12)

## Appendix B: Truncation error and perturbation theory

As stated in the main text, the series solution for run and tumble particles is slowly converging and a low moment approximation is not valid in this case. One way



this magnitude for RTPs, one must truncate the series at

n = 300. For both classes, the number of terms needed

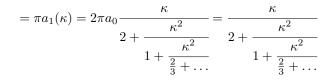
increases as  $\kappa$  gets larger as should be expected.

FIG. 4. (color online) For RTPs a large number of terms in the series must be included. Above shows the percent difference in the value of  $\psi(\theta)$  whether truncating at the nth term or  $n_{th} + 1$  term. Here we examine the value at  $\theta = 0$ . The first point on the horizontal axis represents the percent difference in  $\psi(\theta)$  by truncating the series at n = 2 and n = 3, the next point represents the percent difference when truncating the series at n = 3 and n = 4 this is continued up to the the last point which represents the percent difference by truncating the series at n = 14 and n = 15.

#### Appendix C: Relationship between Correlation and Response

As another measure of the difference between the two classes of active particles one can compute the correlation and response functions. We focus here on the subspace of orientation dynamics (i.e., we have integrated over space and are int the homogeneous limit). Let us begin by considering RTPs in the presence of a polar aligning torque. To compute the correlation and response functions we will need the average of  $\cos(\theta)$ , i.e., the polarization given by the first moment of the angular orientation distribution function.

$$\left\langle \cos(\theta) \right\rangle = \int d\theta \cos(\theta) [a_0 + \sum_{n=1}^{\infty} a_n(\kappa) \cos(n\theta)] \quad (C1)$$



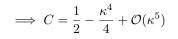
Where we used  $a_0 = 1/2\pi$ . The response function is giving by

$$R = \frac{\partial}{\partial \kappa} \left\langle \cos(\theta) \right\rangle = \frac{1}{2} - \frac{3}{4} \kappa^2 + \mathcal{O}(\kappa^3) \qquad (C2)$$

The response function measures how the order parameter changes in response to a changing field. The correlation function is given by

$$C = \left\langle \cos^2(\theta) \right\rangle - \left\langle \cos(\theta) \right\rangle^2 \tag{C3}$$

$$= \frac{1}{2} + \frac{1}{2}a_2(\kappa) - a_1(\kappa)^2; \quad a_2 = a_1 \frac{\kappa}{1 + \frac{\kappa^2}{\frac{2}{3} + \frac{\kappa^2}{\frac{2}{4} + \dots}}}$$



So up to quadratic order in  $\kappa$  we have

$$\frac{C}{R} = 1 + \frac{3}{2}\kappa^2 + \dots \tag{C4}$$

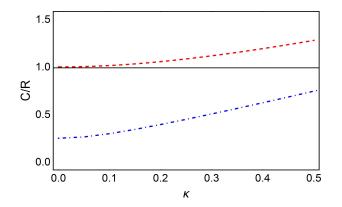


FIG. 5. (color online) The ratio of correlation to response for RTPs in the presence of a polar aligning torque (Red/Dashed) and a nematic aligning torque (Blue/Dot-Dashed) as a function of  $\kappa$ . The constant line at 1 represents the value of this ratio for ABPs

Similary, for a nematic aligning field the relevant quantity is

$$\left\langle \cos(2\theta) \right\rangle = \int d\theta \cos(2\theta) [a_0 + \sum_{n=1}^{\infty} a_{2n}(\kappa) \cos(2n\theta)]$$

$$= \pi a_2(\kappa) = 2\pi a_0 \frac{\kappa}{\frac{1}{2} + \frac{\kappa^2}{\frac{1}{4} + \frac{\kappa^2}{\frac{1}{6} + \dots}}} = \frac{\kappa}{\frac{1}{2} + \frac{\kappa^2}{\frac{1}{4} + \frac{\kappa^2}{\frac{1}{6} + \dots}}}$$
(C5)

Where we used  $a_0 = 1/2\pi$ . The response function is giving by

$$R = \frac{\partial}{\partial \kappa} \left\langle \cos(2\theta) \right\rangle = 2 - 48\kappa^2 + \mathcal{O}(\kappa^3) \tag{C6}$$

The correlation function is given by

$$C = \left\langle \cos^2(2\theta) \right\rangle - \left\langle \cos(2\theta) \right\rangle^2 \tag{C7}$$

$$= \frac{1}{2} + \frac{1}{2}a_4(\kappa) - a_2(\kappa)^2; \qquad a_4 = a_2 \frac{\kappa}{\frac{1}{4} + \frac{\kappa^2}{\frac{1}{6} + \frac{\kappa^2}{\frac{1}{8} + \dots}}}$$

$$\implies C = \frac{1}{2} - 64\kappa^4 + \mathcal{O}(\kappa^5)$$

So up to quadratic order in  $\kappa$  we have

$$\frac{C}{R} = \frac{1}{4} + 6\kappa^2 + \mathcal{O}(\kappa^2) \tag{C8}$$

The exact expression for both aligning torques is explored numerically and shown in Fig.5. Repeating this process for ABPs would yield C/R = 1 irrespective of the value of  $\kappa$ .

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