Electronic Supplementary Information for: Dynamics and polarization of superparamagnetic chiral nanomotors in a rotating magnetic field

Konstantin I. Morozov and Alexander M. Leshansky*

Department of Chemical Engineering and Russel Berrie Nanotechnology Institute (RBNI), Technion – Israel Institute of Technology, Haifa 32000, Israel

(Dated: September 2, 2014)

* lisha@tx.technion.ac.il

I. Rotation matrix

We use the definition of the three Euler angles φ, θ and ψ following Ref. [1]. The components of any vector $\mathbf{W}$ in the body-fixed coordinate system (BCS) and in the laboratory coordinate system (LCS) are determined from the relation $\mathbf{W}^{BCS} = \mathbf{R} \cdot \mathbf{W}$, where $\mathbf{R}$ is the rotation matrix. The rotation matrix is expressed explicitly via the Euler angles [2]

$$\mathbf{R} = \begin{pmatrix} c_\varphi c_\psi - s_\varphi s_\psi c_\theta & s_\varphi c_\psi + c_\varphi s_\psi c_\theta & s_\psi s_\theta \\ -c_\varphi s_\psi - s_\varphi c_\psi c_\theta & -s_\varphi s_\psi + c_\varphi c_\psi c_\theta & c_\psi s_\theta \\ s_\varphi s_\theta & -c_\varphi s_\theta & c_\theta \end{pmatrix} ,$$

where we use the compact notation, $s_\psi = \sin\psi$, $c_\theta = \cos\theta$, etc.

II. Approximate rotational viscous resistance coefficients of a helix

We approximate the rotational viscous resistance coefficients of a helical propeller by the corresponding values for a prolate spheroid approximating the helix. Let a and b be, correspondingly, the longitudinal (along the symmetry axis) and transversal semi-axes of the spheroid. The respective viscous resistances due to rotation about the symmetry axis and in perpendicular direction read [3]

$$\kappa_\parallel = 2\eta V n_\perp^{-1} , \quad \kappa_\perp = 2\eta V \frac{a^2 + b^2}{a^2 n_\parallel + b^2 n_\perp} , \tag{S1}$$

where η is the dynamic viscosity of the liquid, V is the spheroid volume, $n_\parallel$ and $n_\perp = (1 - n_\parallel)/2$ are the depolarizing factors of the spheroid. For the prolate spheroid with $a > b$ and eccentricity $e = \sqrt{1 - b^2/a^2}$ the depolarizing factor along the symmetry axis reads [4]

$$n_\parallel = \frac{1 - e^2}{e^3} \left(\frac{1}{2} \ln \frac{1 + e}{1 - e} - e \right) . \tag{S2}$$

III. Particle-based numerical algorithm

The numerical procedure used to compute the various components of the viscous resistance tensor is based on multipole expansion scheme [5]. The filament is constructed from nearly touching N rigid spheres (“shish-kebab” filament) having the same radius $r = 1$. The no-slip condition at the surface of all spheres is enforced rigorously via the use of direct transformation between solid spherical harmonics centered at origins of different spheres. The method yields a system of $\mathcal{O}(N\mathcal{L}^2)$ linear equations for the expansion coefficients and the accuracy of calculations is controlled by the number of spherical harmonics (i.e. truncation level), $\mathcal{L}$, retained in the series. This approach has been applied before for modeling low-Reynolds-number swimmers, e.g., rotating helix [6, 7] and undulating filament [8].

The spheres composing the helical filament are partitioned along the backbone of the filament $\mathbf{X}(s)$ (see Eq. (21) and Fig. S1) so that the distance between centers of neighboring spheres is set to $2.02r$. The motion of the ith sphere composing a helix can be decomposed into translation $\boldsymbol{U}_i$ and rotation $\boldsymbol{\omega}_i$ about its center, as $\boldsymbol{V}_i = \boldsymbol{U}_i + \boldsymbol{\omega}_i \times \boldsymbol{r}_i$ with $\boldsymbol{r}_i$ being the radius vector with origin at the center of ith sphere. For any prescribed rigid-body-motion of the helix, $\{\boldsymbol{U}_i, \boldsymbol{\omega}_i\}$ are determined uniquely. For instance, for computing the components of the resistance tensor, such as $\xi_\parallel, \kappa_\parallel$ and $\mathcal{B}_\parallel$, associated with translation U and rotation ω about the x_3-axis, one has $\boldsymbol{\omega}_i = \boldsymbol{e}_3\omega$ and $\boldsymbol{U}_i = U\boldsymbol{e}_3 + \omega\boldsymbol{e}_3 \times \boldsymbol{R}_i$, where $\boldsymbol{R}_i$ is a position vector to the ith sphere center.

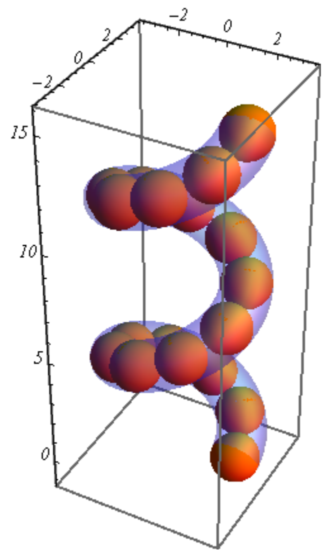

FIG. S1. Illustration of particle-based “shish-kebab” 2-turn helix approximating the regular helix with circular cross section of radius $r = 1$ (transparent blue) with helical radius $R = 2.5$ and pitch angle $\Theta = 65°$.

IV. Demagnetizing factors of infinitely long elliptic cylinder

The demagnetizing factor N of infinitely long cylinder with an elliptic cross-section with corresponding semi-axes $\hat{a}$ and $\hat{b}$ was reported in Ref. [9]:

$$N = (2\pi)^{-1}\left[4\arctan\frac{\hat{a}}{\hat{b}} + \frac{2\hat{b}}{\hat{a}}\ln\frac{\hat{b}}{\hat{a}} + \left(\frac{\hat{a}}{\hat{b}} - \frac{\hat{b}}{\hat{a}}\right)\ln\left(1+\frac{\hat{b}^2}{\hat{a}^2}\right)\right].$$

At $\hat{a} > \hat{b}$ it determines the demagnetization factor N_1 along the short axis. The demagnetizing factor N_2 can be found either by the permutation $\hat{a} \leftrightarrow \hat{b}$ or from the equality $N_1 + N_2 = 1$. For the regular helix with circular cross-section $N_1 = N_2 = 1/2$.

---

[1] Landau, L. D.; Lifshitz, E. M. *Mechanics*, 3rd ed.; Pergamon Press, Oxford, 1976.

[2] Diebel, J. *Representing Attitude: Euler Angles, Unit Quaternions, and Rotation Vectors*; Matrix, Citeseer, 2006.

[3] Jeffrey, G. B. The motion of ellipsoidal particles immersed in a viscous fluid. *Proc. R. Soc. London A* **1922**, *102*, 161–179.

[4] Landau, L. D.; Lifshitz, E. M. *Electrodynamics of Continuous Media*, 2nd ed.; Pergamon Press, Oxford, 1984.

[5] A. V. Filippov, *J. Colloid Interface Sci.*, 2000, **229**, 184–195.

[6] A. M. Leshansky, *Phys. Rev. E*, 2009, **80**, 051911.

[7] K. I. Morozov and A. M. Leshansky, *Nanoscale*, 2014, **6**, 1580–1588.

[8] R. S. Berman, O. Kenneth, J. Sznitman and A. M. Leshansky, *New J. Phys.*, 2013, **15**, 075022.

[9] Brown Jr., W. F. *Magnetostatic Principles in Ferromagnetism*; North-Holland, Amsterdam, 1962.