Supporting Information : Analytical theory and stability analysis of an elongated nanoscale object under external torque

PACS numbers:

I. S1: ESTIMATION OF THE FRICTION COEFFICIENTS AND CRITICAL FREQUENCIES IN THE EXPERIMENTAL SYSTEM

The experimental system is a helical nanostructure, which is shown in Fig. 1 below. The structure is modelled as an ellipsoid with semi major and semi minor axes given by $a = 2.25\,\mu m$ and $b = 0.45\,\mu m$ respectively. The rotational friction coefficients [1] about the short and long axes are given by $\gamma_s = \frac{32\pi\eta}{3}\frac{a^4-b^4}{S(2a^2-b^2)-2a}$; and $\gamma_l = \frac{32\pi}{3}\eta\frac{(a^2-b^2)b^2}{2a-b^2S}$ respectively, where $S = \frac{2}{\sqrt{a^2-b^2}}\ln\left(\frac{a+\sqrt{a^2-b^2}}{b}\right)$, η being the dynamic viscosity of the medium.

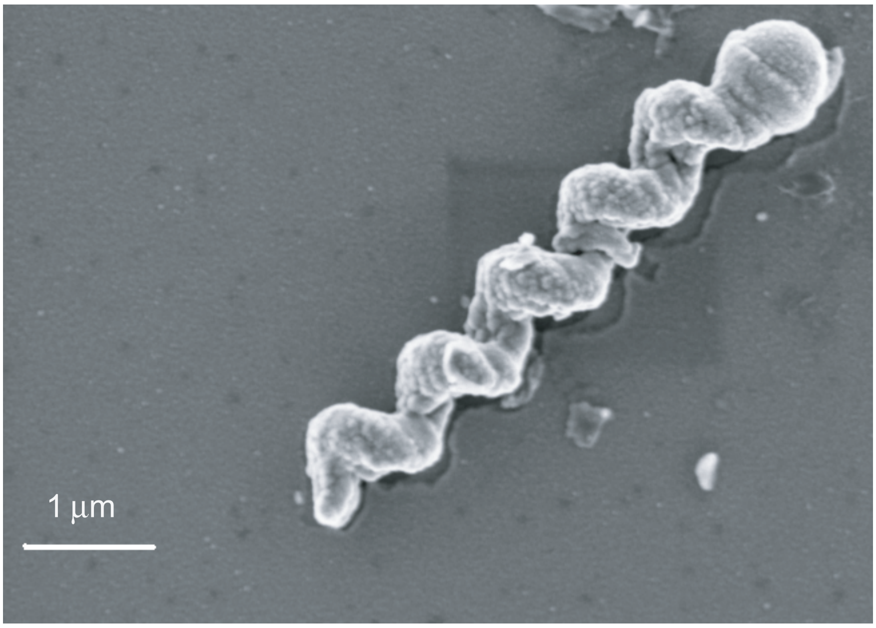

FIG. 1: SEM image of the helical nanostructure used in experiments.

If the medium is assumed to be water at room temperature, $\eta = 8.9 \times 10^{-4} Pa.s$ and hence we have $\gamma_s = 4.73 \times 10^{-20} kg.m^2/s$ and $\gamma_l = 7.2 \times 10^{-21} kg.m^2/s$.

With these values of friction coefficients and $\theta_m = 18°$ (as one example from experimental measurements), the ratio $\frac{\Omega_2}{\Omega_1}$ is given by $\sqrt{1 + \frac{\gamma_s^2}{\gamma_l^2} cot^2(\theta_m)} = 20.25$ (see main text for formulae for Ω_1 and Ω_2). Experimentally obtained ratio is $\frac{\Omega_2^{expt}}{\Omega_1^{expt}} \approx \frac{130}{6} = 21.67$.

II. S2: DETAILS FOR NUMERICAL SIMULATION

In the numerical simulation the same convention has been used as is shown in the main text, while deriving the Euler equations. However quaternions q_0, q_1, q_2, q_3 (which are functions of the

Euler angles ϕ, θ, ψ) have been used to represent the orientation of the rod at any time instant in the numerical calculations. The magnetic moment $\vec{m}$ and the instantaneous magnetic field $\vec{B}$, which rotates at a frequency Ω_B, are expressed as above in the body fixed frame of the rod. The rotation friction coefficient tensor in the body frame is given by

$$\gamma = \begin{bmatrix} \gamma_s & 0 & 0 \\ 0 & \gamma_s & 0 \\ 0 & 0 & \gamma_l \end{bmatrix} \quad (1)$$

Here the object is approximated as a rod or an ellipsoid with appropriate values of γ_s and γ_l as shown in the main text or in section S1. As the Reynolds number under consideration is $\sim 10^{-5}$, the inertial terms can be neglected from the equation of motion. Hence equating the magnetic torque to the viscous torque experienced by the rod we get

$$\vec{m} \times \vec{B} = \gamma\vec{\omega} \Rightarrow \vec{\omega} = \gamma^{-1}(\vec{m} \times \vec{B}) \quad (2)$$

Instantaneous value of $\vec{\omega}$ gives the values of the rate of change of quaternions and hence the Euler angles. Then the instantaneous values of the Euler angles which gives the orientation of the rod is obtained as

$$\phi(t + \Delta t) = \phi(t) + \dot{\phi(t)}\Delta t \quad (3)$$

and similarly for θ and ψ.

It it may be noted that to avoid the common problem of numerical drift in the simulation, we used a renormalization technique,

$$q_i(t + \Delta t) = \frac{q_i(t + \Delta t)}{\sqrt{\sum_i q_i(t + \Delta t)^2}}, \quad (4)$$

where q_i s are the quaternions and Δt is the time interval used in simulations.

Here Δt is a very small time step $\sim 10^{-5}\ s$, which is much smaller than the shortest time scale relevant to the dynamics considered here ($\frac{1}{\Omega_2} \approx 8 \times 10^{-3}\ s$).

III. S3: PRELIMINARY RESULTS FOR SIMULATION WITH NOISE

Fig 4 shows the preliminary results for probability of stable tumbling, where thermal noise is introduced in the numerical simulation.

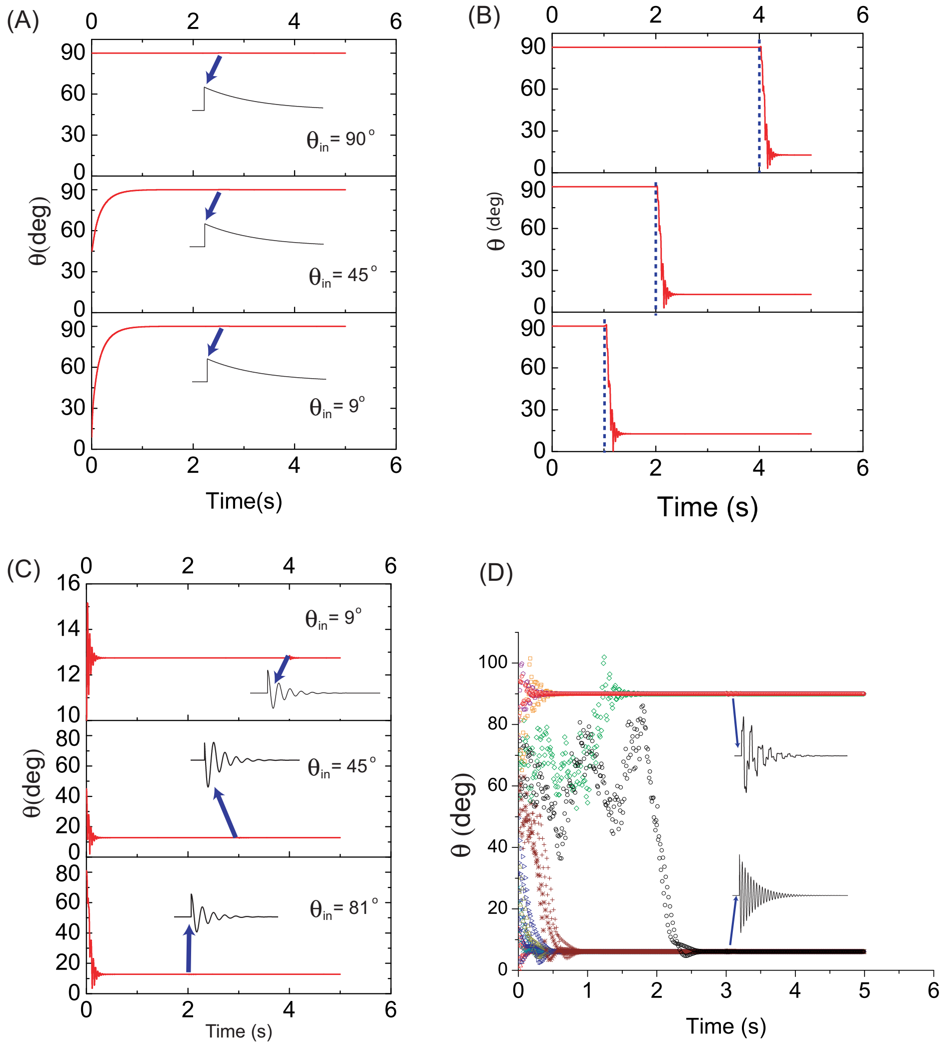

FIG. 2: (color online) (A) Time evolution of the precession angle θ, at a frequency below Ω_1, for different initial conditions θ_{in}, when a perturbation is given at time t = 2.5 s. (B) Time evolution of θ, at a frequency between Ω_1 and Ω_2, for $\theta_{in} = 90°$. Perturbations are given at t = 4 s, 2 s, 1 s. (C) Time evolution of θ, at a frequency between Ω_1 and Ω_2, for different $\theta_{in} \neq 90°$. Perturbations are given at t = 4 s, 3 s, 2 s. (D) Time evolution of θ, at a frequency close to and less than Ω_2, for 15 different θ_{in} values, showing bistable behavior. (Insets show the transients when the perturbation is given to the system. Blue arrows and lines show the time at which the system is perturbed

[1] X. Sun, T. Lin, J. D. Gezelter, *The Journal of Chemical Physics*, 2008, **128**, 234107.

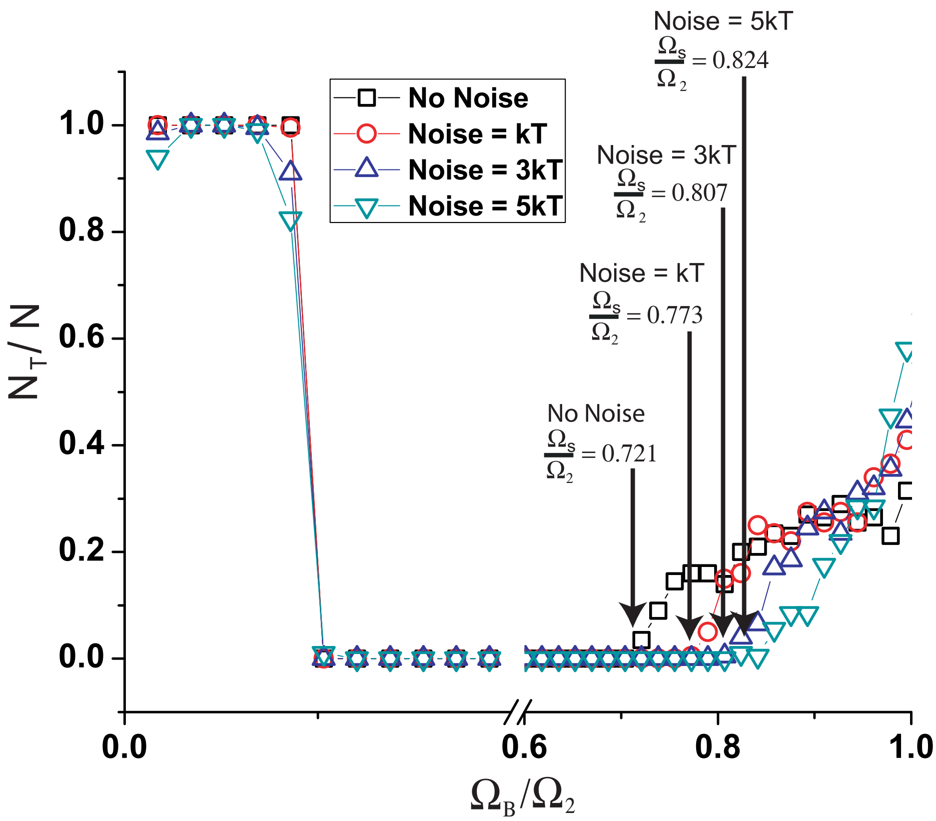

FIG. 3: (color online) Numerical data showing the probability of occurrence of a stable tumbling state for $\theta_m = 40°$ for different values of noise levels as the magnetic field frequency is varied. As the thermal noise is increased in the system, simulation shows that Ω_s also increases. (Here k is Boltzmann's constant and T is assumed to be $300\ K$)