Variational Convergence of Liquid Crystal Energies to Line and Surface Energies

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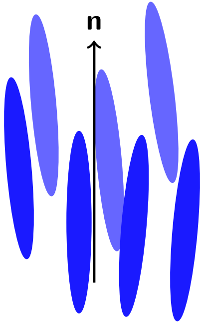
Nematic Liquid Crystals

- State of matter: between liquid and crystalline
- Rod-like molecules: director field $\mathbf{n}$
- Nematic: orientational, but no positional order
- Defects: lines and points



Saturn Ring Effect

- A particle of size r_0 immersed into a nematic liquid crystal
- Homogeneous external magnetic field $\mathbf{H} = h\mathbf{e}_3$

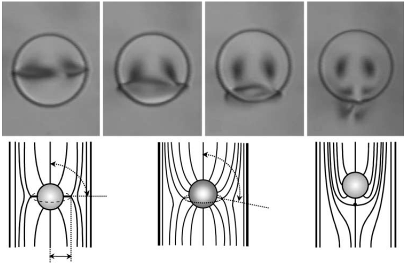


Figure: From: J. Loudet, O. Mondain-Monval and P. Poulin. Line defect dynamics around a colloidal particle. Eur. Phys. J. E 7.3 (2002), pp. 205–208.

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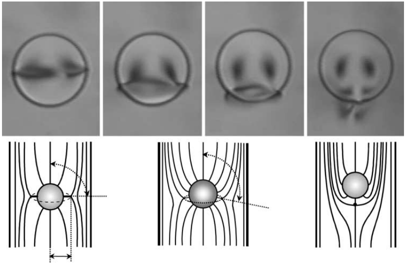

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- Transition between singularities of Saturn ring or dipole type depending on h and r_0

Landau-de Gennes Model

1. Replace director field $\mathbf{n} : \Omega \to \mathbb{R}P^2$ by Q-tensors

$$Q : \Omega \to \mathrm{Sym}_0 = \{A \in \mathbb{R}^{3\times 3} \; : \; A^T = A\,,\; \mathrm{tr}(A) = 0\}\,,$$

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$$Q : \Omega \to \mathrm{Sym}_0 = \{A \in \mathbb{R}^{3\times 3} \;:\; A^T = A\,,\; \mathrm{tr}(A) = 0\}\,,$$
2. and minimize the dimensionless Landau-de Gennes energy
$$\mathcal{E}_{\eta,\xi}(Q) = \int_\Omega \underbrace{\frac{1}{2}|\nabla Q|^2}_{\text{elastic}} + \underbrace{\frac{1}{\xi^2} f(Q)}_{\text{ordering}} + \underbrace{\frac{1}{\eta^2} g(Q)}_{\text{magnetic}}\;\mathrm{d}x$$
on $\Omega = \mathbb{R}^3 \setminus E$,

$$\left.\begin{array}{r} |\nabla Q|^2 \rightsquigarrow Q \text{ constant} \\ f(Q) \rightsquigarrow Q \text{ uniaxial} \\ g(Q) \rightsquigarrow Q \text{ "parallel" } \mathbf{H} \end{array}\right\} Q \equiv Q_\infty = s_* \left(\mathbf{e}_3 \otimes \mathbf{e}_3 - \frac{1}{3}\mathrm{Id}\right)$$

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   on $\Omega = \mathbb{R}^3 \setminus E$,

3. subject to the boundary conditions

$$Q_b = s_* \left(\frac{\mathbf{x}}{|\mathbf{x}|} \otimes \frac{\mathbf{x}}{|\mathbf{x}|} - \frac{1}{3}\mathrm{Id} \right) \qquad \text{on } \mathbb{S}^2 .$$

$\Longrightarrow$ frustrated system, transition layer between Q_b and Q_∞

Main Result (I)

- Suppose $\eta|\ln(\xi)| \to \beta \in (0, \infty)$ as $\eta, \xi \to 0$.
- Assume rotational equivariance of Q w.r.t. the $\mathbf{e}_3$−axis

Main Result (I)

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- Assume rotational equivariance of Q w.r.t. the $\mathbf{e}_3$−axis

Theorem (Alouges, Chambolle, S. (ARMA 2021))

The energy $\eta\,\mathcal{E}_{\eta,\xi}$ converges to $\mathcal{E}_0$ in a variational sense, where the limiting energy $\mathcal{E}_0$ for a set $F \subset \mathbb{S}^2$ is given by

$$\mathcal{E}_0(F) = 2s_*c_* \int_F (1-\cos(\theta))\,\mathrm{d}\omega + 2s_*c_* \int_{F^c} (1+\cos(\theta))\,\mathrm{d}\omega + \frac{\pi}{2}s_*^2\beta|D\chi_F|(\mathbb{S}^2)\,,$$

where s_* depends on f, c_* depends on g and θ is the angle between the outward normal vector ν on $\mathbb{S}^2$ and $\mathbf{e}_3$.

Main Result (II)

More precisely, $\eta\,\mathcal{E}_{\eta,\xi} \to \mathcal{E}_0$ means that

- *Compactness:* $\forall\ Q_{\eta,\xi}$ with $\eta\,\mathcal{E}_{\eta,\xi}(Q_{\eta,\xi}) \leq C \quad \exists\ \mathbf{n}_{\eta,\xi} : \Omega \to \mathbb{S}^2$ and $F \subset \mathbb{S}^2$ of finite perimeter such that

$$\begin{cases} Q_{\eta,\xi} - s_*(\mathbf{n}_{\eta,\xi} \otimes \mathbf{n}_{\eta,\xi} - \frac{1}{3}\mathrm{Id}) \to 0 & \text{in } L^2_{\mathrm{loc}}\,, \\ \{\nu(\omega) \cdot \mathbf{n}_{\eta,\xi} = 1\} \to F & \text{in } \mathrm{BV}\,. \end{cases}$$

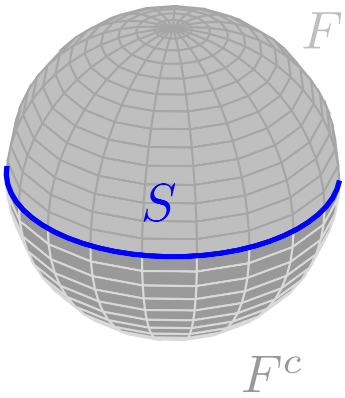
- $\Gamma-$*liminf:* $\forall\ Q_{\eta,\xi} \quad \exists\ F \subset \mathbb{S}^2$ with

$$\liminf_{\eta,\xi\to 0} \eta\,\mathcal{E}_{\eta,\xi}(Q_{\eta,\xi}) \geq \mathcal{E}_0(F)\,.$$

- $\Gamma-$*limsup:* $\forall\ F \subset \mathbb{S}^2 \quad \exists\ Q_{\eta,\xi}$ such that

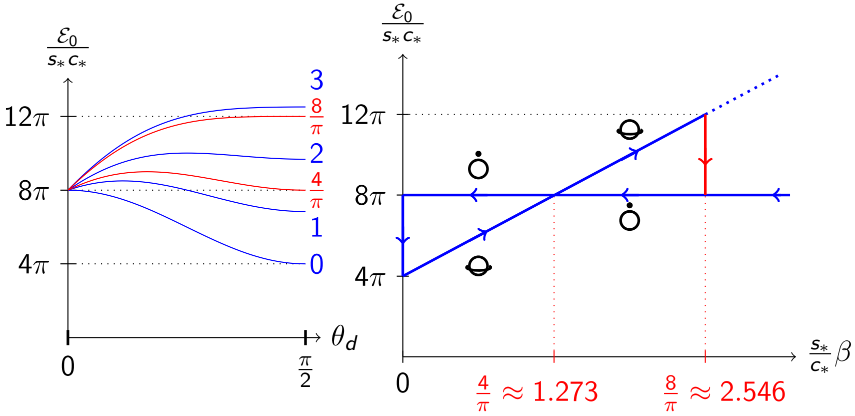
$$\limsup_{\eta,\xi\to 0} \eta\,\mathcal{E}_{\eta,\xi}(Q_{\eta,\xi}) \leq \mathcal{E}_0(F)\,.$$

Main Result (III)



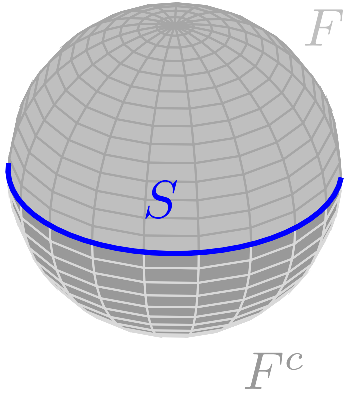
Limit Energy and Hysteresis

- Minimizer of $\mathcal{E}_0$: circle on $\mathbb{S}^2$ at angle θ_d depending on $\frac{s_*}{c_*}\beta$
- Derived numerically by H. Stark



Ongoing Work

- Remove hypothesis of rotational equivariance
- Consider non-spherical and non-convex particles



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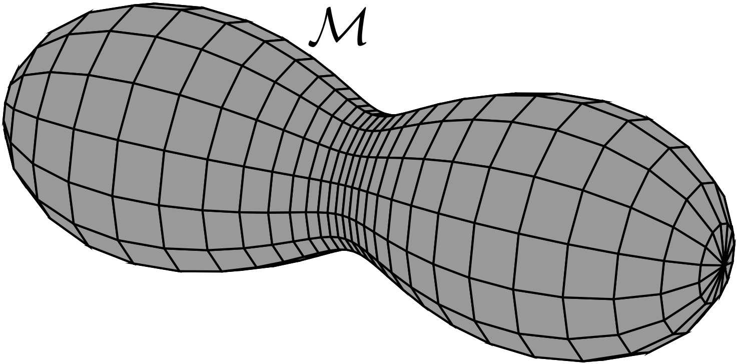

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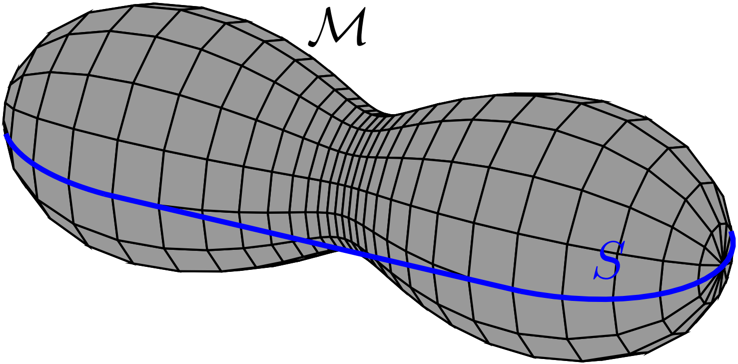

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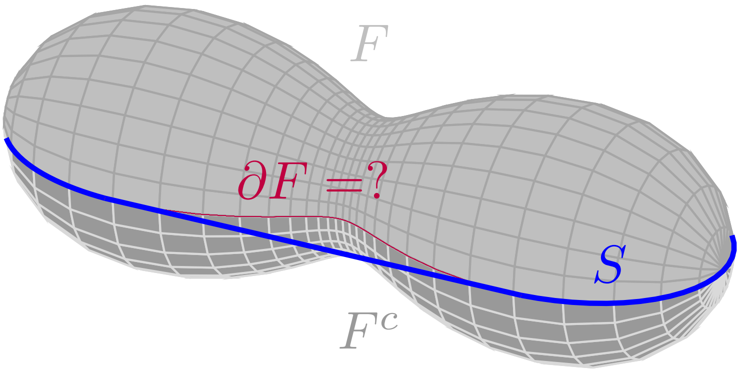

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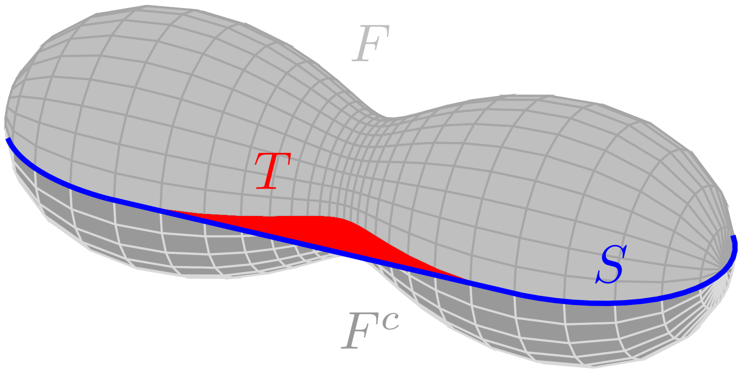

Ongoing Work

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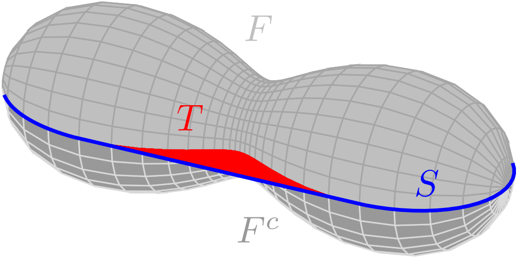
$$\mathcal{E}_0(F, T, S) = 2s_* c_* \int_F (1 - \cos(\theta))\, \mathrm{d}\omega + 2s_* c_* \int_{F^c} (1 + \cos(\theta))\, \mathrm{d}\omega$$
$$+ \frac{\pi}{2} s_*^2 \beta \mathcal{H}^1(S) + 4s_* c_* \mathcal{H}^2(T \llcorner \Omega)\,,$$

where $(\partial T) \llcorner \Omega = S \llcorner \Omega$.



Idea of Proof: Lower Bound and Compactness (I)

Write $Q \in \mathrm{Sym}_0$ as

$$Q = s\left(\left(\mathbf{n}\otimes\mathbf{n} - \frac{1}{3}\mathrm{Id}\right) + r\left(\mathbf{m}\otimes\mathbf{m} - \frac{1}{3}\mathrm{Id}\right)\right) .$$

with $s \geq 0$, $r \in [0,1]$ and $\mathbf{n} \perp \mathbf{m} \in \mathbb{S}^2$.

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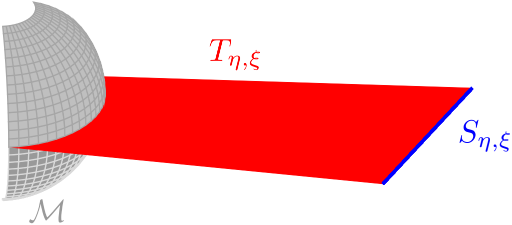
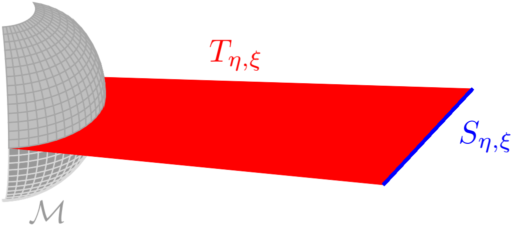
with $s \geq 0$, $r \in [0,1]$ and $\mathbf{n} \perp \mathbf{m} \in \mathbb{S}^2$. Choose

$$S_{\eta,\xi} \approx \underbrace{Q_{\eta,\xi}^{-1}(\{r=1\} \cup \{Q=0\})}_{\text{codim=2} \rightsquigarrow \text{line}}, \qquad T_{\eta,\xi} \approx \underbrace{Q_{\eta,\xi}^{-1}(\{\mathbf{n}_3=0\})}_{\text{codim=1} \rightsquigarrow \text{surface}}.$$



Idea of Proof: Lower Bound and Compactness (II)

Goal: Control size of $S_{\eta,\xi}$ and $T_{\eta,\xi}$ uniformly in ξ, η.



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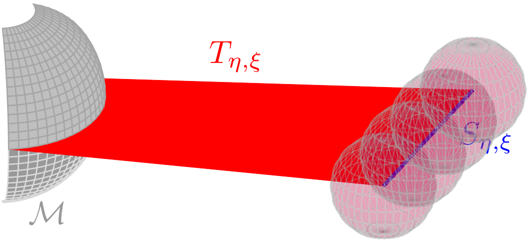

- In most of Ω, r is small:

$$\{r > \delta\} \cup \{Q = 0\} \subset \bigcup_{x \in X_{\xi,\eta}} B_\xi(x) \quad \text{and} \quad \# X_{\xi,\eta} \leq \frac{C_\delta}{\eta}.$$

Idea as in Bethuel (1999)

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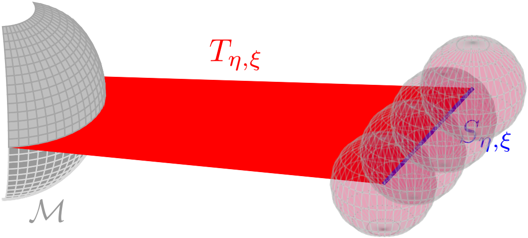

- Cost of the singularity $S_{\eta,\xi}$ around x_0:

$$\int_{B_\eta(x_0)} |\nabla Q_{\eta,\xi}|^2 + \frac{1}{\xi^2} f(Q_{\eta,\xi})\, \mathrm{d}x \geq \frac{\pi}{2} s_*^2 |\ln \xi| \eta - C\eta \,.$$

Generalisation of Sandier (1998) and Canevari (2015)

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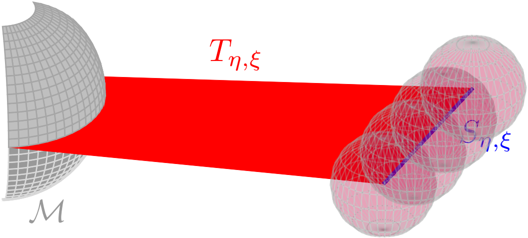
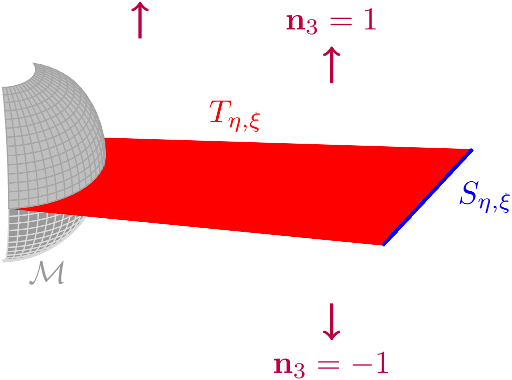


Conclude that

$$\eta\mathcal{E}_{\eta,\xi}(Q_{\eta,\xi}) \geq C \underbrace{\eta|\ln\xi|}_{\to\beta} \underbrace{\eta\#X_{\xi,\eta}}_{\gtrsim\mathcal{H}^1(S)} - C\eta\,.$$

Idea of Proof: Lower Bound and Compactness (III)



- Far from $\mathcal{M}$ and $T_{\eta,\xi}$, $\mathbf{n}_3 \approx \pm 1$.

Idea of Proof: Lower Bound and Compactness (III)

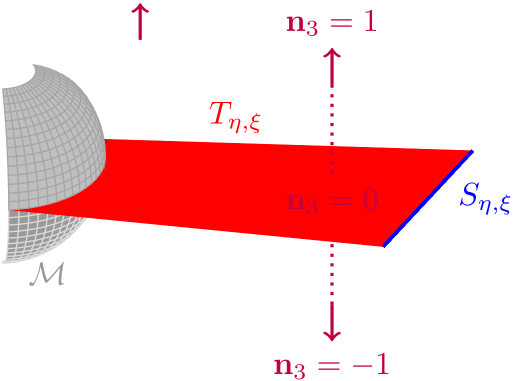
- Minimize $\int \frac{1}{2}|\partial_r Q|^2 + g(Q)\,\mathrm{d}r$ for $r = 0$ or equivalently

$$I(r_1, r_2, a, b) := \inf_{\substack{n_3 \in H^1([r_1,r_2],[0,1]) \\ n_3(r_1)=a,\ n_3(r_2)=b}} \int_{r_1}^{r_2} \frac{s_*^2|n_3'|^2}{1-n_3^2} + c_*^2(1-n_3^2)\,\mathrm{d}r$$

- Alama,Bronsard,Lamy:

$$I(0,\infty,\cos(\theta),\pm 1) = 2s_* c_*(1 \mp \cos(\theta))$$

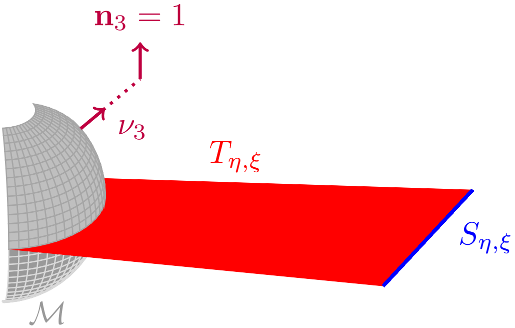
Idea of Proof: Lower Bound and Compactness (III)



- On $T_{\eta,\xi}$ far from the boundary $\mathcal{M}$ we find:

$$\eta \mathcal{E}_{\eta,\xi}(Q_{\eta,\xi}) \geq I(-\sqrt{\eta}, \sqrt{\eta}, -1, 1)\mathcal{H}^2(T_{\eta,\xi}) - C\eta\,.$$

Idea of Proof: Lower Bound and Compactness (III)



- On the surface $\mathcal{M}$

$$\eta \mathcal{E}_{\eta,\xi}(Q_{\eta,\xi}) \geq \int_{\mathcal{M}} I(0, \sqrt{\eta}, \cos(\theta), \pm 1) - C\eta \,.$$

Future Directions

- Study the limit energy: Shape Optimisation

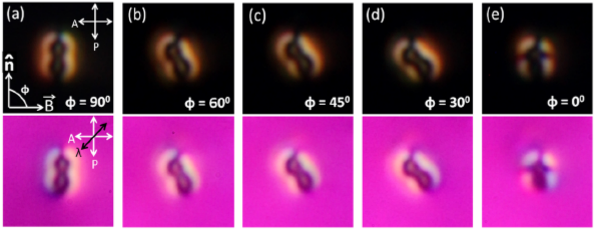


Figure: From: Sahu, D.K., Anjali, T.G., Basavaraj, M.G. et al. Orientation, elastic interaction and magnetic response of asymmetric colloids in a nematic liquid crystal. Sci Rep 9, 81 (2019).

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- Study the limit energy: Shape Optimisation
- Consider more particles: Knots and Links

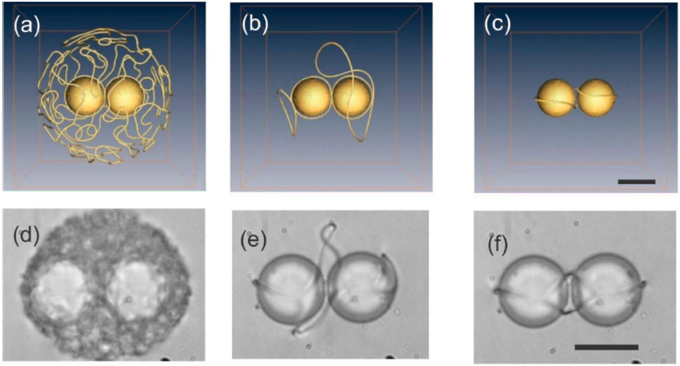

Figure: From: Muševič I. Nematic Liquid-Crystal Colloids. Materials (Basel). 2017;11(1):24. Published 2017 Dec 25.

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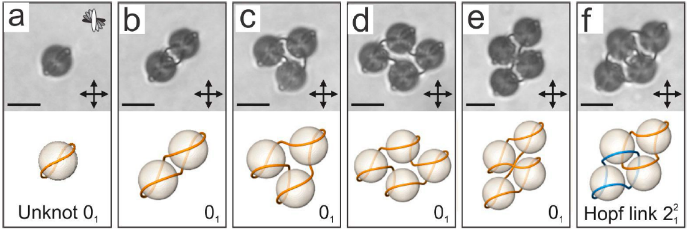

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End

Thank you for your attention!