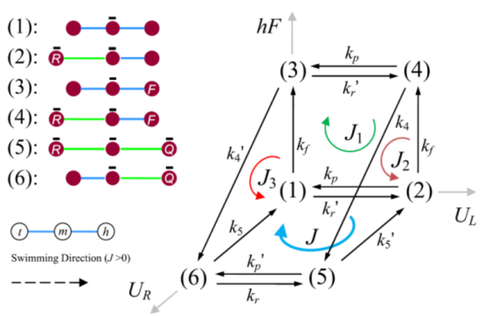
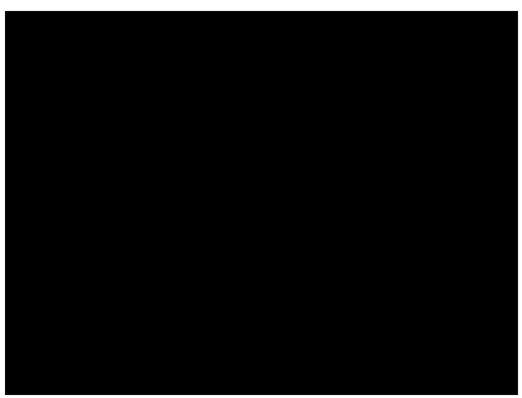
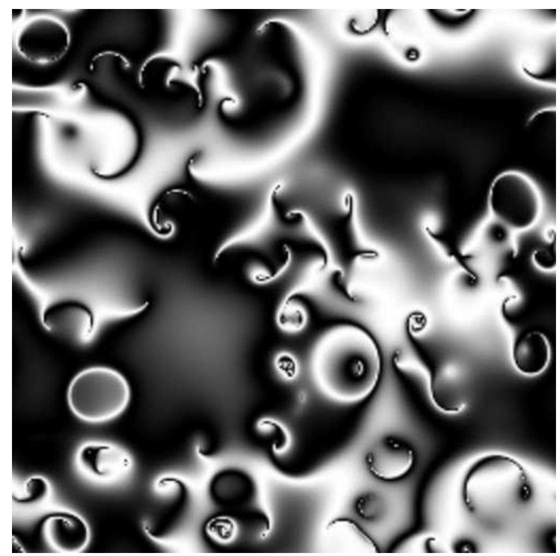
Microswimmers, nanoswimmers, and microfluidic mixers: The roles of hydrodynamic interactions and fluctuations

Ramin Golestanian
Rudolf Peierls Centre for Theoretical Physics







Inspired by Molecular Motors …

Which Are:

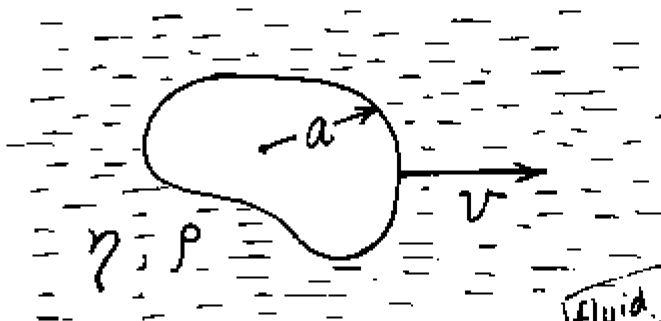
- Nano-scale machines
- Highly accurate despite Brownian agitation
- Capable of converting *chemical* energy directly to *mechanical* work

We Ask:

Can we design such machines?

In particular, Swimmers?

Hydrodynamics at Low Reynolds Number



Purcell (1976)

fluid density

Reynolds Number= $\dfrac{\text{inertial forces}}{\text{viscous forces}} \approx \dfrac{a v \rho}{\eta}$

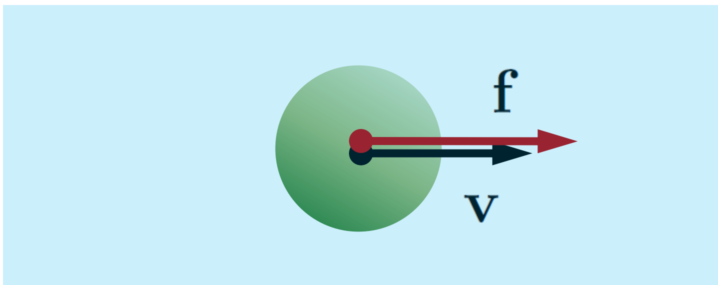
fluid viscosity

Low Reynolds: small size and/or high viscosity

Low Re Hydrodynamics is Dominated by Viscous Forces

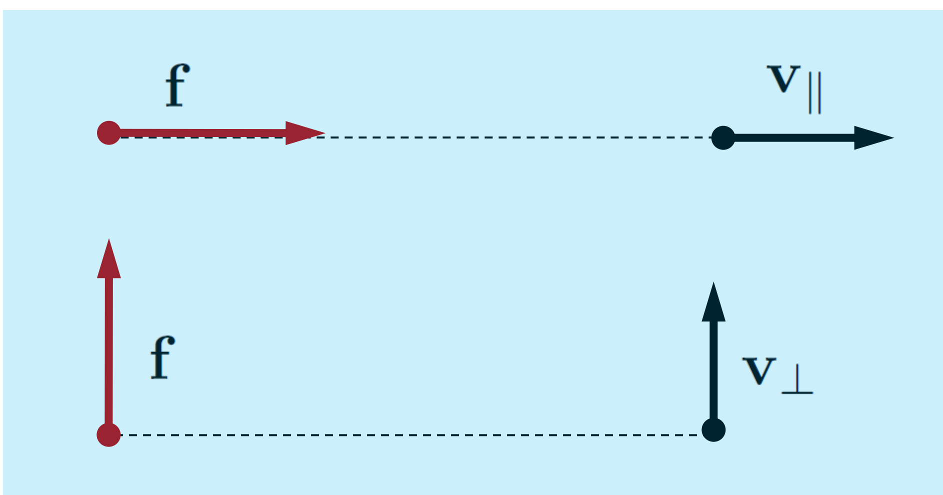
Viscous Hydrodynamics

Hydrodynamic Friction: Stokes (1851)



$$\mathbf{v} = \frac{1}{6\pi\eta a}\,\mathbf{f}$$

Hydrodynamic Interaction: Oseen (1927)



$$\mathbf{v}_{\|} = \frac{1}{4\pi\eta r}\,\mathbf{f}$$

$$\mathbf{v}_{\perp} = \frac{1}{8\pi\eta r}\,\mathbf{f}$$

Stokes Equation

$$-\eta\partial^2 v_i = -\partial_i p + g_i$$

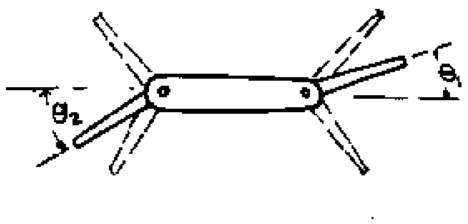
$$\partial_j v_j = 0 \qquad\qquad p = \left(\tfrac{1}{\partial^2}\right)\partial_j g_j$$

$$-\eta\partial^2 v_i = \left(\delta_{ij} - \frac{\partial_i\partial_j}{\partial^2}\right) g_j$$

$$v_i(\mathbf{r}) = \frac{1}{8\pi\eta r}\left(\delta_{ij} + \frac{r_i r_j}{r^2}\right) F_j$$

Minimal Low Re Swimmers

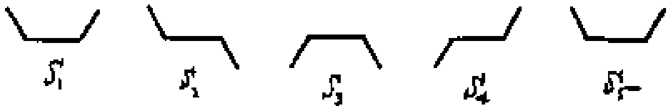
- Purcell Swimmer (1976)



  - **One**, is not enough:

    Scallop Theorem

  - **Two**, will just do!



- Three-Sphere Swimmer

  Two Translational Degrees of Freedom

A. Najafi & RG, PRE **69**, 062901 (2004)

Analysis of the Motion

$$v_1 = \frac{f_1}{6\pi\eta a_1} + \frac{f_2}{4\pi\eta L_1} + \frac{f_3}{4\pi\eta(L_1 + L_2)}$$

$$V = \frac{1}{3}(v_1 + v_2 + v_3)$$

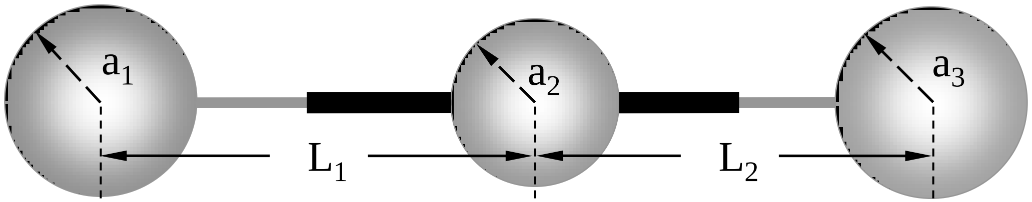
$$v_2 = \frac{f_1}{4\pi\eta L_1} + \frac{f_2}{6\pi\eta a_2} + \frac{f_3}{4\pi\eta L_2}$$

$$\dot{L}_1 = v_2 - v_1$$

$$v_3 = \frac{f_1}{4\pi\eta(L_1 + L_2)} + \frac{f_2}{4\pi\eta L_2} + \frac{f_3}{6\pi\eta a_3}$$

$$\dot{L}_2 = v_3 - v_2$$

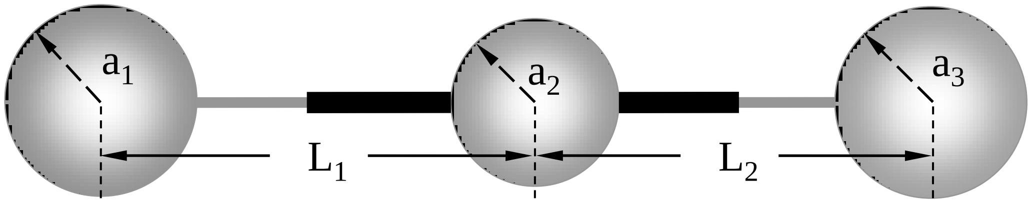
$$f_1 + f_2 + f_3 = 0$$



Swimming Velocity

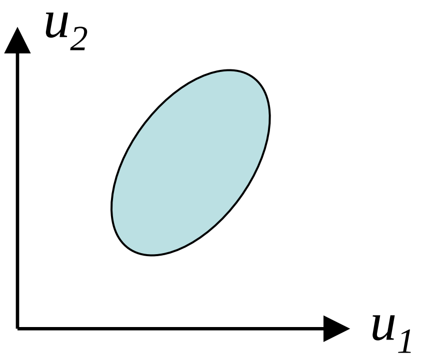
- Perturbative Analysis

$$L_1 = \ell + u_1$$
$$L_2 = \ell + u_2$$



$$\overline{V} = \frac{7}{24}\frac{a}{\ell^2}\overline{(u_1\dot{u}_2 - \dot{u}_1 u_2)}$$

- Geometric Interpretation



RG & A. Ajdari, PRE **77**, 036308 (2008)

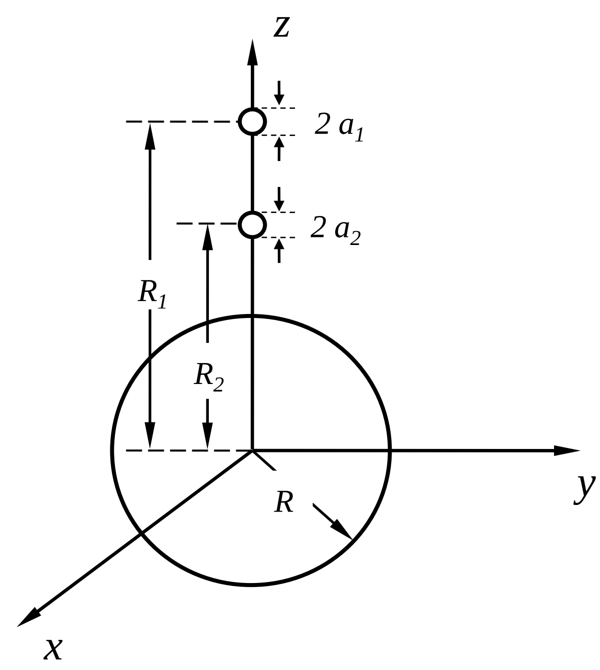
Swimmer with Cargo

- Swimming Velocity

$$\overline{V} = \frac{9}{4}\left(\frac{a_1 a_2}{R^3}\right)\frac{\ell_2^2\,(3\ell_1 + 2\ell_2)}{\ell_1^2\,(\ell_1 + 2\ell_2)}\,\overline{(\dot{u}_1 u_2 - \dot{u}_2 u_1)}$$

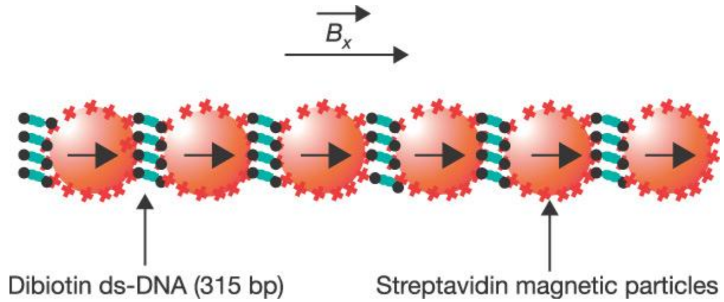
- Size Dependence

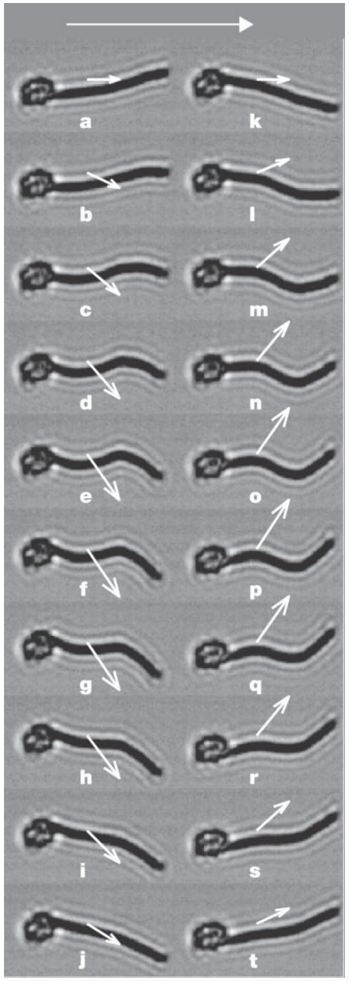
balancing "internal force"
with "Stokes Friction"
is WRONG



RG, EPJE **25,** 1 (2008)

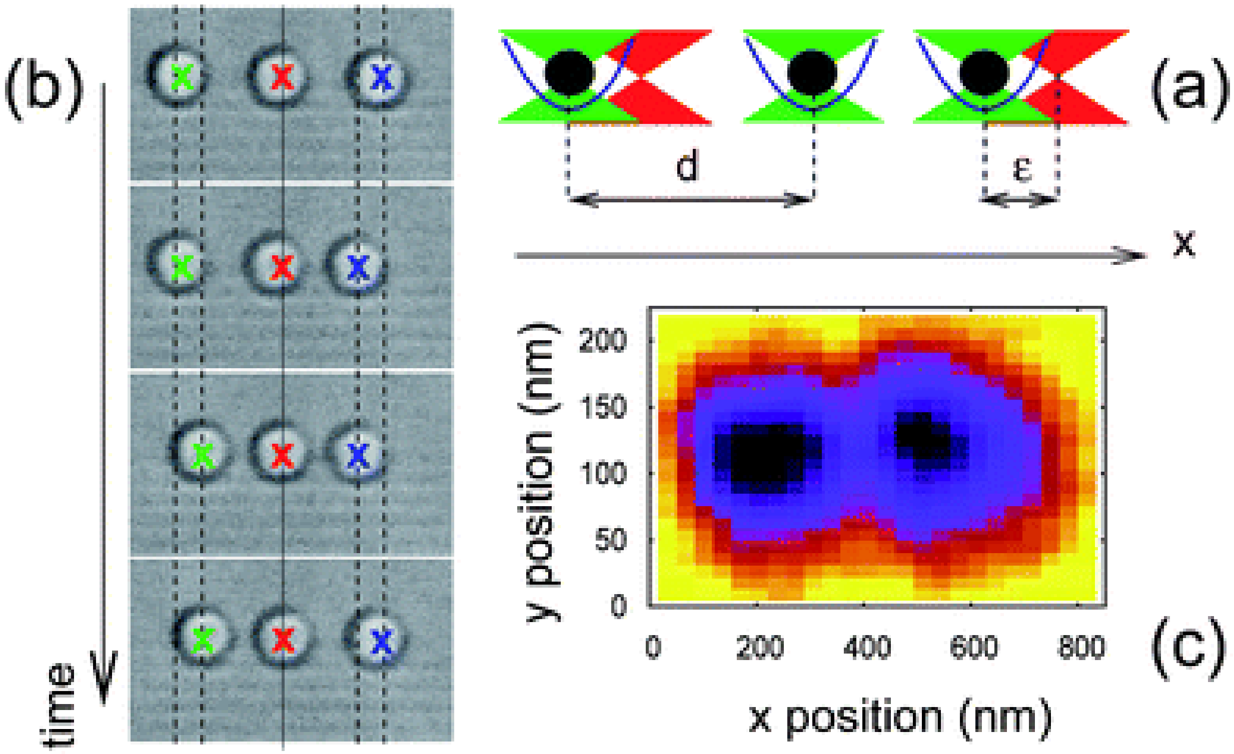
Paris Swimmer





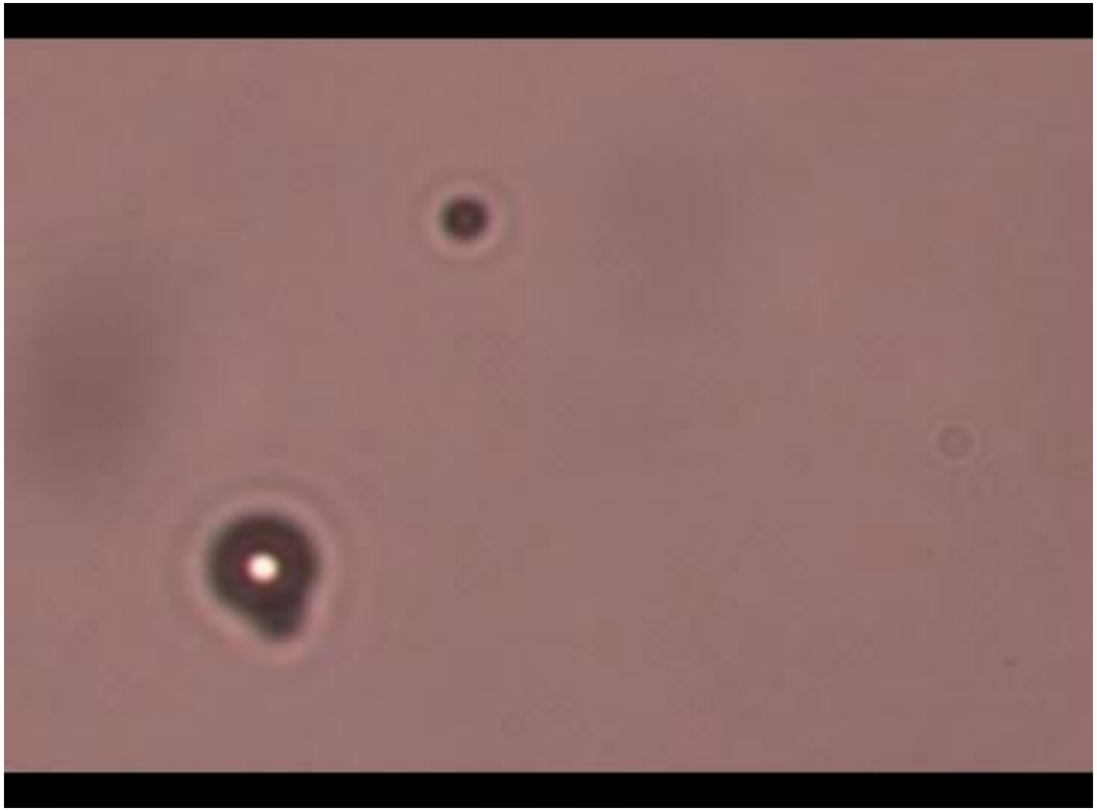
R. Dreyfus, J. Baudry, M.L. Roper, M. Fermigier, H.A. Stone & J. Bibette, Nature **437**, 862 (2005)

Cambridge “Swimmer”

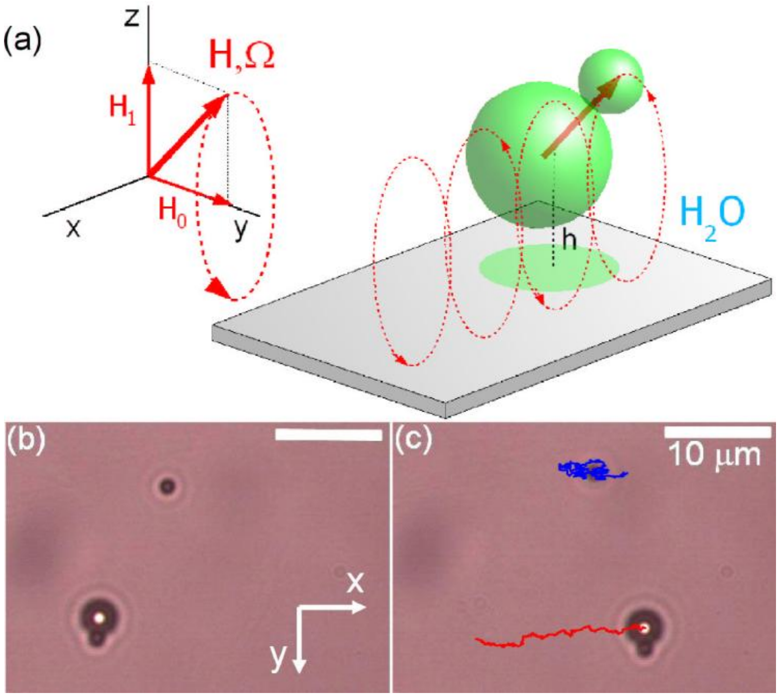


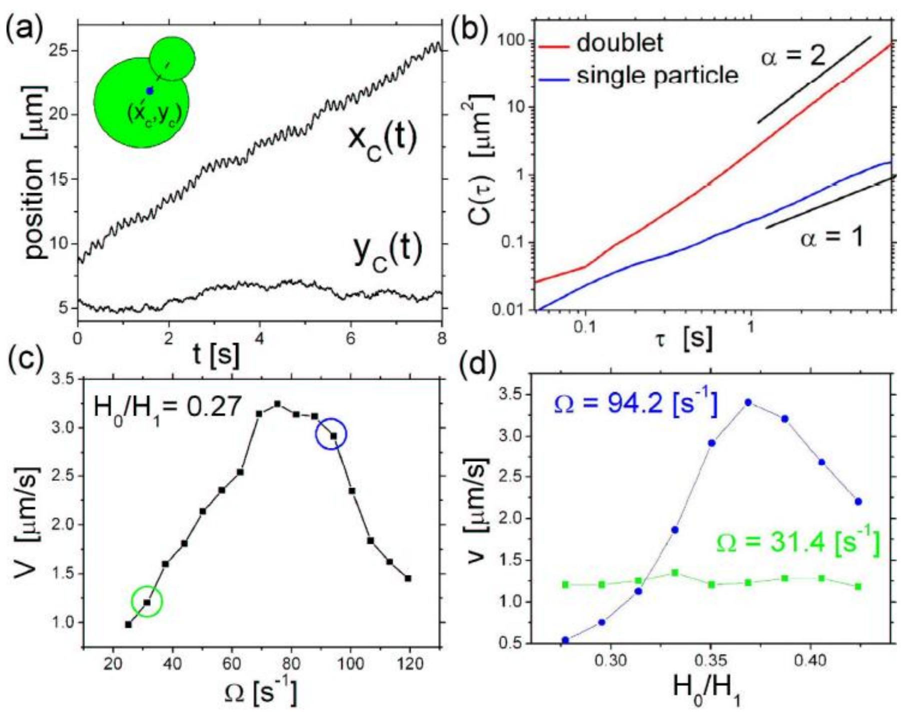
M. Leoni, J. Kotar, B. Bassetti, P. Cicuta, and M. C. Lagomarsino, Soft Matter **5**, 472 (2009)

Barcelona Swimmer



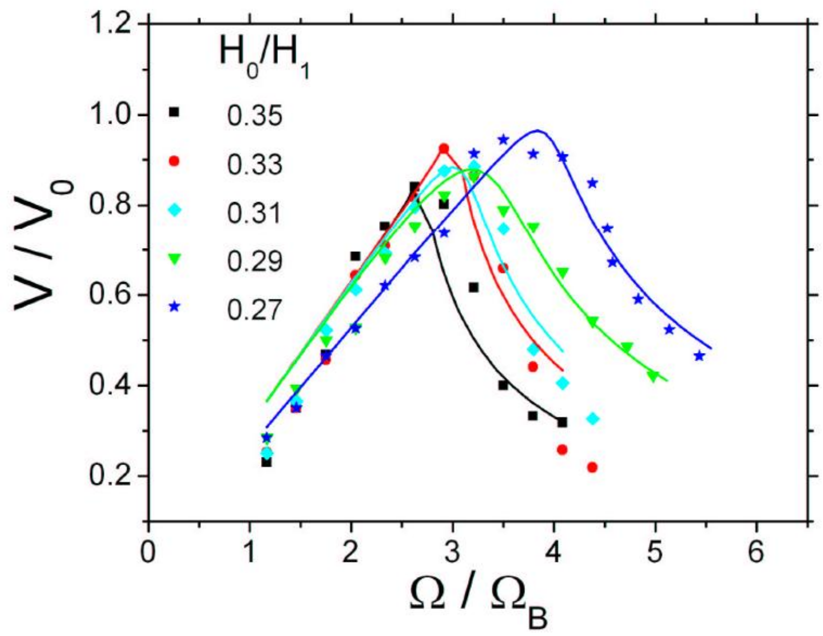
Motion of the *Unicycle*





P. Tierno, RG, I. Pagonabarraga, & F. Sagues, PRL **101**, 218304 (2008)

Swimming Velocity of the Unicycle



$$\gamma \equiv b/a$$

$$\Lambda_\pm \equiv a(1+\gamma)/[h(1+\gamma^{\pm 3})]$$

$$\Omega_B \equiv \mu_0 m H_0/\zeta_r$$

$$V_0 = \frac{9}{16}\frac{a\gamma(\gamma^2-\gamma+1)}{1+\gamma}\Omega_B$$

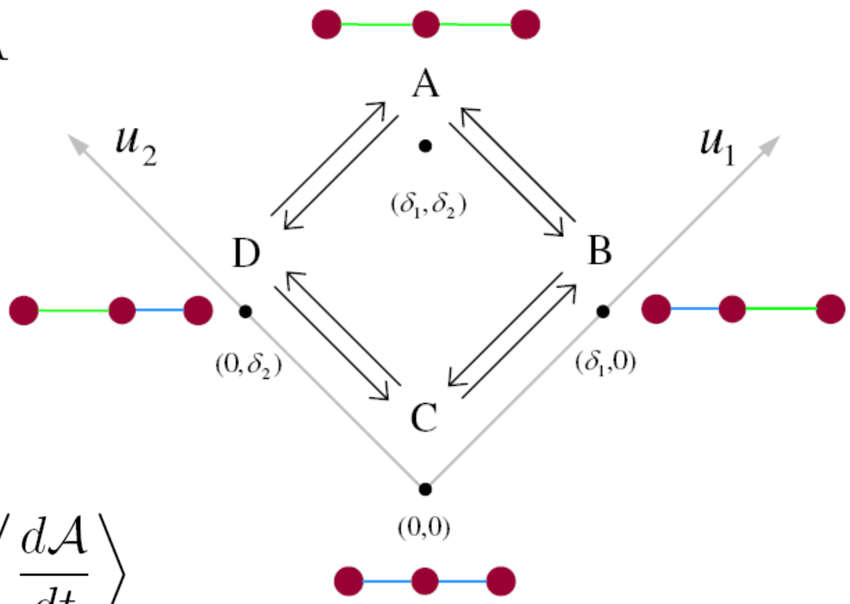
$$\frac{\langle V_x\rangle}{V_0} = \frac{\Omega}{\Omega_B}\left(-\gamma-\gamma^{-3}+\frac{\gamma}{\sqrt{1-\Lambda_+^2\sin^2\theta}}+\frac{\gamma^{-3}}{\sqrt{1-\Lambda_-^2\sin^2\theta}}\right)$$

$$\sin^2\theta = 1-\frac{1}{2}\frac{\Omega_B^2}{\Omega^2}\left[\frac{\Omega^2}{\Omega_B^2}-\frac{H_1^2}{H_0^2}-1+\sqrt{\left(1+\frac{H_1^2}{H_0^2}-\frac{\Omega^2}{\Omega_B^2}\right)^2+4\frac{\Omega^2}{\Omega_B^2}}\right]$$

Stochastic Swimming

- Conformational Transitions

$$\mathrm{A} \underset{k_{AB}}{\overset{k_{BA}}{\rightleftharpoons}} \mathrm{B} \underset{k_{BC}}{\overset{k_{CB}}{\rightleftharpoons}} \mathrm{C} \underset{k_{CD}}{\overset{k_{DC}}{\rightleftharpoons}} \mathrm{D} \underset{k_{DA}}{\overset{k_{AD}}{\rightleftharpoons}} \mathrm{A}$$



$$V \equiv \langle v \rangle = \frac{K}{2}\langle \dot{u}_1 u_2 - \dot{u}_2 u_1 \rangle = K \left\langle \frac{d\mathcal{A}}{dt} \right\rangle$$

RG & A. Ajdari, PRL **100**, 038101 (2008)

General Theory of Stochastic Swimming

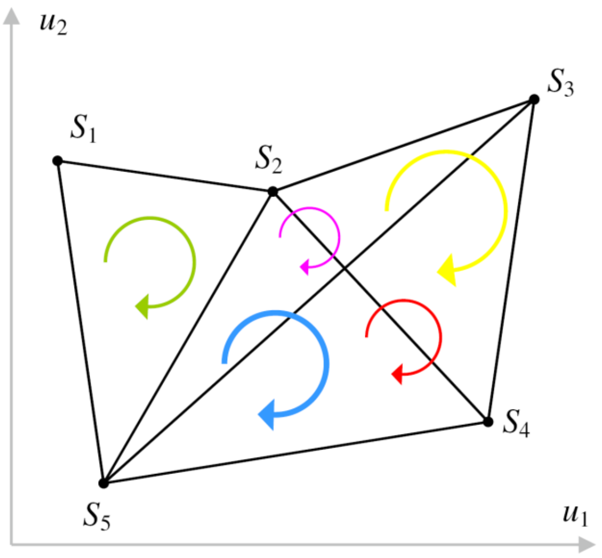
- Master Equation Formulation

$$J_{\langle nm \rangle} = k_{mn} P_n - k_{nm} P_m \qquad \sum_n P_n = 1$$

$$\sum_m J_{\langle nm \rangle} = 0$$

- ``Parallel'' Arrangement

$$\left\langle \frac{\Delta \mathcal{A}}{\Delta t} \right\rangle = \sum_\alpha \mathcal{A}(\alpha) J(\alpha)$$

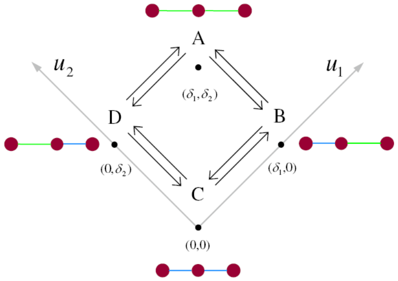


RG & A. Ajdari, JPCM **21**, 204104 (2008)

Stationary State

- Average Swimming Velocity

$$V = K\delta_1\delta_2 J \qquad\qquad T = J^{-1}$$



$$J = \frac{k_{AD}k_{DC}k_{CB}k_{BA} - k_{AB}k_{BC}k_{CD}k_{DA}}{\sum_{\text{replace A by B, C, D}}(k_{AD}k_{DC}k_{CB} + k_{AB}k_{BC}k_{CD} + k_{AB}k_{AD}k_{DC} + k_{AD}k_{AB}k_{BC})}$$

Breaking the detailed balance

- \`\`Series" Arrangement

$$k_{BA} \gg k_{AB},\ etc.$$

$$T = k_{AD}^{-1} + k_{DC}^{-1} + k_{CB}^{-1} + k_{BA}^{-1}$$

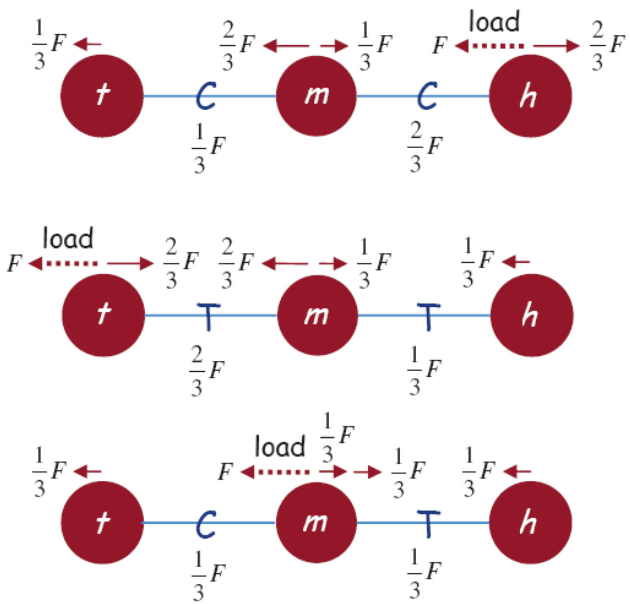
- Example:

$$k_{BA} = 1 + \epsilon$$

$$J = \epsilon/(16 + 6\epsilon)$$

Mechanical Response

- Two types:
  - Contribution to *hydrodynamic* force balance
  - Changing the *kinetics* of the conformational transitions



- Force-Velocity Relation

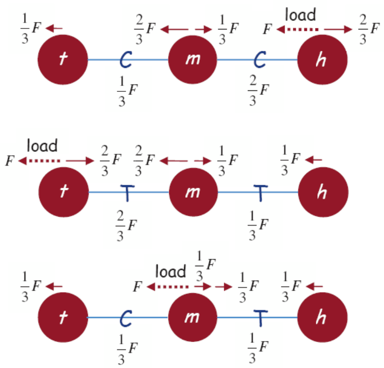
$$V(F) = -\frac{F}{18\pi\eta a_R} + V_0\, J(F)/J(0)$$

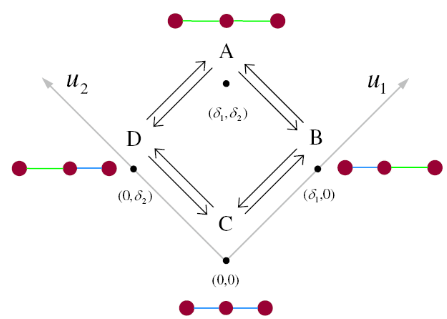
Mechanical Response

- Transition Rates

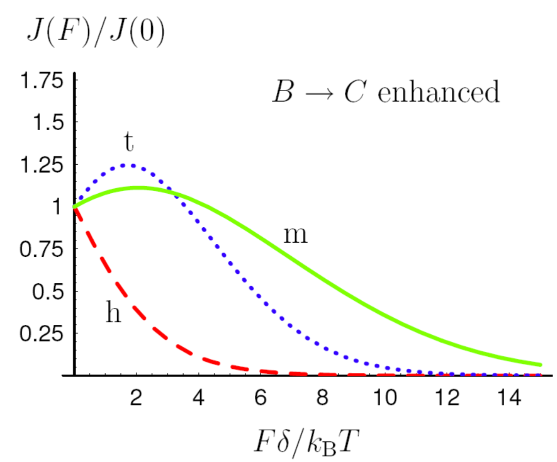
$$k_{\beta\alpha} = k_{0\beta\alpha}\ \exp\left(\frac{1}{2}\frac{f_{\beta\alpha}\delta_i}{k_{\mathrm{B}}T}\right)$$

Transition	Head	Tail	Middle
$A \longrightarrow B$	$+\frac{1}{3}F$	$-\frac{2}{3}F$	$+\frac{1}{3}F$
$B \longrightarrow C$	$+\frac{2}{3}F$	$-\frac{1}{3}F$	$-\frac{1}{3}F$
$C \longrightarrow D$	$-\frac{1}{3}F$	$+\frac{2}{3}F$	$-\frac{1}{3}F$
$D \longrightarrow A$	$-\frac{2}{3}F$	$+\frac{1}{3}F$	$+\frac{1}{3}F$

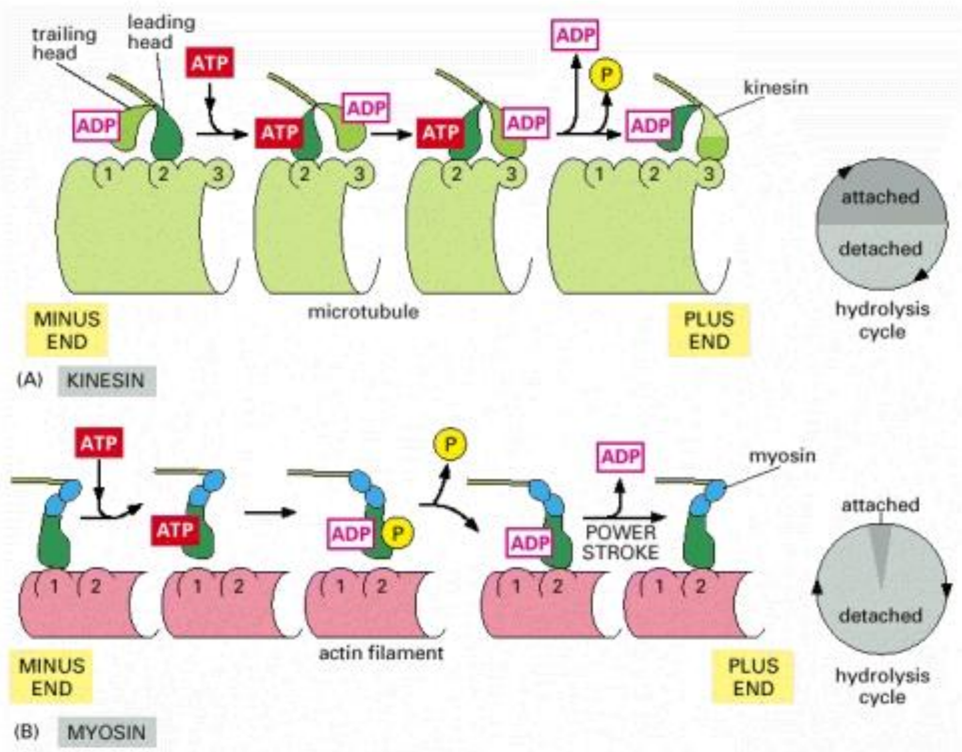




- Motor “Performance”



Mechanochemical Coupling



Alberts et al., *Molecular Biology of The Cell*

Can we design something like that?

Synthetic Molecular Swimmers

$$F + h \rightarrow hF \rightarrow hQ^{-} + G^{+} \rightarrow h + Q^{-} + G^{+}$$

$$R^{-} + P^{+} + t \rightarrow tR^{-} + P^{+} \rightarrow t + S$$

Electrostatic Actuation

$h = \mathrm{CA}$ *carbonic anhydrase*

$t = \mathrm{SOD}$ *superoxide dismutase*

$F = CO_2$

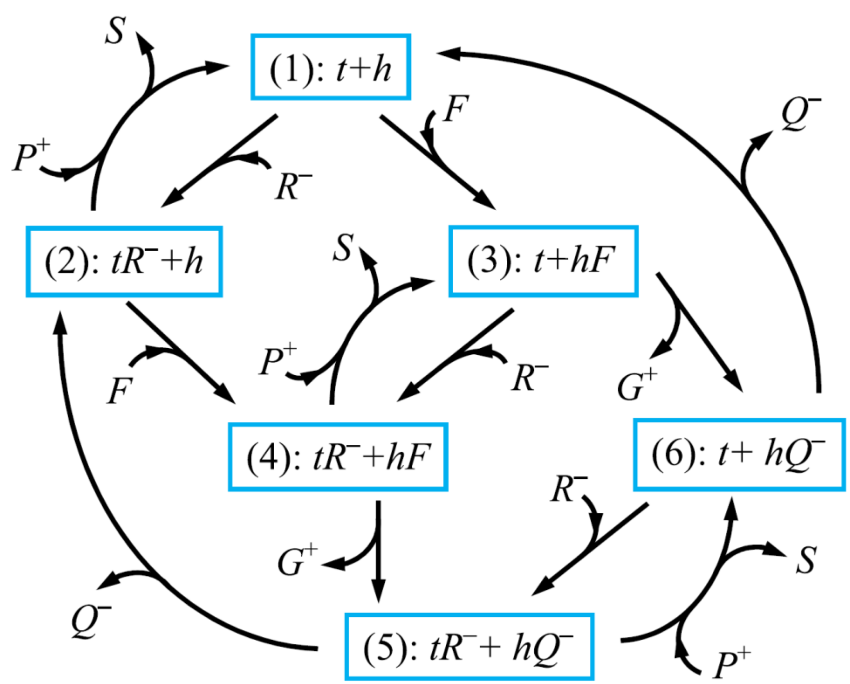
$Q^{-} = HCO_3^{-}$ bicarbonate

$G^{+} = H^{+}$

$R^{-} = O_2 \cdot^{-}$ superoxide anion

$P^{+} = H^{+}$

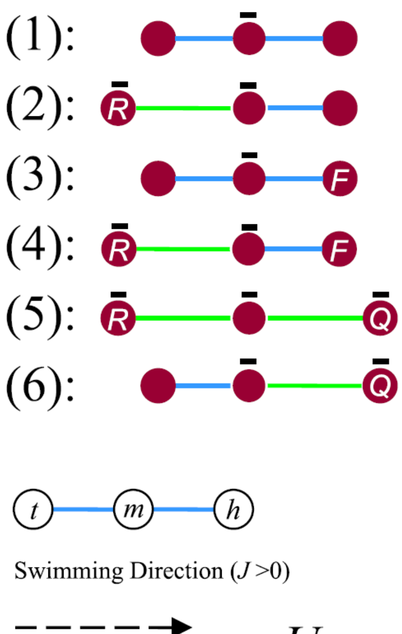
$S = \frac{1}{2}H_2O_2 + \frac{1}{2}O_2$

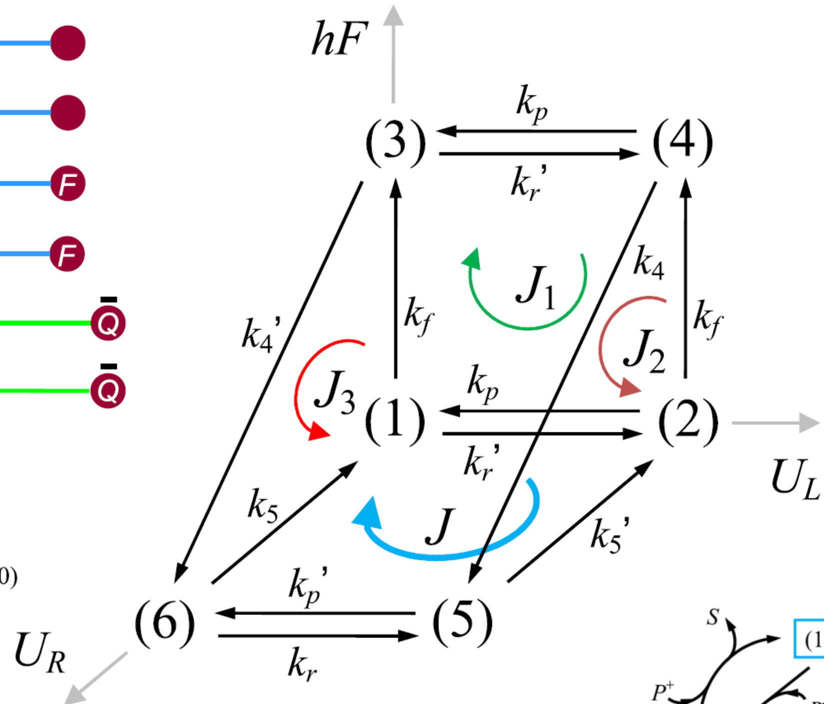


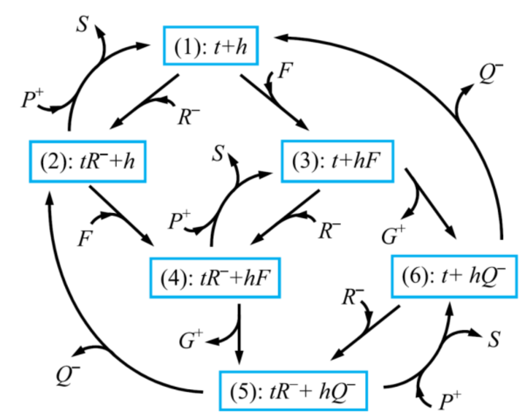
RG, PRL **105**, 018103 (2010)

(bio-) chemical cycle

Mechanochemical Swimmers





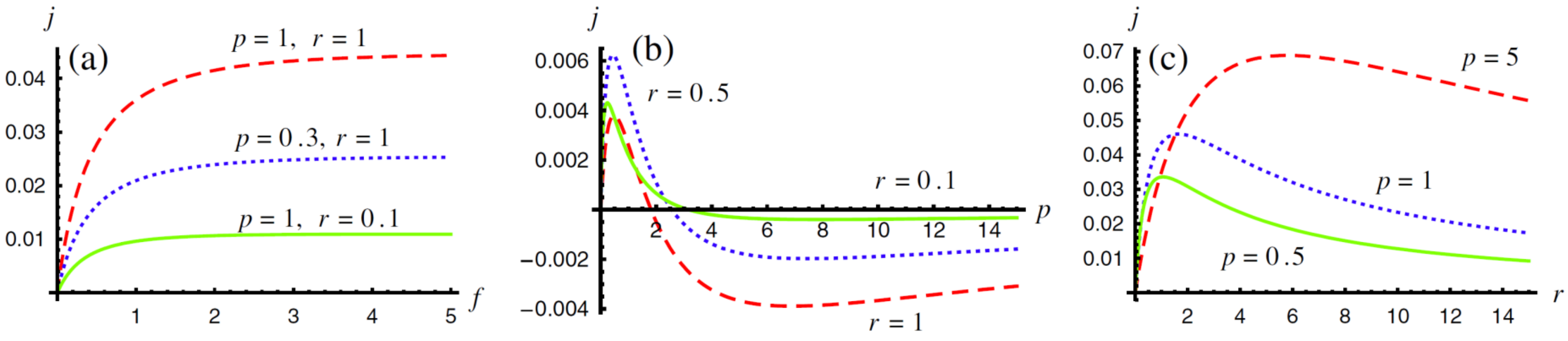


mechanochemical cycle

Concentration Dependence

Swimming Velocity

$$V = \frac{gDAk_5}{L^2}\, j\left(\frac{k_f[F]}{k_5}, \frac{k_r[R^-]}{k_5}, \frac{k_p[P^+]}{k_5}\right)$$



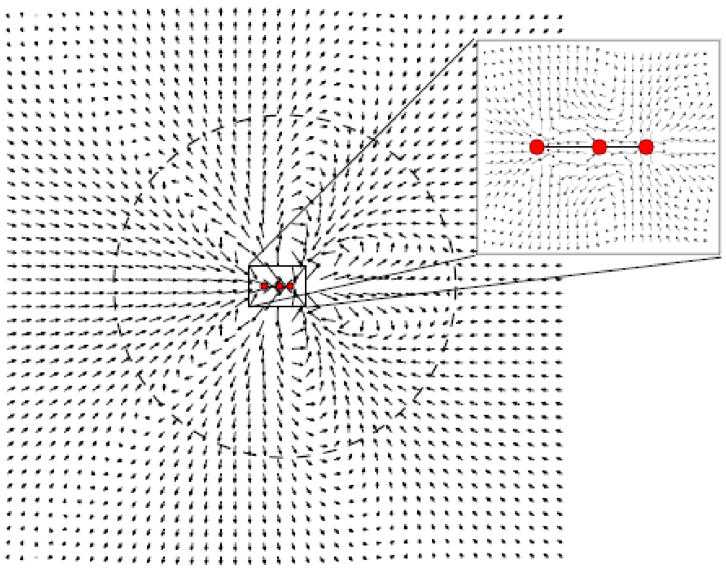
a) Michaelis-Menten behavior

b) Sign change of the velocity as a function of concentration

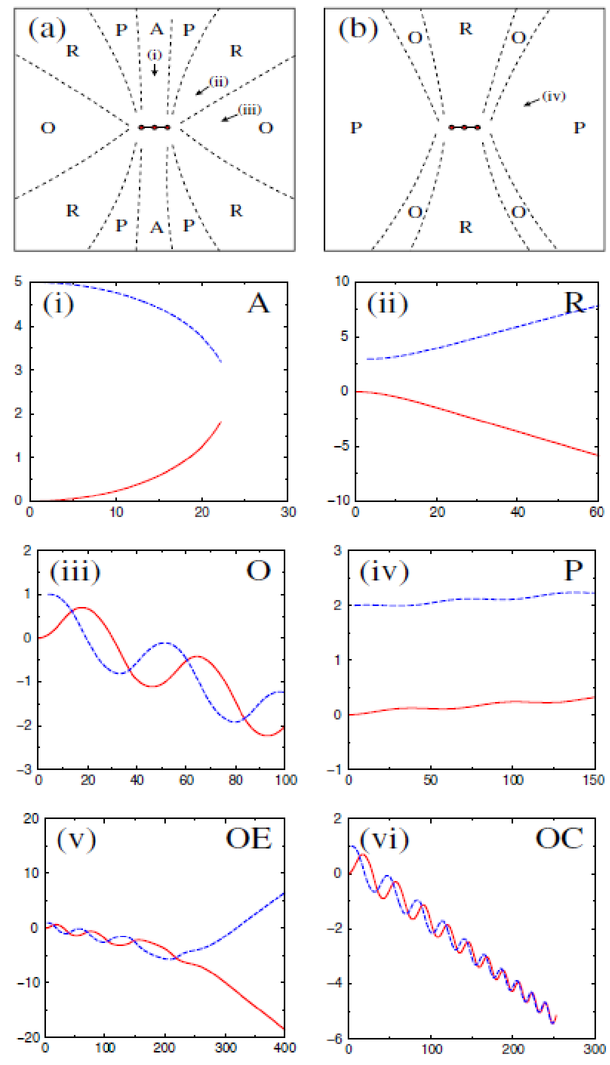
c) Non-monotonic concentration dependence; optimal concentration

Interaction between Swimmers

- Flow Field



- Hydrodynamic Interaction



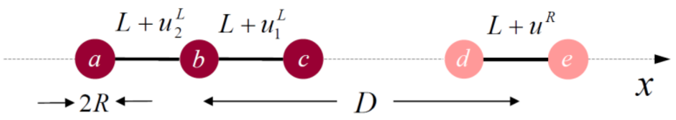
C. M. Pooley, G. P. Alexander, and J. M. Yeomans, PRL **99,** 228103 (2007)

Hydro Coupling for Stochastic Swimmers

- Coupled 3-Sphere & 2-Sphere System

$$V^L = \frac{7}{12}\frac{R}{L^2}\left\langle \dot{u}_1^L u_2^L \right\rangle - \frac{1}{2}\frac{RL}{D^3}\left[\left\langle u_1^L \dot{u}^R \right\rangle - \left\langle u_2^L \dot{u}^R \right\rangle\right]$$

$$V^R = \frac{RL}{D^3}\left[-2\left\langle \dot{u}_1^L u_2^L \right\rangle + \frac{3}{2}\left\langle u_1^L \dot{u}^R \right\rangle + \frac{3}{2}\left\langle u_2^L \dot{u}^R \right\rangle\right]$$

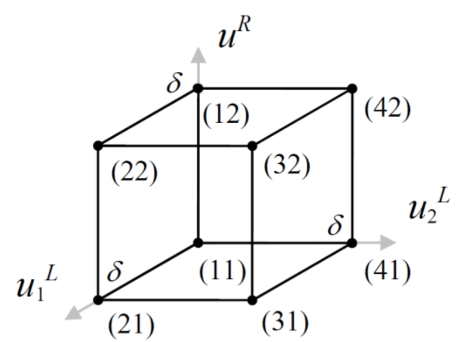


- Phase and Coherence

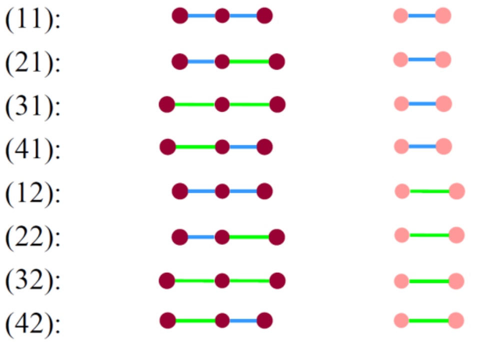
$$\left\langle \dot{u}_1^L u_2^L \right\rangle = \frac{1}{2} d^2 \Omega \sin(\varphi_1^L - \varphi_2^L)$$

$$\left\langle u_1^L \dot{u}^R \right\rangle = \frac{1}{2} d^2 \Omega \sin(\varphi^R - \varphi_1^L)$$

$$\left\langle u_2^L \dot{u}^R \right\rangle = \frac{1}{2} d^2 \Omega \sin(\varphi^R - \varphi_2^L)$$



- 8-State Configuration

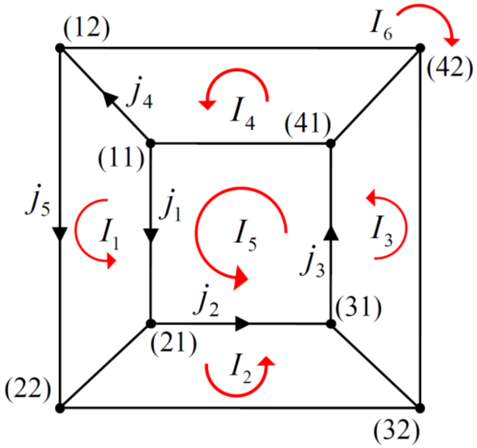


A. Najafi & RG, EPL **90**, 68003 (2010)

Coherence in Stochastic Swimming

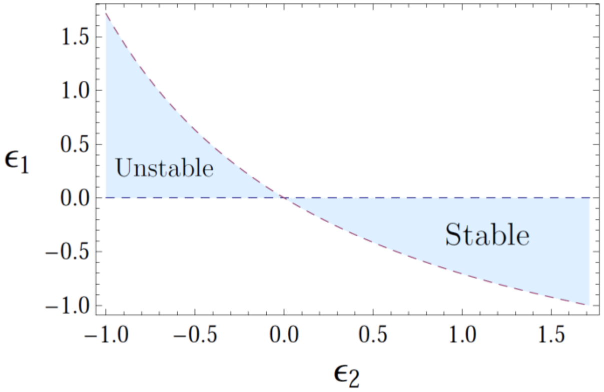
- Probabilities & Currents

$$\langle \dot{u}_1^L u_2^L \rangle = \delta^2 (I_6 - I_5)$$
$$\langle u_1^L \dot{u}^R \rangle = \delta^2 (I_3 - I_1)$$
$$\langle u_2^L \dot{u}^R \rangle = \delta^2 (I_4 - I_2)$$



- Hydrodynamic Bound-State

$$D_{\mathrm{eq}} = L \left(\frac{24}{7}\right)^{1/3} \left[\frac{-\epsilon_1(24 + 5\epsilon_2)}{12(\epsilon_1 + \epsilon_2) + 5\epsilon_1\epsilon_2}\right]^{1/3}$$



Phoretic Motion

- Electrophoresis

  Smoluchowski (1903)

- Thermophoresis

  Ludwig (1856), Soret (1879)

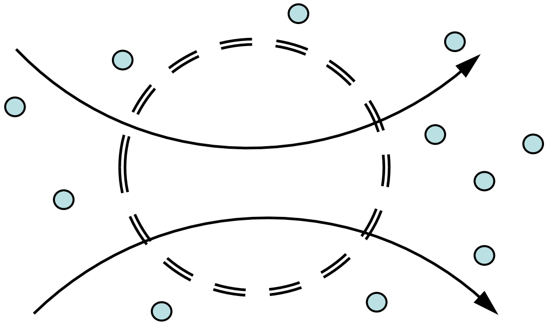
- Osmiophoresis

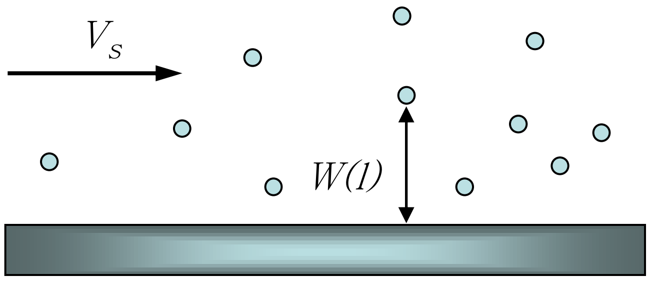
  Sackmann *et al* (1999)

- Diffusiophoresis

  Derjaguin *et al* (1961),

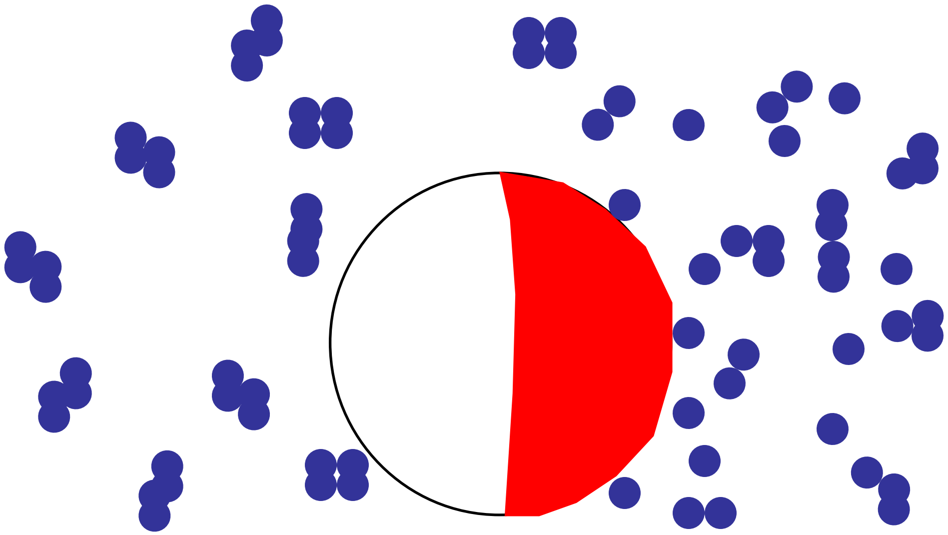
  Anderson & Prieve (1984)





Reaction-Driven Propulsion

Self-diffusiophoresis



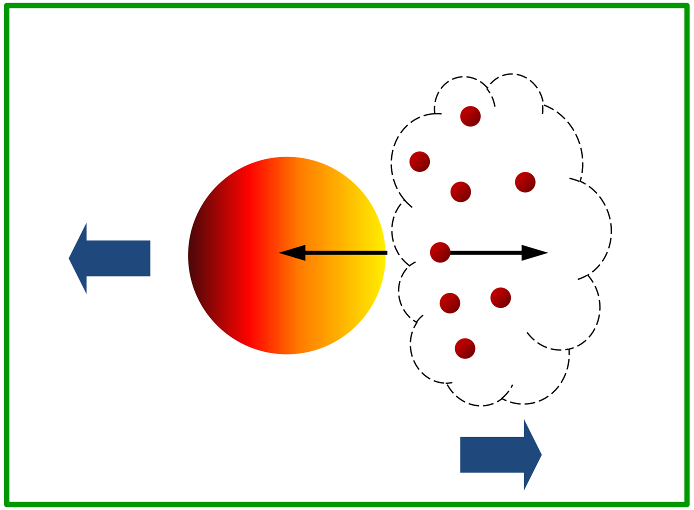
Chemical reaction produces more products than reactants

Propulsion (repulsive interaction)

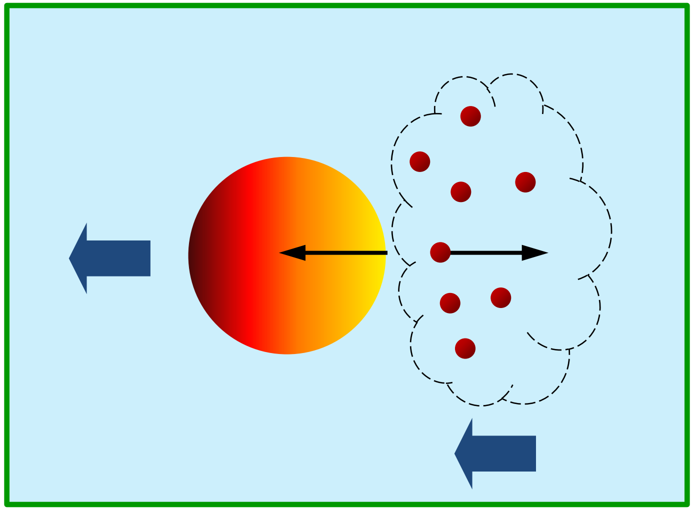
Particle half-coated with catalyst

RG, T.B. Liverpool & A. Ajdari, PRL **94,** 220801 (2005)

Who is Going Where?



Without Solvent



With Solvent

In solvent, balancing "Osmotic Pressure" with "Stokes Friction" is WRONG

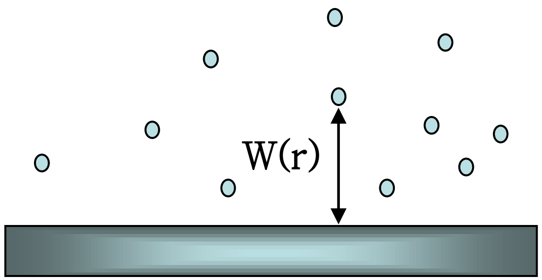
See, e.g.: U.M. Córdova-Figueroa and J.F. Brady, PRL **100,** 150303 (2008)

What is Diffusiophoresis?

For Solute:

$$\begin{cases} \mathbf{J} = -\mu k_\mathrm{B} T \nabla c + \mu c(-\nabla W) + c\mathbf{v} \\ \partial_t c + \nabla \cdot \mathbf{J} = 0 \end{cases}$$

$$D = \mu k_\mathrm{B} T \qquad \mathbf{F} = -\nabla W(\mathbf{r})$$



For Solvent:

$$\begin{cases} -\eta \nabla^2 \mathbf{v} = -\nabla p + \mathbf{f} \\ \nabla \cdot \mathbf{v} = 0 \\ \mathbf{f} = c\mathbf{F} = c(-\nabla W) \end{cases}$$

$$-\nabla^2 p + \nabla \cdot \mathbf{f} = 0$$

Stationary State: $-D\nabla^2 c + \mathbf{v} \cdot \nabla c + \mu \nabla \cdot \mathbf{f} = 0$

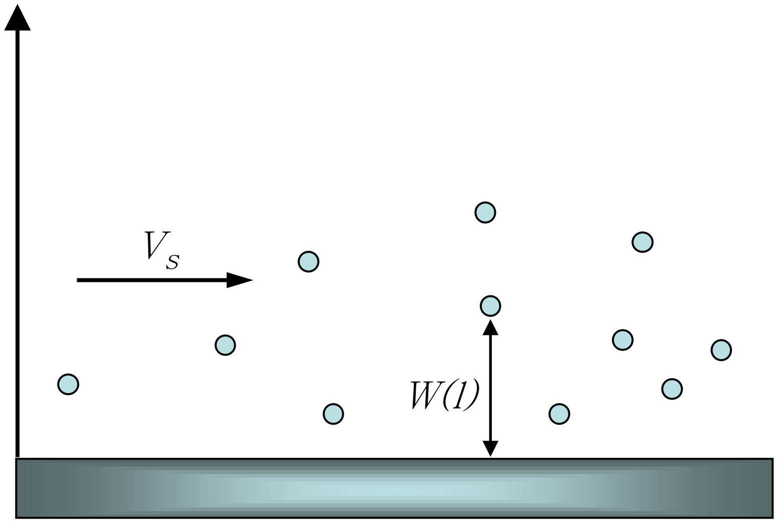
$$\boxed{\nabla^2 \left[p - k_\mathrm{B} T c\right] + \frac{1}{\mu} \mathbf{v} \cdot \nabla c = 0}$$

What is Diffusiophoresis?

Hydrostatic+Osmotic pressure balance:

No external pressure gradient	external concentration gradient
$p_{\mathrm{out}} = \mathrm{const.}$	$\nabla C_{\mathrm{out}} \neq 0$

$$p - k_{\mathrm{B}} T\, C \approx \mathrm{const.}$$



Depletion due to interaction

$\nabla p_{\mathrm{s}} \neq 0$

$C_{\mathrm{s}} = 0$

pressure gradient in the interaction zone

Fluid Slip inside the Interaction Domain

For a slightly different, and more general discussion, see: F. Julicher and J. Prost, EPJE **29**, 27 (2009)

Analysis of the Motion

- Slip Velocity $\mu = k_{\mathrm{B}} T \lambda^2 / \eta$

$$\lambda_D^2 = \int_0^\infty dl\ l \left[1 - \mathrm{e}^{-W(l)/k_{\mathrm{B}}T}\right]$$

$$\mathbf{v}_{\mathrm{s}}(\mathbf{r}_{\mathrm{s}}) = \mu(\mathbf{r}_{\mathrm{s}})(\mathbf{I} - \mathbf{nn}) \cdot \nabla c(\mathbf{r}_{\mathrm{s}})$$

- Surface Reaction

$$D\nabla^2 c = 0$$

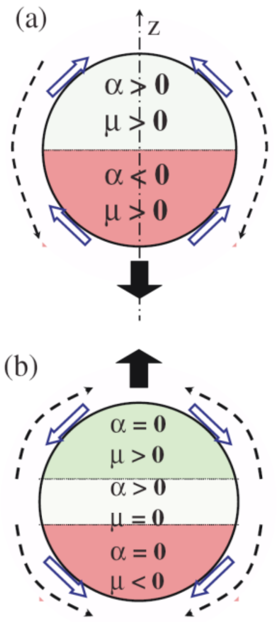
$$-D\mathbf{n} \cdot \nabla c(\mathbf{r}_{\mathrm{s}}) = \alpha(\mathbf{r}_{\mathrm{s}})$$

Characteristics of the Motion

- Swimming Velocity

$$V \sim \alpha\mu/D \qquad \mu = k_{\rm B}T\lambda^2/\eta$$

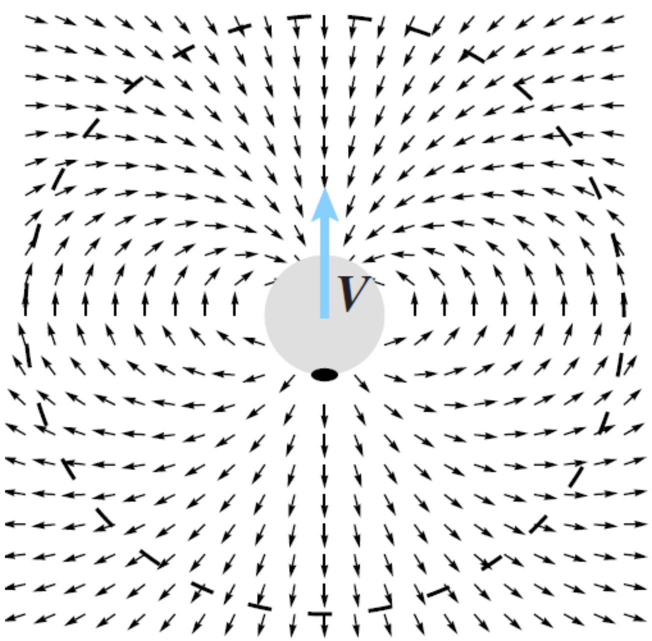
- Design-related Questions
  - Symmetry breaking
  - Relative importance of activity/mobility
  - Effect of Geometry



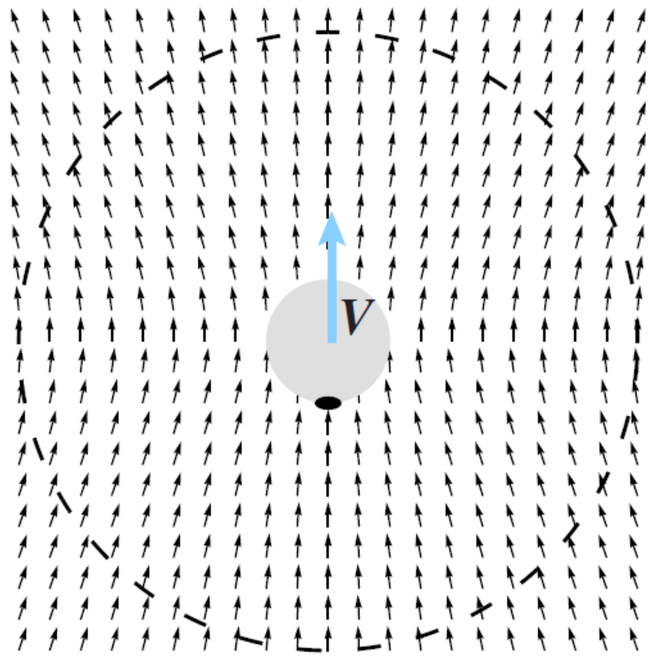
- Generic for Any Phoresis

RG, T.B. Liverpool & A. Ajdari, New J Phys **9,** 126 (2007)

Flow Field Pattern



Phoretic

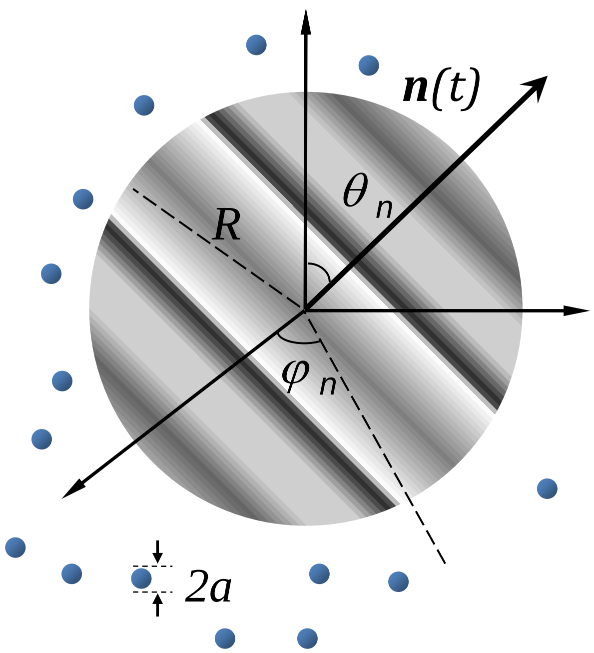


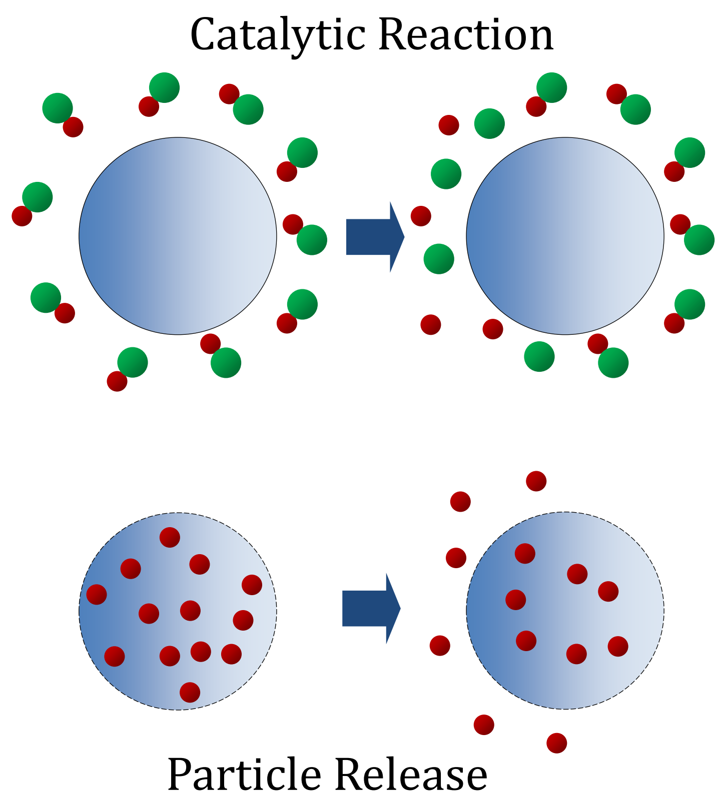
"Osmotic Pressure" Picture

Image from: M.N. Popescu, S. Dietrich, and G. Oshanin, JCP **130,** 194702 (2009)

For a thorough discussion, see: F. Julicher and J. Prost, EPJE **29**, 27 (2009)

Stochastic Dynamics of Phoretic Swimmers





Activity: $$\alpha(\theta,\phi,t) = \sum_{\ell,m} \left(\frac{4\pi}{2\ell+1}\right) \alpha_\ell \, Y^*_{\ell m}(\theta_n(t),\phi_n(t)) Y_{\ell m}(\theta,\phi)$$

RG, PRL **102,** 188305 (2009)

Relevant Time Scales

- Colloid Rotational Diffusion

$$\tau_r = 4\pi\eta R^3/k_{\mathrm{B}}T$$

$$\tau_r = 3\ (R/1\mu\mathrm{m})^3\ \mathrm{s}$$

- Solute Diffusion

$$\tau_d = R^2/D$$

$$\tau_d = 10^{-3}\ (R/1\mu\mathrm{m})^2\ \mathrm{s}$$

- Hydrodynamic

$$\tau_h = R^2/\nu$$

$$\tau_h = 10^{-6}\ (R/1\mu\mathrm{m})^2\ \mathrm{s}$$

$$\nu = \eta/\rho$$

$$\tau_h \ll \tau_d \ll \tau_r$$

Symmetric Contribution

- Short Time Behavior

$$\Delta L^2_{\rm sym} \simeq \frac{8\alpha_0\mu^2}{3\pi^{3/2}D^{3/2}R^3}\, t^{3/2} \quad ; \; t \ll \tau_d$$

$$\Delta L^2 \sim v^2 t^2$$

$$v \sim \mu \nabla C \sim \mu \delta C / R$$

$$\Delta L^2 \sim \mu^2 \langle \delta C(t) \delta C(0) \rangle t^2 / R^2$$

$$\langle \delta C(t) \delta C(0) \rangle = \langle \delta C^2 \rangle k(t)$$

$$k(t) \sim 1/(Dt)^{3/2}$$

$$\langle \delta C^2 \rangle \sim C_{\rm av}$$

$$C_{\rm av} \sim (\alpha_0 R^2 t)/R^3$$

- Long Time Behavior

$$c_1 = 1.17810$$

$$\Delta L^2_{\rm sym} \simeq \frac{2c_1\alpha_0\mu^2}{\pi^2 D^2 R^2}\, t \quad ; \; t \gg \tau_d$$

Asymmetric Contribution

- Memory Effect

$$v_0 = -\alpha_1 \mu/(3D)$$

$$\mathbf{v}(t) = \frac{v_0}{\tau_d} \int_{-\infty}^{t} dt' \mathcal{M}(t-t')\mathbf{n}(t')$$

$$\mathcal{M}(t) \simeq \tfrac{2}{\sqrt{\pi}}(t/\tau_d)^{-1/2} \text{ for } t \ll \tau_d$$

$$\mathcal{M}(t) \simeq \tfrac{3}{8\sqrt{\pi}}(t/\tau_d)^{-5/2} \text{ for } t \gg \tau_d$$

- Rotational Diffusion

$$\langle \mathbf{n}(t) \cdot \mathbf{n}(0) \rangle = e^{-t/\tau_r}$$

Asymmetric Contribution

- Short Time Behavior

$$\Delta L^2_{\text{asym}} \simeq v_0^2 t^2 \left[1 - \frac{4c_2}{\pi}\left(\frac{\tau_d}{\tau_r}\right)\right] \quad ; \; t \ll \tau_d \ll \tau_r$$

$c_2 = 0.642699$

- Intermediate Time Behavior

$$\Delta L^2_{\text{asym}} \simeq v_0^2 t^2 - \left(\frac{8}{3\sqrt{\pi}}\right) \frac{v_0^2 \tau_d^{3/2}}{\tau_r} \, t^{3/2} \quad ; \; \tau_d \ll t \ll \tau_r$$

- Long Time Behavior

$$\Delta L^2_{\text{asym}} \simeq 2 v_0^2 \tau_r \, t \quad ; \; \tau_d \ll \tau_r \ll t$$

Hydrodynamic Contribution

- Short Time Behavior

$$\Delta L^2_{\rm hyd} \simeq 3\left(\frac{k_{\rm B}T}{M_{\rm eff}}\right)t^2 \quad ;\ t \ll \tau_h$$

- Long Time Behavior

$$\Delta L^2_{\rm hyd} \simeq 6D_0 t - \frac{2k_{\rm B}T\rho^{1/2}}{\pi^{3/2}\eta^{3/2}}\,t^{1/2} \quad ;\ t \gg \tau_h$$

Bare Diffusion Coefficient of the Colloid: $D_0 = k_{\rm B}T/(6\pi\eta R)$

Hydrodynamic long-time tail: Alder-Wainwright 1967; Zwanzig-Bixon 1970

Effect of All Contributions

- Summary of the Different Regimes

Asymmetric Contribution	$\sim t^2$ *inertial*	$\sim t^2$ *propulsive*	$\sim t^2 - \gamma\, t^{3/2}$ *propulsive + anomalous*	$\sim t$ *diffusive*
Symmetric Contribution	$\sim t^2$ *inertial*	$\sim t^{3/2}$ *anomalous*	$\sim t$ *diffusive*	
Hydrodynamic Contribution	$\sim t^2$ *inertial*	$\sim t - \beta\, t^{1/2}$ *diffusive + anomalous*		

τ_h $\quad$ τ_d $\quad$ τ_r

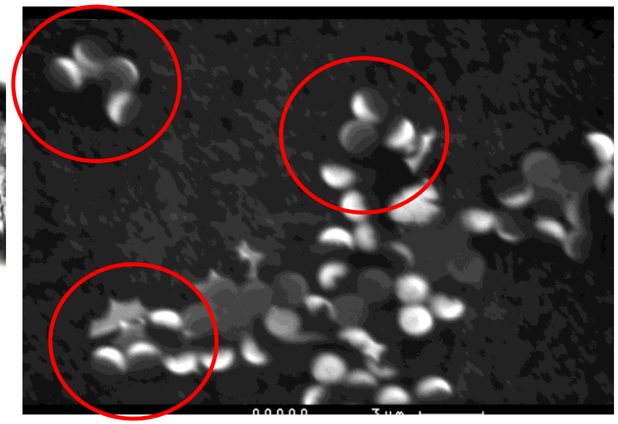
- Effective Diffusion at Long Times

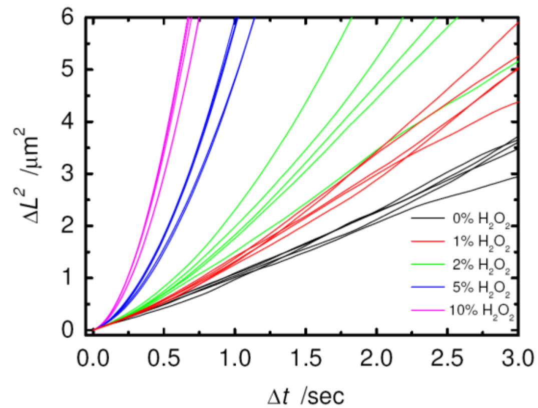
$$D_{\text{eff}} = \frac{k_{\text{B}}T}{6\pi\eta R} + \frac{4\pi\alpha_1^2\mu^2\eta R^3}{27D^2k_{\text{B}}T} + \frac{c_1\alpha_0\mu^2}{3\pi^2D^2R^2}$$

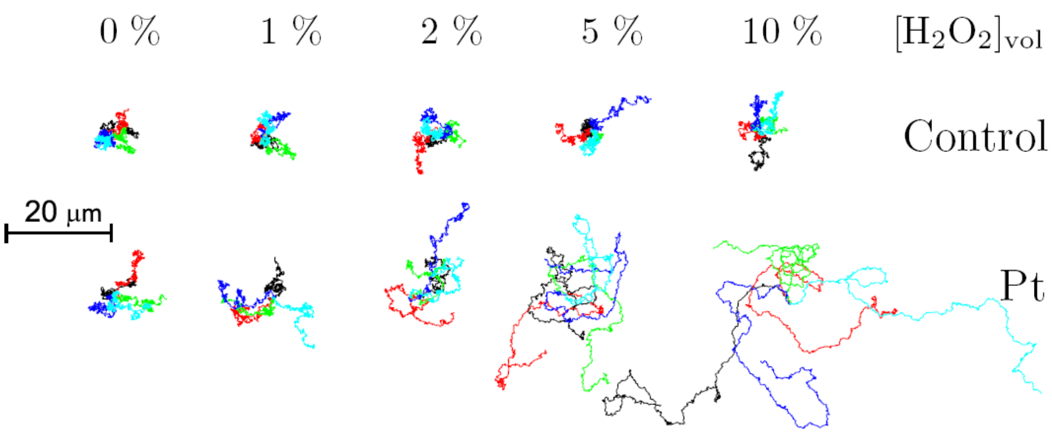
Non-monotonic Size Dependence

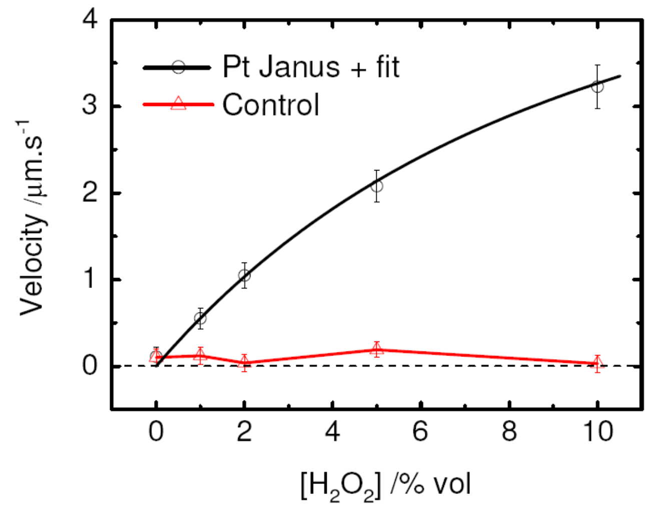
Sheffield Swimmer

half-Pt coated spherical
PS beads in aqueous
hydrogen peroxide solution



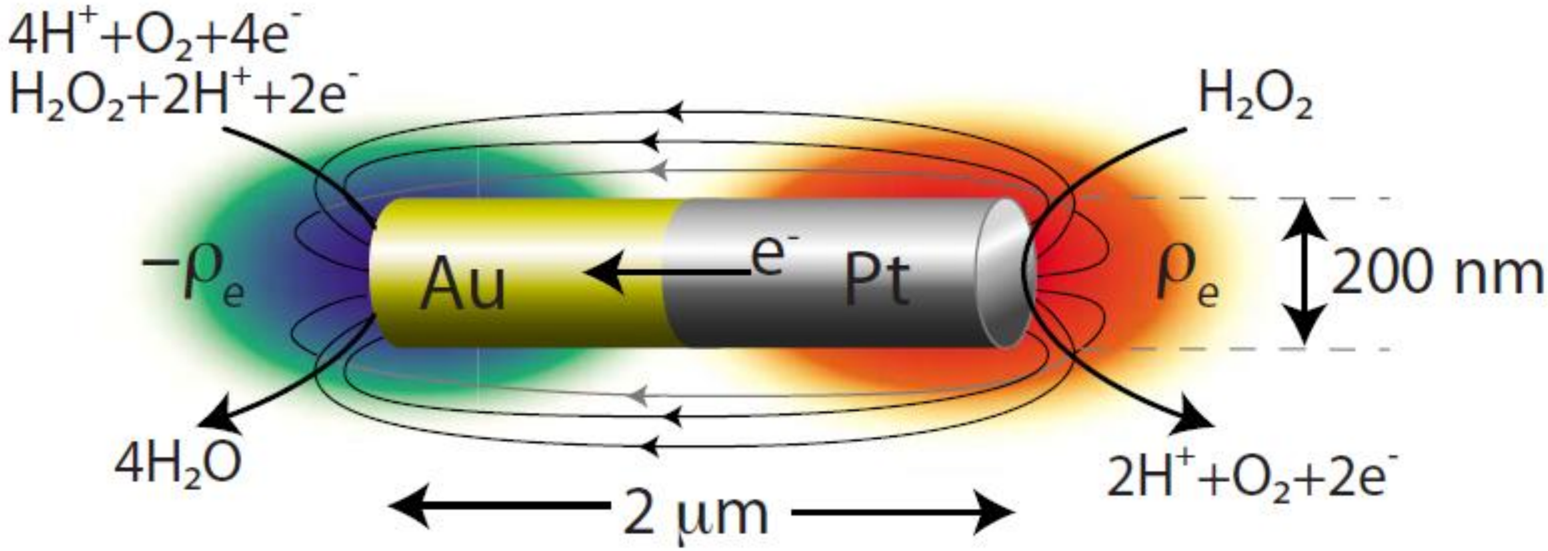






J. Howse, R.A.L. Jones, A.J. Ryan, T. Gough, R. Vafabakhsh, & RG, PRL **99,** 048102 (2007)

Penn Swimmer

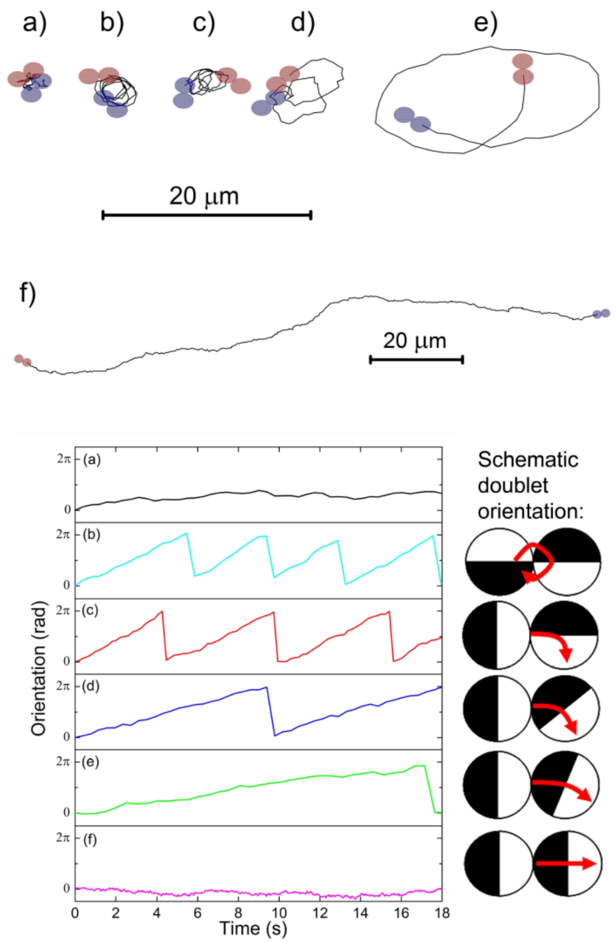


W.F. Paxton, *et al* JACS **126**, 13424 (2004) [Ayusman Sen Group]

A short circuited inverted battery!

Theoretical Analysis: J. L. Moran, P.M. Wheat, and J.D. Posner, PRE **81,** 065302(R) (2010)

Sheffield II: Runners and Tumblers

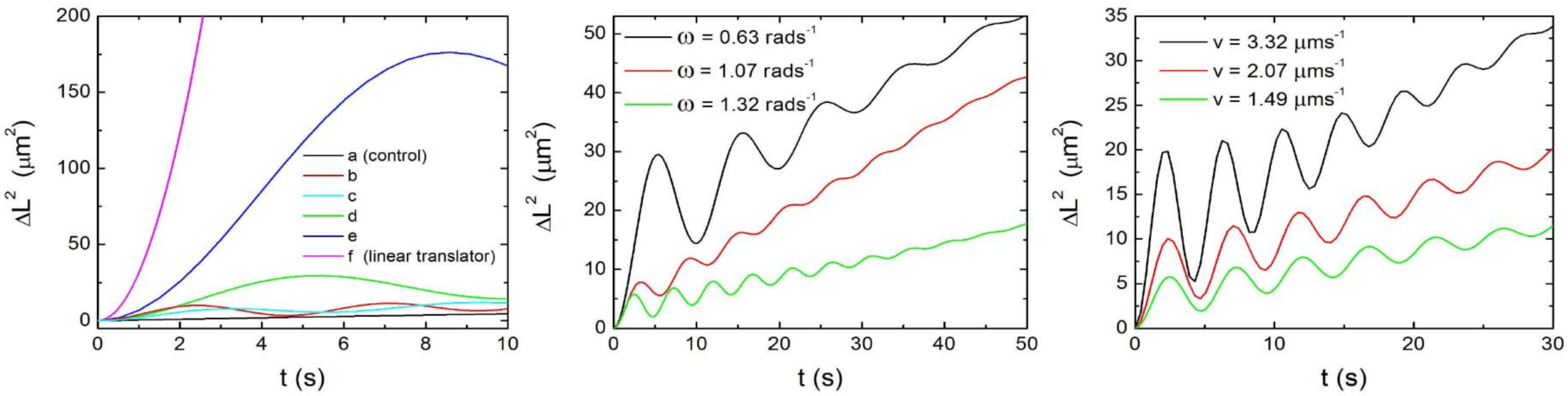


Two half-Pt coated spherical PS beads attached at an angle in aqueous hydrogen peroxide solution

Translational and **Rotational** Propulsion

S. Ebbens, R.A.L. Jones, A.J. Ryan, RG & J.R. Howse, PRE **82,** 015304 (R) (2010)

Mean-Square Displacement

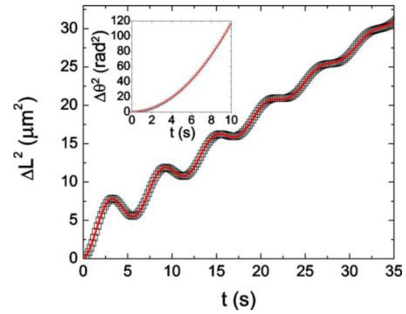


Crossover:

1. from **Ballistic**
2. to **Oscillatory+decay**
3. to **Diffusive** behavior

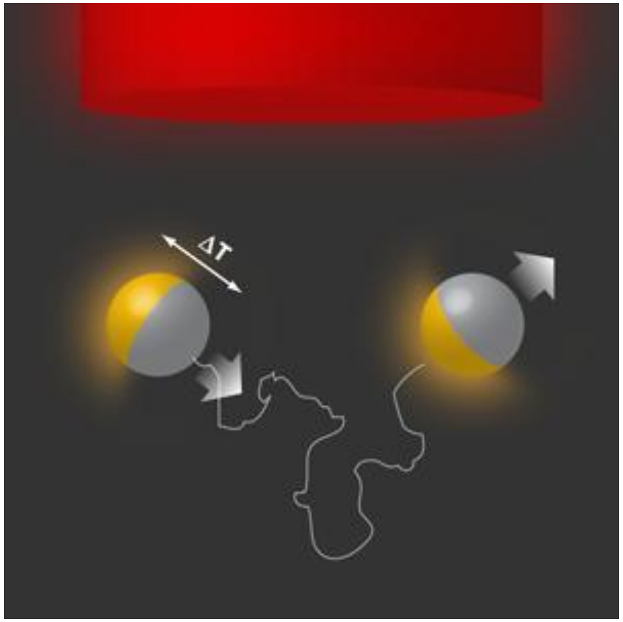
$$\Delta L^2(t) = 4Dt + \frac{2v^2 D_r t}{D_r^2+\omega^2} + \frac{2v^2(\omega^2 - D_r^2)}{(D_r^2+\omega^2)^2} + \frac{2v^2\, e^{-D_r t}}{(D_r^2+\omega^2)^2}\left[(D_r^2-\omega^2)\cos\omega t - 2\omega D_r \sin\omega t\right]$$

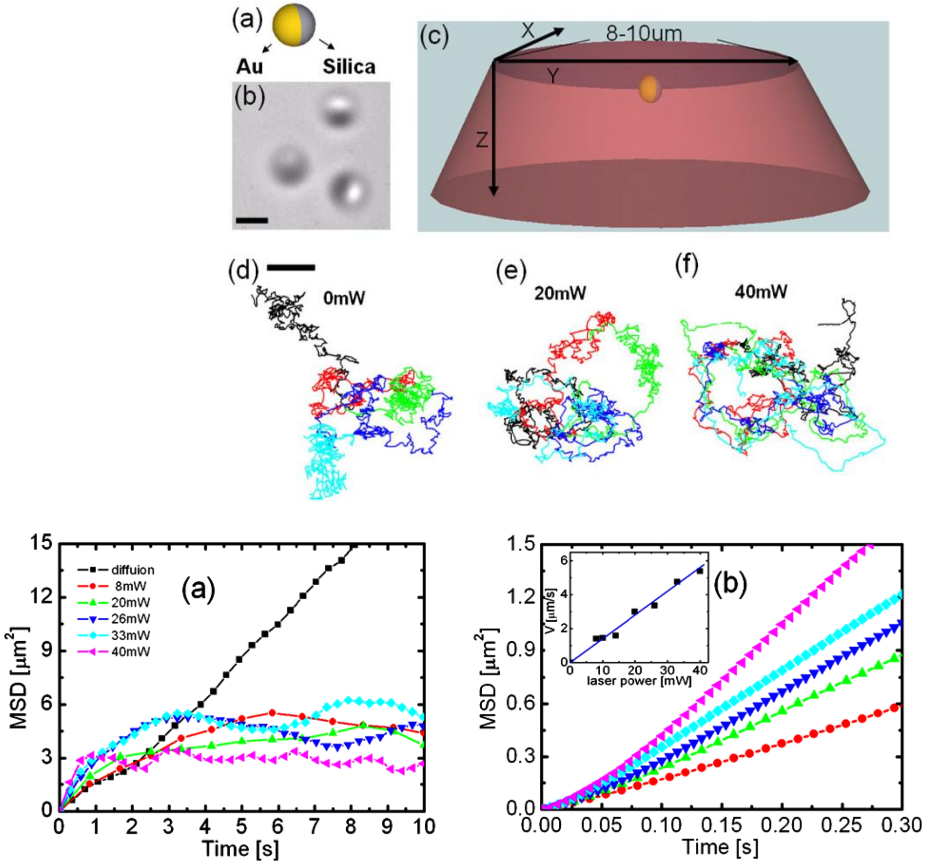
Trajectory	ω (rad s^{-1}) from MSAD	τ_r (s) from MSAD	τ_r (s) from MSD	D (μm^{2}s^{-1}) from MSD	v (μm s^{-1}) from MSD	ω (rad s^{-1}) from MSD
a	0	14.5	n/a	0.10	0	0
b	1.32	11.1	19.2	0.06	2.07	1.35
c	1.08	16.4	15.6	0.15	1.30	1.07
d	0.63	22.7	21.3	0.07	1.66	0.63
e	0.39	20.5	24.5	0.03	2.80	0.49
f	0	21.8	14.1	0.09	5.99	0



Tokyo Swimmer

Self-thermophoresis





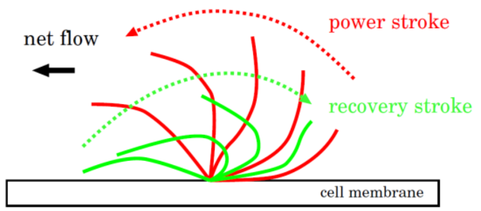
H-R. Jiang, N. Yoshinaga, and M. Sano,
Phys. Rev. Lett. **105**, 268302 (2010)

Active Hydrodynamics at Low Re

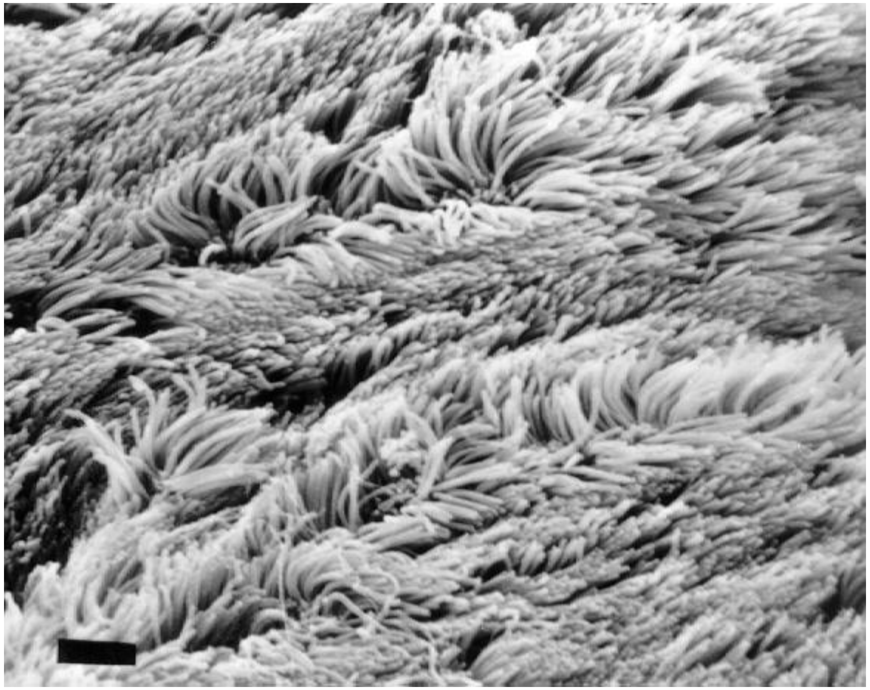
Active components (cilia, flagella, …) couple via long-ranged hydrodynamic interactions, leading to interesting emergent behaviors.

metachronal waves

beating pattern

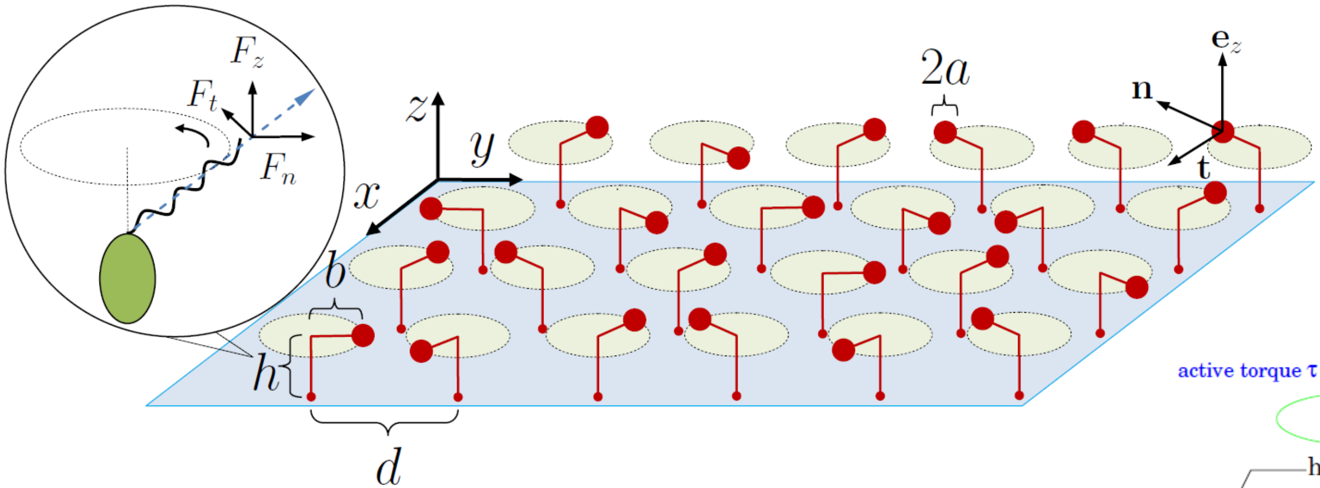


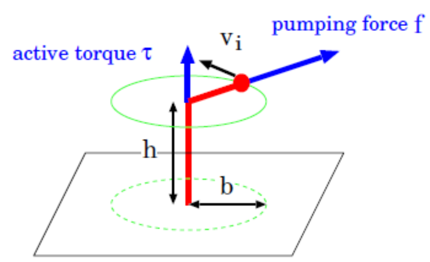
Mike Sanderson



A Simple Model for Metachrony

Generic for microfluidic rotors on a substrate, coupled via hydrodynamic interactions





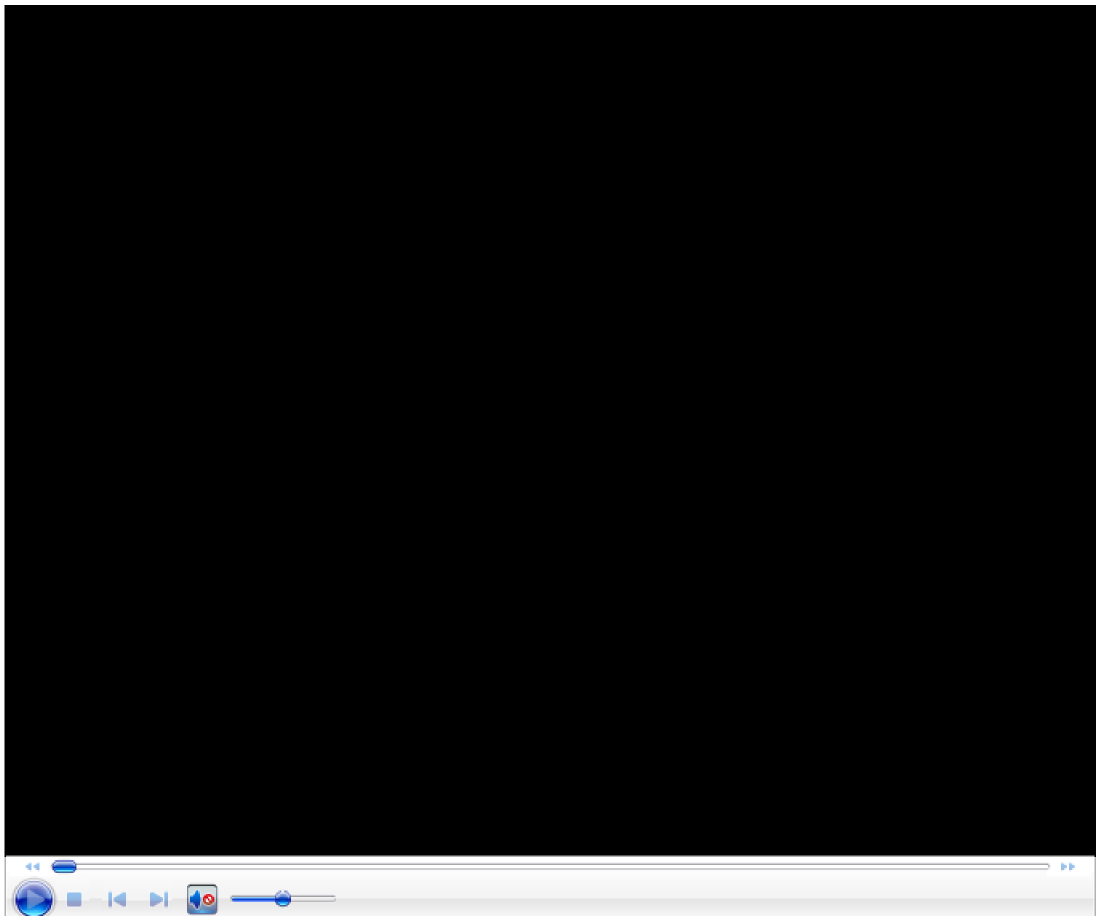
→ Can they synchronize?

→ Can they form patterns and dynamic structures?

N. Uchida & RG, PRL **104**, 178103 (2010)

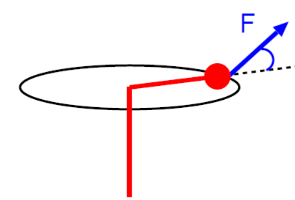
Symmetric Pumping

Complete synchronization for δ=0, via **defect coarsening**



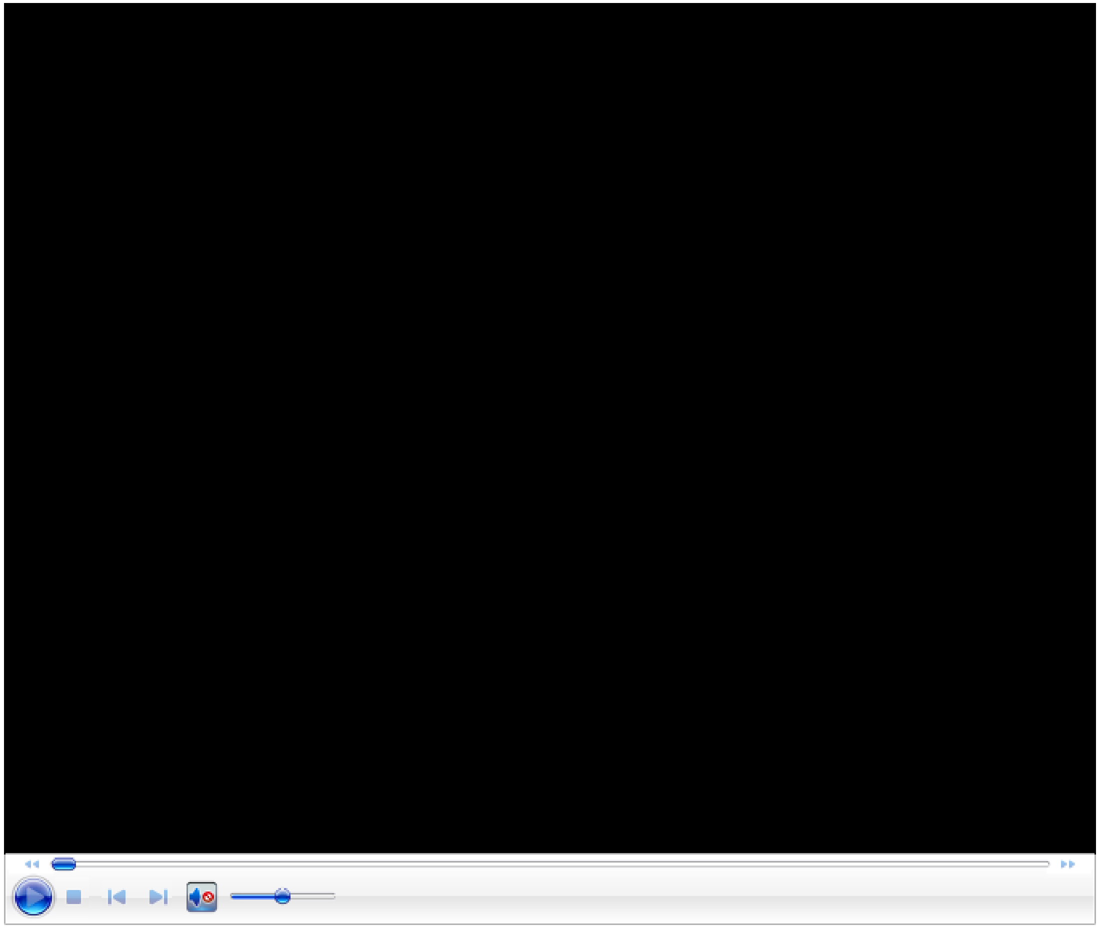
256×256

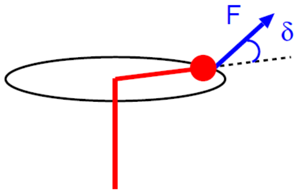
greyscale: $\cos\left(\phi(\boldsymbol{r}) - \langle\phi\rangle\right)$



Turbulent Spiral Waves

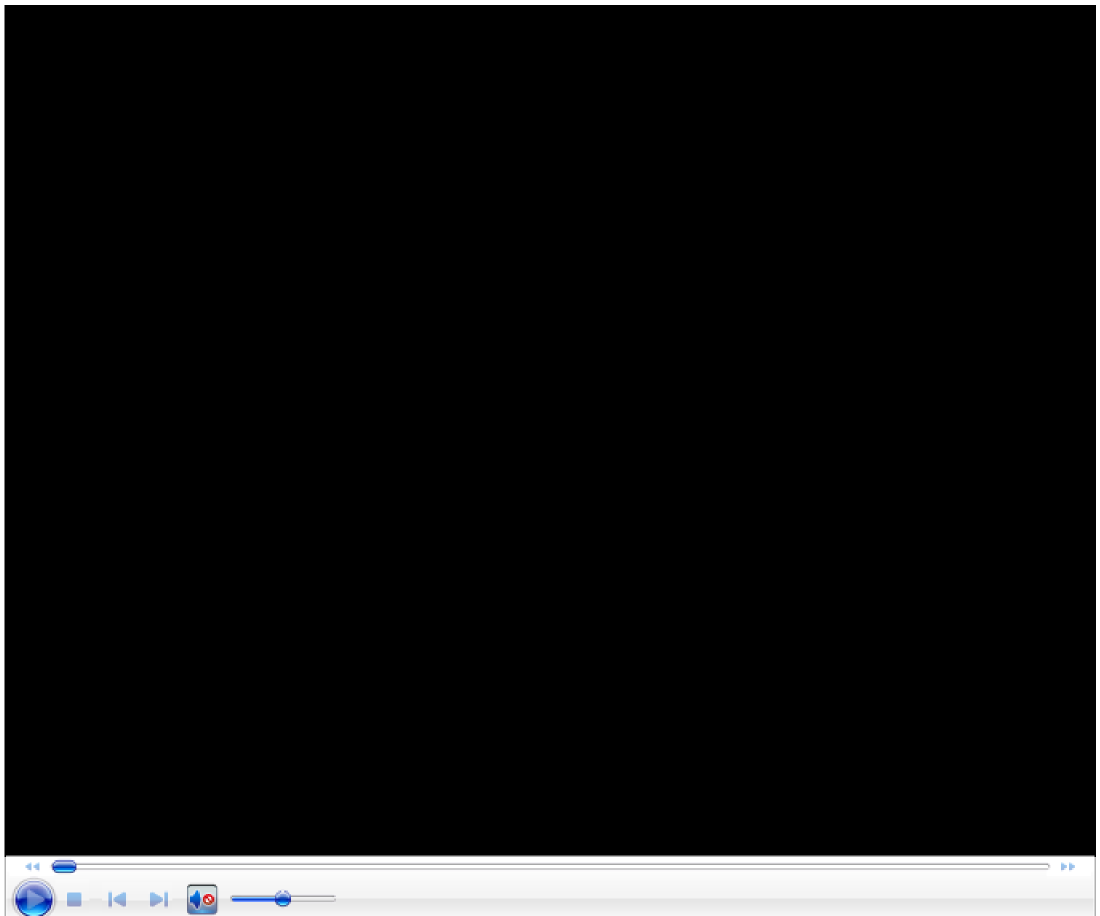
Synchronization NOT possible for $40<\delta<90$: $\delta=45$

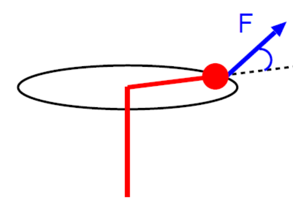




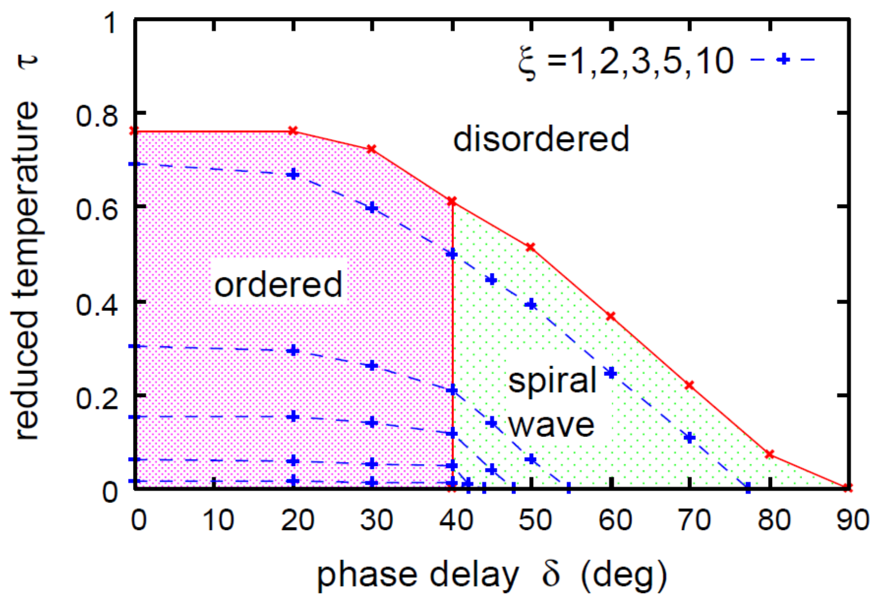
Turbulent Spiral Waves

Synchronization NOT possible for $40<\delta<90$: $\delta=60$





The Effect of Thermal Noise



In agreement with a mean-field theory result:

B. Guirao and J-F. Joanny, Biophys. J. **92**, 1900 (2007)

$$\omega \sim 10^2 \text{ Hz}$$

$$d \sim 10 \ \mu\text{m}$$

$$\tau = \frac{D_r d^3}{\gamma\omega} = \frac{k_B T d^3}{36\pi^2 \eta a^2 b^2 h^2 \omega}$$

$$a \sim b \sim h \sim 1 \ \mu\text{m}$$

Living systems operate close to the transition boundary $\quad \tau \sim 10^{-1}$

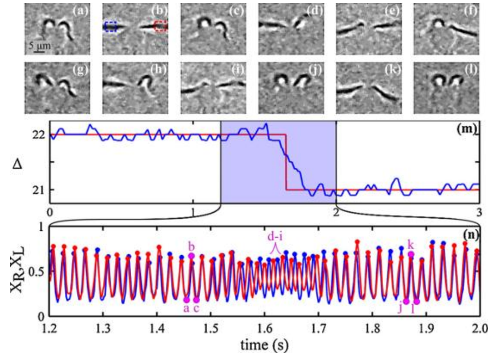
Hydrodynamic Synchronization

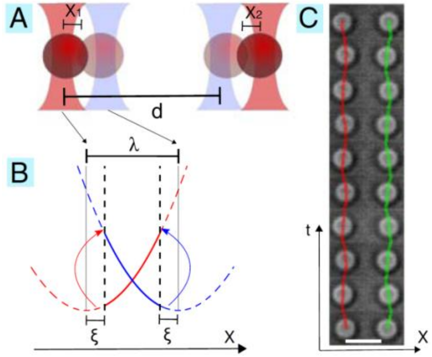
When do we have hydrodynamic synchronization or coordination?

- When the trajectories are asymmetric? How asymmetric?
- When the beating patterns are jerky? How jerky?

Numerical modeling of ciliary systems as elastic objects with realistic and complicated beating patterns does not answer the above questions.

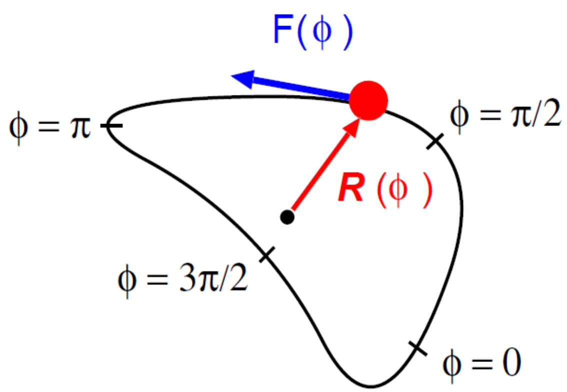
Recent Experiments from Goldstein and Cicuta Labs in Cambridge opened new doors…





Conditions for Hydro Synchronization

Q: When do objects with fixed trajectories synchronize via hydrodynamic interaction?



$$\mathbf{r}_i(\phi) = \mathbf{r}_{i0} + \mathbf{Q}_i \cdot \mathbf{R}(\phi)$$

Hydro Coupling:

$$H(\phi_1, \phi_2) \;=\; \mathbf{Q}_1 \cdot \mathbf{t}(\phi_1) \cdot \zeta \mathbf{G}_{12} \cdot \mathbf{Q}_2 \cdot \mathbf{t}(\phi_2)$$

Growth Rate:

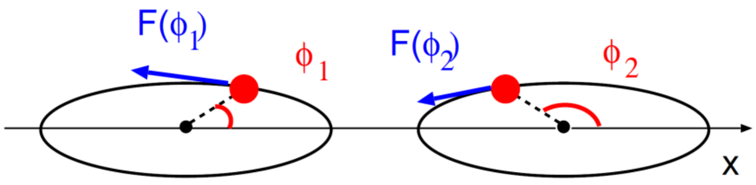
$$\boxed{\Gamma = -\frac{2}{T}\int_0^{2\pi} d\phi \, [\ln F(\phi)]' H(\phi, \phi)}$$

Condition for Synchronization: $\Gamma \; < \; 0$

N. Uchida & RG, PRL **106**, 058104 (2011)

Example: Circular Trajectories

$$\mathbf{R}(\phi) = b(\cos\phi, \sin\phi, 0)$$

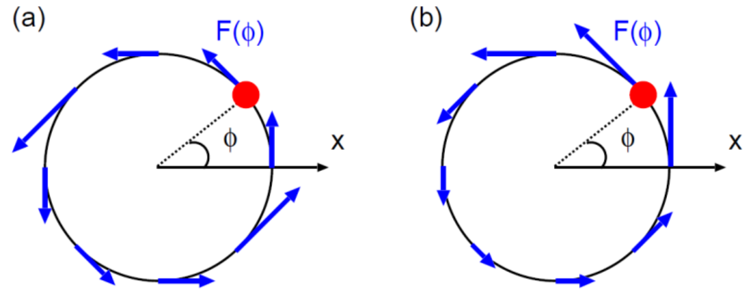


Hydro Coupling for parallel circles:

$$H(\phi,\phi) = G_D(d)\sin^2\phi = -\tfrac{1}{2}G_D(d)\cos(2\phi) + \mathrm{const}$$

Beating force profile:

$$F(\phi) = F_0[1 - \tfrac{1}{2}\sin(2\phi)]$$



$$F(\phi) = F_0\left[1 + \tfrac{1}{2}\sin\left(\phi + \tfrac{\pi}{4}\right)\right]$$

In general, *logarithm of Force* should have a negative 2nd sine-Fourier coefficient!

Acknowledgements

Experimental Collaborators:

S. Ebbens (Sheffield)
J. Howse (Sheffield)
R.A.L. Jones (Sheffield)
A.J. Ryan (Sheffield)
T. Gough (Bradford)
R. Vafabakhsh (Zanjan)
P. Tierno (Barcelona)
F. Sagues (Barcelona)

Theory Collaborators:

A. Najafi (Zanjan)
T.B. Liverpool (Bristol)
A. Ajdari (Paris)
I. Pagonabarraga (Barcelona)
N. Uchida (Tohoku)

Sheffield II,
the grey goo,
at your service...

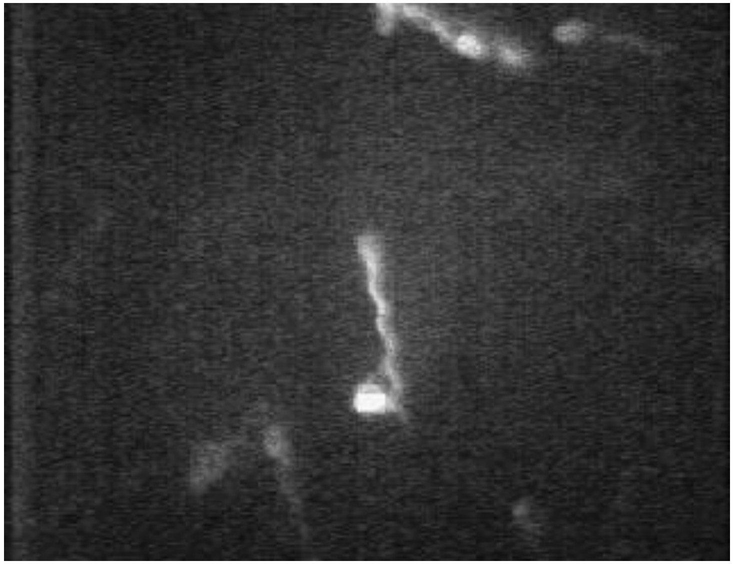
THANK YOU

Conclusion

- At small scales the conformational changes will be random, and we will need to cleverly "bias" them towards our desired outcome
- The stochastic nature can lead to novel mechanical responses of the "engine"
- Electrostatic actuation could be used to design synthetic molecular swimmers
- Coherence can be defined for stochastic swimmers
- Stochastic motion of phoretic swimmers is anomalous, depending on time scale
- Phoretic swimmers can be made to follow a variety of trajectories
- Phase ordering, defects, turbulent spiral waves, and much more in a model of microfluidic rotors
- Quantitative prescriptions for designing beating patterns that lead to synchronization

Bacterial Swimming

- *E. coli* driven by rotating flagella



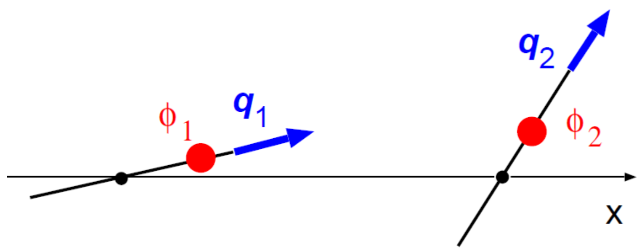
L. Turner, W.S. Ryu, and H.C. Berg, J. Bacteriol. **182**, 2793-2801 (2000)

- G.I. Taylor (1951)

Swimming at low Reynolds number

Example: Linear Trajectories

$$\mathbf{R}(\phi) = R(\phi)\mathbf{e}_x$$



Hydro Coupling: $$H(\phi,\phi) = -2R(\phi)\Big[G_I'(d)(\mathbf{q}_1\cdot\mathbf{q}_2)p_x + G_D'(d)q_{1x}q_{2x}p_x + \frac{G_D(d)}{d}(q_{1x}\mathbf{q}_2\cdot\mathbf{p} + q_{2x}\mathbf{q}_1\cdot\mathbf{p})\Big] + \text{const}$$

$$\mathbf{p} = \mathbf{q}_1 - \mathbf{q}_2$$

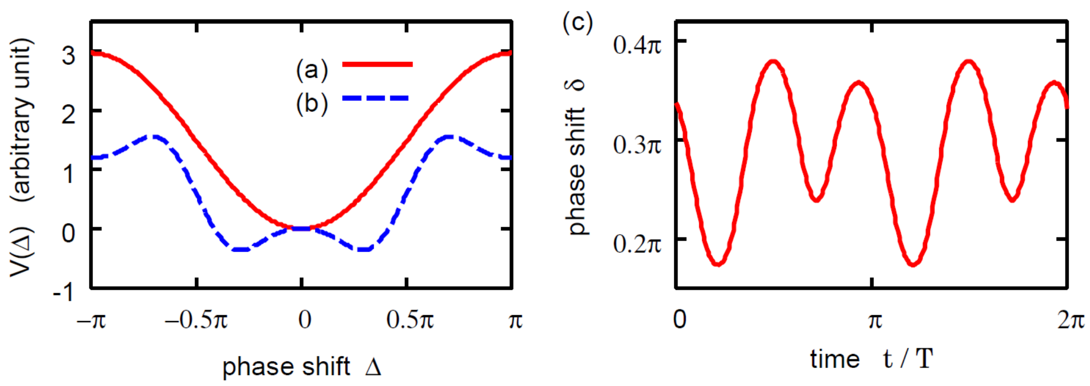
No monopole-monopole contribution for linear trajectories.

Assuming: $R(\phi) = b\cos\phi$

logarithm of Force should have a negative 1st sine-Fourier coefficient!

Nonlinear Stability Analysis

Cycle-averaged Eqn: $\dot{\Delta} = -V'(\Delta)$ $\Delta = \Phi_1 - \Phi_2$



Hydrodynamic synchronization is possible:

- in-phase
- out-of-phase
- at intermediate phases
- with varying phase shift