IAS Program on Frontiers of Soft Matter Physics: Tutorial

From Brownian to Driven and Active Dynamics of Colloids: Energetics and Fluctuations Part I

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Outline of Talk

Part I:

- Introduction to Brownian motion, Fluctuation Dissipation Theorem
- Stochastic Energetics (by K. Sekimoto, 1997)
- Fluctuation Theorems, Jarzynski Equality, etc. (1993-1996) → (Tuesday: by Hyunggyu Park)
- Measuring energy dissipation in small systems

Part II:

- Information Feedback control and thermodynamics
- Self-propelled particles, Active Matter

Einstein's Derivation of the Relation for Brownian Motion

 Consider colloidal suspension in an equilibrium state under the balance between external field and diffusion.



(1)

Equilibrium condition:
$$j = 0$$

 $\rho v_f = D \frac{\partial \rho}{\partial x}$

Osmotic pressure due to particle concentration

$$p = k_B T \rho$$

• Force due to osmotic pressure balances with the external force f

$$\frac{\partial p}{\partial x} = \rho f \qquad \longrightarrow \qquad k_B T \frac{\partial \rho}{\partial x} = \rho f \qquad (2)$$

Stokes's law of drag force:
$$f = \gamma v_f$$

 $\gamma = 6\pi\eta a \,$: Drag coefficient

From eq. (1) and (2)

$$\frac{k_B T}{\gamma} \frac{\partial \rho}{\partial x} = \rho v_f = D \frac{\partial \rho}{\partial x}$$

Einstein-Stokes Relation:

$$D = \frac{RT}{N_A} \frac{1}{6\pi\eta a} = \frac{k_B T}{\gamma}$$

Mesoscopic relation connecting between atomic scale and macroscopic scale

Brownian motion and Langevin equation

• Langevin equation

$$\dot{v}(t) = -\gamma v(t) + \frac{\xi(t)}{m} \tag{1}$$

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = 2\epsilon\delta(t-t')$$
 (2)

Integrating this equation

$$v(t) = v(t_0)e^{-\gamma(t-t_0)} + \frac{1}{m}\int_{t_0}^t e^{-\gamma(t-s)}\xi(s)ds$$

Multiplying v(t) and integrating it,

$$\langle v(t)^2 \rangle = \frac{\epsilon}{m^2 \gamma} (1 - e^{-2\gamma t}) + \langle v^2 \rangle e^{-\gamma t}$$

$$t \to \infty \qquad \langle v(t)^2 \rangle = \epsilon / (m^2 \gamma) \qquad \longrightarrow \qquad m \langle v(t)^2 \rangle = k_B T$$
Using equipartition
$$\vdots \qquad \epsilon = k_B T m \gamma$$
Fluctuation \mathfrak{K} . Dissipation

Fluctuation \propto Dissipation

• Diffusion coefficient:

$$D \equiv \lim_{t \to \infty} \frac{x(t)^2}{2t} = \int_0^t \int_0^t \langle v(t_1)v(t_2) \rangle dt_1 dt_2$$
$$D = \frac{\epsilon}{(m\gamma)^2} = \frac{k_B T}{m\gamma} = \mu k_B T$$
$$\mu \equiv 1/(m\gamma) \qquad : \text{mobility}$$

FDT (Fluctuation Dissipation relation of 1st kind)

$$\mu = \frac{1}{k_BT} \int_0^\infty \langle v(0)v(t)\rangle dt$$

Integrating (2) gives

FDT (Fluctuation Dissipation relation of 2nd kind)

$$m\gamma = \frac{1}{2k_BT} \int_0^\infty \langle \xi(0)\xi(t)\rangle dt$$

Theories on Non-equilibrium Systems



Mesoscopic level

Macroscopic level

Stochastic Energetics

Underdamped Langevin equation:

External control parameter

$$\frac{d^{2}x}{dt^{2}} = -\frac{\partial U(x;a)}{\partial x} - \gamma \frac{dx}{dt} + \xi(t)$$
$$\left\langle \xi(t)\xi(t') \right\rangle = 2\gamma k_{B}T\delta(t-t')$$

by K. Sekimoto, JPSJ (1997)

See also, Ken Sekimoto, "Stochastic Energetics", Lecture Notes in Physics 799. (Springer)

Heat:
$$dQ \equiv \left(-\gamma \frac{dx}{dt} + \xi(t)\right) \circ dx =$$

Force exerted from heat bath x displacement

Then, 1 st Law of Thermodynamics holds for Langevin equations

$$d\left(\frac{p^2}{m} + U(x;a)\right) = dQ + \frac{\partial U}{\partial a} \circ da$$

$$dE = dQ + dW$$
$$E \equiv \frac{p^2}{m} + U(x;a)$$
$$dW \equiv \frac{\partial U}{\partial x} \circ da$$

How to derive

$$dQ = \left(\frac{dp}{dt} + \frac{\partial U}{\partial x}\right) \circ dx = \frac{dp}{dt} \circ \frac{p}{m} dt + dU - \frac{\partial U}{\partial x} \circ da$$
$$= d\left(\frac{p^2}{2m}\right) + dU - \frac{\partial U}{\partial x} \circ da$$
Separate conservative forces and non-conservative forces

$$d\left(\frac{p^2}{m} + U(x;a)\right) = dQ + \frac{\partial U}{\partial a} \circ da$$

$$dE = dQ + dW$$

$$E \equiv \frac{p^2}{m} + U(x;a)$$

1 st Law of Thermodynamics for Langevin Dynamics

$$dW \equiv \frac{\partial U}{\partial x} \circ da$$

Ito Integral and Stratonovich Integral in Stochastic Differential Equations

Wiener process:
$$B_t \int_0^t \xi(s) ds = \sqrt{2\gamma k_B T} [B_t - B_0]$$

Computing $\int f(s) dB_s$

Ito's definition

$$f(s) \cdot dB_s \equiv f(s) \left[B_{s+\Delta s} - B_s \right]$$

Stratonovich's defintion

$$f(s) \circ dB_s \equiv \frac{f(s + \Delta s) + f(s)}{2} \left[B_{s + \Delta s} - B_s \right]$$

Mesoscopic Nonequilibrium Systems

Some New Results

• Jarzynski Equality (1997)

(Relation connecting Equilibrium and Nonequilibrium)

 $W \ge \Delta F$: irreversible processes

$$\exp(-\beta\,\Delta F) = \overline{\exp(-\beta\,W)}$$

Ex.: Unfolding of RNA

• Fluctuation Theorem (1993-)

$$\frac{P(\sigma)}{P(-\sigma)} = e^{\sigma\tau}$$

 σ : entropy production rate

(Probability of negative entropy production, Proof of the second law in thermodynamics)

Harada-Sasa Equality (2005)

FDT violation = Irreversible Production of Heat

Ex: efficiency of molecular motors

Example: Small Particle Driven by External Forces

Langevin Simulation of Active Transport: ex. Brownian Ratchet





Langevin Equation (overdamped case)

$$0 = -\gamma \dot{x} - \frac{\partial U(x,t)}{\partial x} + f(t) + \hat{\xi}(t)$$

$$\left\langle \hat{\xi}(t) \right\rangle = 0, \quad \left\langle \hat{\xi}(t) \hat{\xi}(0) \right\rangle = 2\gamma k_{\rm B} T \delta(t)$$

Energy Dissipation

 Energy dissipation rate (energy flow from the Brownian particle to the environment) can be defined as

$$J(t)dt \equiv \left[\gamma \dot{x}(t) - \hat{\xi}(t)\right] \circ dx(t)$$
$$= \left[-\frac{\partial U(x,t)}{\partial x} + f(t)\right] \circ dx(t)$$

But difficult to measure.

according to Sekimoto(JPSJ, 1997).

Optical Trapping (LASER Tweezers)





Toyabe & Sano (2006)



Multi-beam Laser Trap





How to make Nonequilibrium State ?



Switching

Surfing



Swinging

Tool: Laser Tweezers and Colloid System

- It is possible to capture and manipulate small particles.
- Particles feel **harmonic potential** around the focal point of the LASER.





$$F_{opt} = k \Delta x = k(x_{opt}(t) - x(t))$$

$$J(t) = F_{opt}(t) v_{opt}(t)$$
$$\sigma_t = \frac{1}{k_B T} \int_0^t F_{opt}(t) v_{opt} dt$$

Fluctuation Theorem (steady state)





Negative Entropy Production

Measuring Energy Dissipation in Small Systems

Harada-Sasa's relation, P.R.L. (2005):

$$\langle J \rangle = \gamma \int_{-\infty}^{\infty} \left[\tilde{C}(\omega) - 2k_{\rm B}T\tilde{R}'(\omega) \right] \frac{d\omega}{2\pi}$$

Heat = Degree of Violation of FDT

Equilibrium State

$$D = \mu k_{\rm B} T$$

$$\longrightarrow \overline{C}(\omega) = 2k_B T \overline{R}(\omega)$$

Einstein's Relation (1905)

Correlation Function:

Response Function:

$$C(t) \equiv \langle \dot{x}(t) \dot{x}(0) \rangle$$

 $\langle \dot{x}(t) \rangle_{\epsilon} = \epsilon \int_{-\infty}^{t} R(t-s) f^{p}(s) ds + O(\epsilon^{2})$ $C(\tau) = \frac{1}{2\pi} \int C(\omega) e^{i\omega\tau} d\omega$

The Equality is generalized for more complex systems

- Time independent driving force with U(x)
- Flushing potential
- Periodically switching of potential : U(x,t+T)=U(x,t)
- Many particles (Colloidal suspension)

$$\gamma \dot{x}_i(t) = F_i(\Gamma(t)) + \xi_i(t) + \varepsilon f_i^{\rm p}(t),$$

$$F_{i}(\Gamma) = \sum_{\mu=1}^{N} f \delta_{i,3\mu-2} - \partial_{x_{i}} \sum_{\mu=1}^{N} U(\boldsymbol{r}_{\mu}) - \partial_{x_{i}} \sum_{\mu,\nu=1}^{N} U_{\mu\nu}^{\text{int}}(|\boldsymbol{r}_{\mu} - \boldsymbol{\bar{r}}_{\nu}|)/2$$
$$\langle \xi_{i}(t)\xi_{j}(s)\rangle_{0} = 2\gamma T \delta_{ij}\delta(t-s).$$
$$\langle J\rangle_{0} = \sum_{i=1}^{3N} \gamma \Big[\langle \dot{x}_{i} \rangle_{0}^{2} + \int_{-\infty}^{\infty} [\tilde{C}_{ii}(\omega) - 2T\tilde{R}_{ii}'(\omega)] \frac{d\omega}{2\pi} \Big],$$

How to make Nonequilibrium Steady State (NESS)?



(c)

Equilibrium Case

Check of FDT(Fluctuation Dissipation Theorem)

FDT

$$\tilde{C}(\omega) = 2k_{\mathsf{B}}T\tilde{R}'(\omega)$$



Shape of the potential



2,654,127 POINTS

Equilibrium State (Check of Fluctuation-Dissipation Theorem)



Non-Equilibrium Case

- Flushing: Switch LASER position between two positions temporally with a **poisson process**.
- Every 10ms, decide if switch or not randomly.



Measurement of Response Functions



Correlation Functions & Responses





Verification of Harada-Sasa Equality

LHS can be measured in this system



More general case (Memory effect)



Colloid in polymer solution: viscosity has
memory effect
$$\rightarrow$$
 generalized Langevin
eq.
 $\int_{-\infty}^{t} \gamma(t-s)\dot{x}(s)ds = F(x(t),t) + \xi(t)$
 $\widetilde{T}(\omega) = \widetilde{\Gamma}'(\omega) [\widetilde{C}(\omega) - 2kT\widetilde{R}'(\omega)]$

$$I(t) = \frac{\langle F(x(t),t) \circ v(0) \rangle_0 + \langle F(x(0),0) \circ v(t) \rangle_0}{2}$$

Ohkuma & T. Ohta (2006)

Narayan, Deutche PRE (2006)

Micro-Rheology

Measure viscosity from fluctuations





FDT:

$$\tilde{C}_{x}(\omega) \equiv \langle |\tilde{x}(\omega)|^{2} \rangle = \frac{2k_{\mathrm{B}}T\tilde{\alpha}''(\omega)}{\omega},$$

$$\tilde{x}(\omega) = \tilde{\alpha}(\omega)\tilde{f}(\omega).$$

$$\tilde{\alpha}'(\omega) = \frac{2}{\pi}P\int_{0}^{\infty}\frac{\zeta\tilde{\alpha}''(\zeta)}{\zeta^{2}-\omega^{2}}d\zeta$$

$$\tilde{G}(\omega) = \frac{1}{6\pi a\alpha(\omega)},$$

$$\int_{0}^{10} \int_{0}^{10} \int_{0}^{0} \int_{0$$

 ω [rad/s]






Simplified proof !! $J(t)dt = (\gamma v(t) - \xi(t)) \circ dx(t)$ $J(t) = \gamma v(t)^2 - \xi(t) \circ v(t)$ $\langle v(t)^2 \rangle = v_s^2 + \langle (v(t) - v_s)^2 \rangle_0$ 1st term: $= v_s^2 + \int_{-\infty}^{\infty} C(\omega) \frac{d\omega}{2\pi}$ $v(t) = \int_{-\infty}^{t} R(t-s)\xi(s)ds$ response: $V(\omega) = \int_{-\infty}^{\infty} R(\omega) \Sigma(\omega) e^{i\omega t} \frac{d\omega}{2}$ $\langle \xi(t)v(t) \rangle = \int_{-\infty}^{\infty} \xi(t)dt \int_{-\infty}^{\infty} R(\omega)\Xi(\omega)e^{i\omega t}\frac{d\omega}{2\pi}$ 2nd term: $= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} R(\omega) \Xi(\omega) \int_{-\infty}^{\infty} \xi(t) e^{i\omega t} dt$ $= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} R(\omega) \Xi(\omega) \Xi^{*}(\omega)$ $= \int_{-\infty}^{\infty} 2k_B T \gamma R(\omega) \frac{d\omega}{2\pi}$

Molecular Rotary Motor > F₁-ATPase



S. Toyabe et al. Phys. Rev. Lett. 104, 198103 (2010)

Results > Violation of FDT



S. Toyabe et al. Phys. Rev. Lett. 104, 198103 (2010)

Results > Harada-Sasa equality



$$ilde{C}(f o\infty) orac{2\gamma}{T}$$

Results > Heat Dissipation



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From Brownian to Driven and Active Dynamics of Colloids: Energetics and Fluctuations Part II

Masaki Sano* Shoichi Toyabe¹ Hong-ren Jiang² Ryo Suzuki^{*3} *The University of Tokyo ¹Ludwig Maximilians University Munich ²National Taiwan University ³Techinical University of Munich

Outline of Part I

- Stochastic Thermodynamics was introduced
- Degree of the violation FDT relation is equal to heat flux to the environment in Langevin systems. Such small heat flux can be experimentally evaluated by using a new theory.

Jarzynski Equality

Importance of fluctuations

2 nd law of thermodynamics and FDT can be derived from JE





New Theories in Statistical Mechanics



Initial conditions producing positive entropy production is much more frequent than the negative entropy production

Confirmed for driven Brownian particles, electric current, etc.



Fluctuation Theorem

Jarzynski equality

- $W\,$:Work performed to the system
- F :Free energy gain of the system

2nd law of thermodynamics:

$$e^{-(W-\Delta F)/k_{BT}} = 1$$
$$e^{-x} \ge 1-x$$

$$\langle W \rangle - \Delta F \ge 0$$

Generalized Jarzynski equality including information

 $\langle W \rangle \geq \Delta F - kT \langle I \rangle$

Correspondingly generalized Jarzynski equality:

I : mutual information measurement and control have errors



Maxwell's demon

Violation of the second law of thermodynamics

(1871)





James Clerk Maxwell (1831-1879)

Opening & closing door do not perform work to atoms.

- ⇒ 2nd law really violate?
- ⇒ controversial state lasted more than 150 years.

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The simplest and analyzable Maxwell's demon



Schematic illustration of the experiment



Toyabe, Sagawa, Ueda, Muneyuki, Sano, Nature Physics, 6, 988, (2010))

Experimental Setup

- > Dimeric polystyrene particle (300nm) is linked on the substrate with a biotin.
- Particles exhibit a rotational Brownian motion.



1 µm (1/1000 mm)

How to produce a spiral-stair-like potential



Estimating a potential function from the data



Feedback control based on information contents



Trajectories under feedback control



Calculation of Free Energy



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Φ

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Efficiency of Information-Energy Conversion

Information gained by the observation:

$$I = -p \ln p - (1-p) \ln((1-p))$$



Efficiency of Information-Energy Conversion :

$$\vartheta = \frac{\Delta F - W}{k_B T I}$$





Experimental test of generalized Jarzynski equality



Feedback Efficacy

• A fundamental principle to relate energy and information feedback



How to measure the feedback efficacy



 $\gamma = p_{sw} + p_{ns} \le 1$

Consistency with 2nd Law



- 2nd law holds for the total system.
- Information-energy conversion is realized when we look at the small system.

Self-propelled dynamics of Janus particle

- By a local temperature gradient: Self-Thermophoresis
- By electric field:

Induced Charge Electro-Osmosis (ICEO)

Self-propulsion of Janus particle I : Temperature field



Rotation of Chiral Doublet: Thermophoresis



HR Jiang, Yoshinaga, Sano, PRL (2010)



Induced flow visualized by tracer particles around the fixed Janus particle

Temperature distribution :

$$T(R) = T_{\infty} + \sum_{n=1}^{\infty} \frac{q_n R}{(n+1)\kappa_o + n\kappa_i} P_n(\cos\theta).$$
$$q(\theta) = \kappa \mathbf{e}_n \cdot \nabla T$$
$$\Delta T = 3\epsilon IR/2(2\kappa_o + \kappa_i)$$

Temperature distribution around a Janus Particle



Seed of self-thermophoresis of Janus particle is related to the response to the external gradient

$$V = -\frac{1}{4}D(S_T^0 + S_T^G)\frac{\epsilon I}{2\kappa_o + \kappa_i}.$$

Self-thermophoresis



Viewpoint in Physics, PRL (2010)

Light is absorbed on the metal side:

$$-\kappa_o \mathbf{n} \cdot \nabla T_o + \kappa_i \mathbf{n} \cdot \nabla T_i = q(\theta).$$
$$T(R) = T_0 + \sum_{n=0}^{\infty} \frac{q_n R}{(n+1)\kappa_o + n\kappa_i} P_n(\cos\theta)$$

Theoretical calculation by N. Yoshinaga

Effective slip velocity: $m{v}_s=v_sm{e}_ heta=\mu|
abla T|_sm{e}_ heta$ $\mu=-(k_B/\eta)\Gamma\lambda$

Characteristic length: $\lambda = \Gamma^{-1} \int c_0 y (e^{-\beta U_0} - 1) dy$ U_0 : Interaction potential between the surface and fluid

$$\Gamma = \int c_0 (e^{-\beta U_0} - 1) dy \qquad V = -\frac{1}{2} \int_0^\pi v_s \sin^2 \theta d\theta.$$



Migration in an uniform external temperature gradient

$$\begin{split} V &= -\mu T_1 = -DS_T T_1 \quad T_1 \text{ : Temperature diff.} \\ \mu &= DS_T \quad \text{across the particle} \\ V &= -\frac{1}{4} D(S_T^0 + S_T^G) \frac{\epsilon I}{2\kappa_o + \kappa_i}. \end{split}$$

Migration speed is determined by the average of Soret coeff.

Stochastic Dynamics of Active particle

Langevin equation:

Fokker-Planck equation:

$$\gamma \boldsymbol{v} = -\frac{\partial U}{\partial \boldsymbol{r}} + \beta \boldsymbol{n} + \boldsymbol{\xi}(t)$$



 $\frac{\partial P(\mathbf{r}, \mathbf{n})}{\partial t} = -\frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{v}P) - \mathcal{R} \cdot (\omega P)$ $\mathbf{v} = -D\frac{\partial}{\partial \mathbf{r}} (k_B T \ln P + U) + \alpha \mathbf{n}.$

$$\mathbf{R} = \mathbf{n} \times \frac{\partial}{\partial \mathbf{n}}$$

$$\label{eq:weight} \boldsymbol{\omega} = \frac{1}{\zeta_r} \mathbf{N} = -\frac{1}{\zeta_r} \mathcal{R}(k_B T \ln P + U),$$

 $\frac{\partial P(\mathbf{r},\mathbf{n},t)}{\partial t} = \frac{\partial}{\partial \mathbf{r}} \cdot D\left(\frac{\partial P}{\partial \mathbf{r}} + \frac{P}{k_B T}\frac{\partial U}{\partial \mathbf{r}}\right) - \alpha \frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{n}P) + D_r \mathcal{R} \cdot \left(\mathcal{R}P + \frac{P}{k_B T}\mathcal{R}U\right).$

$$D = \frac{k_B T}{6\pi\eta a} \qquad D_r = \frac{k_B T}{8\pi\eta a^3}$$

$$U = \frac{1}{2}kr^2 \qquad \mathcal{R}U = 0.$$

Correlation function of the polarity direction:

$$<\mathbf{n}(t)\cdot\mathbf{n}(0)>=\int d\mathbf{n}d\mathbf{n}'d\mathbf{r}d\mathbf{r}'\left[\mathbf{n}\cdot\mathbf{n}'G(\mathbf{n},\mathbf{n}',t)P_{eq}(\mathbf{r}',\mathbf{n}')\right]$$

Equilibrium distributionc

$$P_{\rm eq}(\mathbf{r}, \mathbf{n}) = \frac{1}{4\pi} \left(\frac{k}{2\pi k_B T} \right)^{-3/2} e^{-\frac{k\mathbf{r}^2}{2k_B T}}.$$

Rotational Diffusion:

$$\langle \mathbf{n}(t) \cdot \mathbf{n}(0) \rangle = \exp(-2D_r t).$$

$$\frac{\partial}{\partial t} < (\mathbf{r}(t) - \mathbf{r}(0))^2 > = \int d\mathbf{r} d\mathbf{n}' d\mathbf{r} d\mathbf{r}' \left[(\mathbf{r} - \mathbf{r}')^2 \frac{\partial G}{\partial t} P_{eq} \right].$$

MSD of active particle:

$$|\nabla \hat{\mathbf{r}}_{\text{active particle:}}| < (\mathbf{r}(t) - \mathbf{r}(0))^2 > = \frac{6k_BT}{k} + \frac{2\alpha^2}{\tilde{D}}e^{-2D_rt} - \left(\frac{2\alpha^2}{\tilde{D}}t + \frac{6k_BT}{k} + \frac{2\alpha^2}{\tilde{D}}\right)e^{-Dkt/(k_BT)},$$
$$\tilde{D} = \frac{-2D_rk_BT + Dk}{\tilde{D}}$$

2.5

Without potential:

for k = 0

$$D = \frac{1}{k_B T}$$

$$< (\mathbf{r}(t) - \mathbf{r}(0))^2 >= 6Dt + \frac{\alpha^2}{2D_r^2} \left(e^{-2D_r t} + 2D_r t - 1 \right),$$



Motion of Janus Particle: Top View



How do they move?

1) Surface charges are induced by the AC electric field \dot{E}

- 2) Counter-ions gathers around the induced charges.
- 3) Flow of fluid containing counter-ions is induced by $ec{E}$



Self-propulsion of Janus particle II : Electric field





Ε



b



Formation of Chains at frequency higher than fc







Doublet



Triplet



Linear Chain fixed front particle



Oscillation, Wave






Role of Thermal fluctuation

- How does the driving force corr fluctuations?
- Use of Eluctuation Theorem $\ln[P(\Delta\theta)/P(-\Delta\theta)] = \tau \Delta\theta/k_{B}T$

Precise determination of torque is possible

R. Suzuki, HR Jiang, M. Sano, Archive







Deformable self-propelled chain



Waving motion

Spiraling motion



Induced Polarization: $P_{eff} = 4\pi a^3 \epsilon_2 Re[K(\omega) Ee^{i\omega t}]$

 $\epsilon_1 - \epsilon_2$

Electric charging time



Chemotaxis of Bacteria





http://www.sciencemag.org/content/334/6053/238.abstrac

Information and Feedback in Different Systems

	Fluctuation	Information	Feedback	Outcome
Maxwell's demon	Thermal	Speed, position	Biased Choice of fluctuations	Gain Free Energy
Active Particle	Thermal			Enhanced Diffusion
Bacteria (<u>Escherichia coli</u>)	tumbling	Chemotactic Signal	Change tumbling freq.	Chemotaxis
Amoeboid cell (<i>Dictyostelium</i> <i>Discoideum</i>)	Instability of cell shape	Chemotactic Signal	Biased Choice of random protrusion	Chemotaxis

Summary

- Information thermodynamics can be tested and demonstrated in colloidal systems.
- Different kinds of phoresis can be used to create self-propelled particles and control interaction of particles.

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- Information Feedback Control and Generalized Jarzynski Equality
- Introduction to Active particle, Active Matter

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$$T(R) = T_0 + \sum_{n=0}^{\infty} \frac{q_n R}{(n+1)\kappa_o + n\kappa_i} P_n(\cos\theta)$$

Theoretical calculation by N. Yoshinaga

Effective slip velocity: $m{v}_s=v_sm{e}_ heta=\mu|
abla T|_sm{e}_ heta$ $\mu=-(k_B/\eta)\Gamma\lambda$

Characteristic length: $\lambda = \Gamma^{-1} \int c_0 y (e^{-\beta U_0} - 1) dy$ U_0 : Interaction potential between the surface and fluid

$$\Gamma = \int c_0 (e^{-\beta U_0} - 1) dy \qquad V = -\frac{1}{2} \int_0^\pi v_s \sin^2 \theta d\theta.$$



Migration in an uniform external temperature gradient

$$\begin{split} V &= -\mu T_1 = -DS_T T_1 \quad T_1 \text{ : Temperature diff.} \\ \mu &= DS_T \quad \text{across the particle} \\ V &= -\frac{1}{4} D(S_T^0 + S_T^G) \frac{\epsilon I}{2\kappa_o + \kappa_i}. \end{split}$$

Migration speed is determined by the average of Soret coeff.

Stochastic Dynamics of Active particle

Langevin equation:

Fokker-Planck equation:

$$\gamma \boldsymbol{v} = -\frac{\partial U}{\partial \boldsymbol{r}} + \beta \boldsymbol{n} + \boldsymbol{\xi}(t)$$



 $\frac{\partial P(\mathbf{r}, \mathbf{n})}{\partial t} = -\frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{v}P) - \mathcal{R} \cdot (\omega P)$ $\mathbf{v} = -D\frac{\partial}{\partial \mathbf{r}} (k_B T \ln P + U) + \alpha \mathbf{n}.$

$$\mathbf{R} = \mathbf{n} \times \frac{\partial}{\partial \mathbf{n}}$$

$$\label{eq:weight} \boldsymbol{\omega} = \frac{1}{\zeta_r} \mathbf{N} = -\frac{1}{\zeta_r} \mathcal{R}(k_B T \ln P + U),$$

 $\frac{\partial P(\mathbf{r},\mathbf{n},t)}{\partial t} = \frac{\partial}{\partial \mathbf{r}} \cdot D\left(\frac{\partial P}{\partial \mathbf{r}} + \frac{P}{k_B T}\frac{\partial U}{\partial \mathbf{r}}\right) - \alpha \frac{\partial}{\partial \mathbf{r}} \cdot (\mathbf{n}P) + D_r \mathcal{R} \cdot \left(\mathcal{R}P + \frac{P}{k_B T}\mathcal{R}U\right).$

$$D = \frac{k_B T}{6\pi\eta a} \qquad D_r = \frac{k_B T}{8\pi\eta a^3}$$

$$U = \frac{1}{2}kr^2 \qquad \mathcal{R}U = 0.$$

Correlation function of the polarity direction:

$$<\mathbf{n}(t)\cdot\mathbf{n}(0)>=\int d\mathbf{n}d\mathbf{n}'d\mathbf{r}d\mathbf{r}'\left[\mathbf{n}\cdot\mathbf{n}'G(\mathbf{n},\mathbf{n}',t)P_{eq}(\mathbf{r}',\mathbf{n}')\right]$$

Equilibrium distributionc

$$P_{\rm eq}(\mathbf{r}, \mathbf{n}) = \frac{1}{4\pi} \left(\frac{k}{2\pi k_B T}\right)^{-3/2} e^{-\frac{k\mathbf{r}^2}{2k_B T}}.$$

Rotational Diffusion:

$$\langle \mathbf{n}(t) \cdot \mathbf{n}(0) \rangle = \exp(-2D_r t).$$

$$\frac{\partial}{\partial t} < (\mathbf{r}(t) - \mathbf{r}(0))^2 > = \int d\mathbf{r} d\mathbf{n}' d\mathbf{r} d\mathbf{r}' \left[(\mathbf{r} - \mathbf{r}')^2 \frac{\partial G}{\partial t} P_{eq} \right].$$

MSD of active particle:

$$|\nabla \hat{\mathbf{r}}_{l}(\mathbf{r}(t) - \mathbf{r}(0))^{2} \rangle = \frac{6k_{B}T}{k} + \frac{2\alpha^{2}}{\tilde{D}}e^{-2D_{r}t} - \left(\frac{2\alpha^{2}}{\tilde{D}}t + \frac{6k_{B}T}{k} + \frac{2\alpha^{2}}{\tilde{D}}\right)e^{-Dkt/(k_{B}T)},$$

$$\tilde{D} = \frac{-2D_{r}k_{B}T + Dk}{\tilde{D}}$$

2.5

Without potential:

for k = 0

$$D = \frac{1}{k_B T}$$

$$< (\mathbf{r}(t) - \mathbf{r}(0))^2 >= 6Dt + \frac{\alpha^2}{2D_r^2} \left(e^{-2D_r t} + 2D_r t - 1 \right),$$



Motion of Janus Particle: Top View



How do they move?

1) Surface charges are induced by the AC electric field \dot{E}

- 2) Counter-ions gathers around the induced charges.
- 3) Flow of fluid containing counter-ions is induced by $ec{E}$



Self-propulsion of Janus particle II : Electric field





Ε



b



Formation of Chains at frequency higher than fc






Doublet



Triplet



Linear Chain fixed front particle



Oscillation, Wave







Role of Thermal fluctuation

- How does the driving force corr fluctuations?
- Use of Eluctuation Theorem $\ln[P(\Delta\theta)/P(-\Delta\theta)] = \tau \Delta\theta/k_{B}T$

Precise determination of torque is possible

R. Suzuki, HR Jiang, M. Sano, Archive







Deformable self-propelled chain



Waving motion

Spiraling motion



Induced Polarization: $P_{eff} = 4\pi a^3 \epsilon_2 Re[K(\omega) Ee^{i\omega t}]$

 $\epsilon_1 - \epsilon_2$

Electric charging time



Collective motion of self-propelled string



Chemotaxis of Bacteria





http://www.sciencemag.org/content/334/6053/238.abstrac

Information and Feedback in Different Systems

	Fluctuation	Information	Feedback	Outcome
Maxwell's demon	Thermal	Speed, position	Biased Choice of fluctuations	Gain Free Energy
Active Particle	Thermal			Enhanced Diffusion
Bacteria (<u>Escherichia coli</u>)	tumbling	Chemotactic Signal	Change tumbling freq.	Chemotaxis
Amoeboid cell (<i>Dictyostelium</i> <i>Discoideum</i>)	Instability of cell shape	Chemotactic Signal	Biased Choice of random protrusion	Chemotaxis

Summary of Part II

- Information thermodynamics can be tested and demonstrated in colloidal systems.
- Different kinds of phoresis can be used to create self-propelled particles and control interaction of particles.