# entropy production & linear response in active Brownian particles

*Debasish Chaudhuri*
*Institute of Physics, Bhubaneswar*

ICTS - 2017

# thermodynamics 01

- describes macroscopic system in thermal equilibrium
- Laws of thermodynamics : first & second law

- first law : energy conservation
- 2nd law : *Clausius relation*

spontaneous process → total entropy increases

$$\delta S \geq \delta Q/T$$

$$\delta S_t = \delta S + \delta S_r \geq 0, \quad \delta S_r = -\delta Q/T$$

# thermodynamics 02

- linear response & fluctuation-dissipation theorem :

$$R_A(t_2 - t_1) = \beta \frac{\partial}{\partial t_1} \langle A(t_2)[-\partial_h H(t_1)]_{h=0} \rangle_{eq}$$

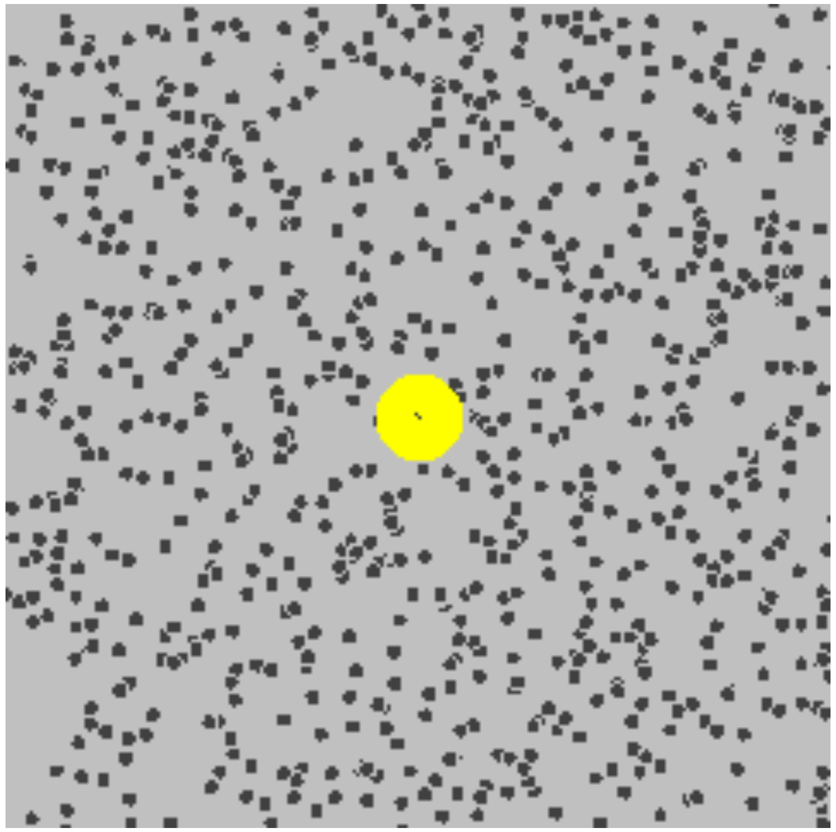
- Einstein relation : $R_v(\tau) = \beta \langle v(\tau) v(0) \rangle_{eq}$

→ mobility $\mu = \int d\tau R_v(\tau) = \beta D$

stochastic thermodynamic description for active Brownian particles?

# Brownian motion

- large particle in a bath of small particles
- time and length scale separation



# Brownian motion

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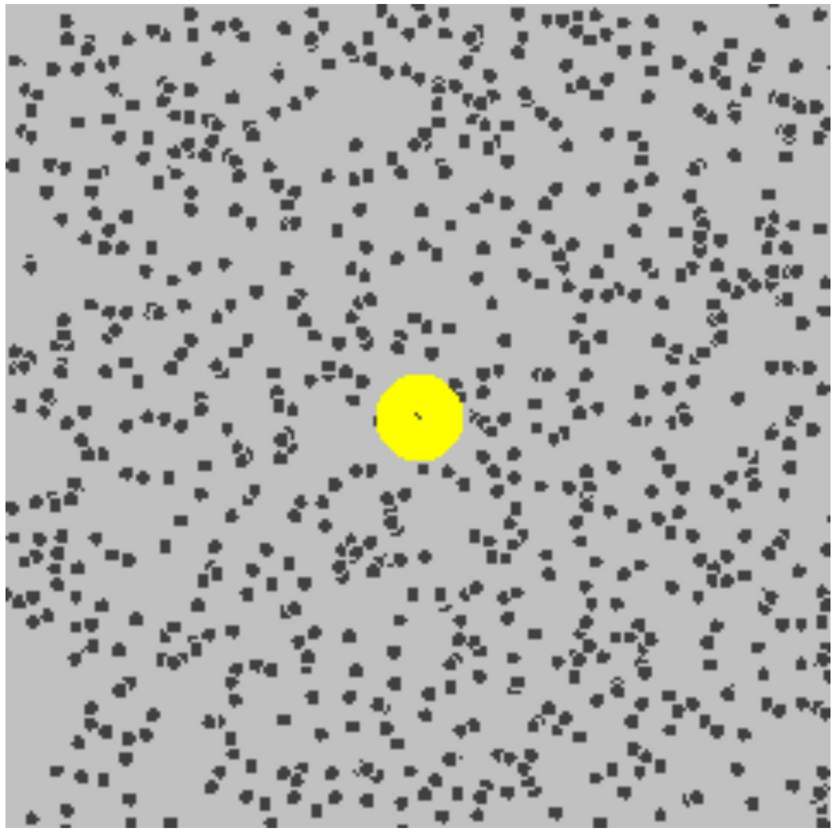


$$\dot{x} = v$$

$$\dot{v} = -\gamma v + \eta(t)$$

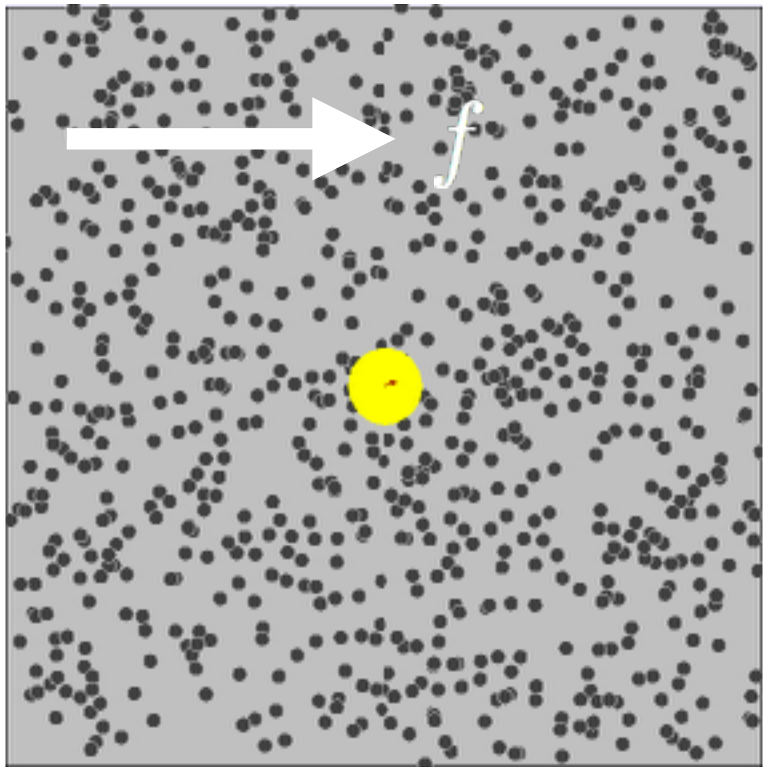
$$\langle \eta(t)\eta(0)\rangle = 2D_0\delta(t) \;, \quad D_0 = \gamma k_B T$$

stochastic energy conservation

$$d(v^2/2)/dt = v \cdot (-\gamma v + \eta(t)) \equiv \dot{q}$$

# drive : entropy production

- directed drive
- breaking of time reversal symmetry
- entropy production




Langevin equation $\dot{v} = -\gamma v + \eta(t) + f$

stochastic energy conservation $d(v^2/2)/dt = \dot{q} + \dot{W}$

rate of work done $\dot{W} = f \cdot v$

# entropy from Fokker-Planck equation

$$\partial_t P(x,v,t) = -\nabla \cdot (\mathbf{j_r} + \mathbf{j_r}) \;, \quad \nabla \equiv (\partial_x, \partial_v)$$

$$\mathbf{j}_r = \{vP, fP\}, \quad \mathbf{j}_d = \{0, -\gamma v P - D_0 \partial_v P\}$$

entropy production $S = -k_B \int P \ln P d\Gamma \;\Rightarrow\; \dot{S} = k_B \int d\Gamma \ln P \, \nabla \cdot (\mathbf{j}_r + \mathbf{j}_d)$

$$\int d\Gamma \ln P \, \nabla \cdot \mathbf{j}_r = \left\langle \nabla \cdot \left( \frac{\mathbf{j}_r}{P} \right) \right\rangle \qquad \int d\Gamma \ln P \, \nabla \cdot \mathbf{j}_d = \int d\Gamma \left( \frac{(j_d^v)^2}{P D_0} + \frac{\gamma v j_d^v}{D_0} \right)$$

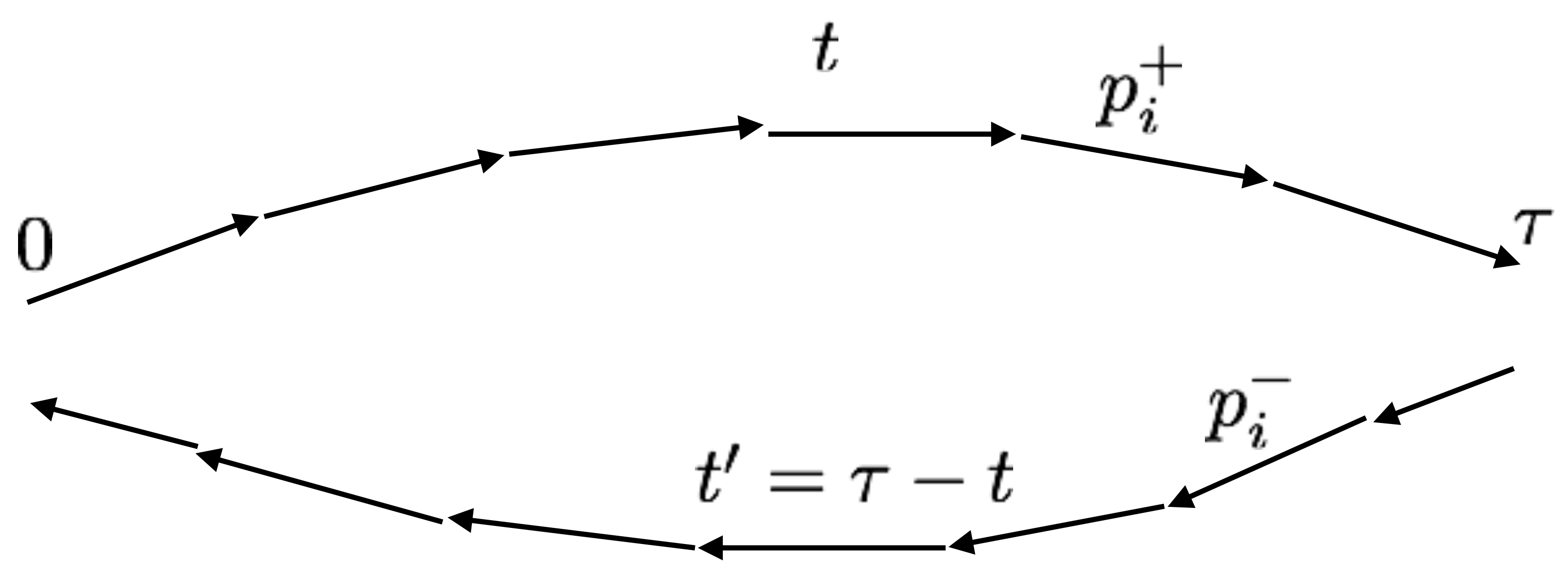
using current components $\dot{S} + \dot{S}_r = \int d\Gamma (j_d^v)^2 / P D_0 \geq 0$

where, $\dot{S}_r = -\int d\Gamma \, \gamma v j_d^v / D_0 = -\langle \dot{q} \rangle / k_B T$

$\langle \dot{q} \rangle$ averaging over trajectory and distribution

U. Seifert, *Phys Rev Lett.* (2005)

# entropy from path probability




forward and reverse protocols

$$X^{\dagger} = [x'(t'), v'(t'), f'(t')] = [x(\tau_0 - t), -v(\tau_0 - t), f(\tau_0 - t)]$$

$$p_i^+ = J_{\eta_i, v_i} \int d\eta_i \, P(\eta_i) \delta(\dot{x}_i - v_i) \delta(\dot{v}_i - \mathcal{F}_i)$$ and $$P(\eta_i) = (\delta t / 4\pi D_0)^{1/2} \exp(-\delta t \, \eta_i^2 / 4 D_0).$$

ratio of forward and reverse path probabilities on i-th segment

$$\ln(p_i^+ / p_i^-) = -\beta \delta t [\dot{q}]_i$$

ratio of forward and reverse path probabilities over time $\tau$

$$\ln(\mathcal{P}_f / \mathcal{P}_r) = -\beta \int^{\tau} dt \dot{q}$$

# entropy from path probability - 2

stochastic entropy of initial and final states

$$s_0 = -k_B \ln p_0, \quad s_\tau = -k_B \ln p_\tau$$

breaking of time reversal symmetry,

$$\Delta s_t = k_B \ln[p_0 \mathcal{P}_f / p_\tau \mathcal{P}_r] = \Delta s + \Delta s_r$$

where,

$$\Delta s = s_\tau - s_0, \quad \Delta s_r = \int^\tau dt \; \dot{q}/T$$

*Clausius form*

leading to detailed fluctuation theorem (Crook’s)

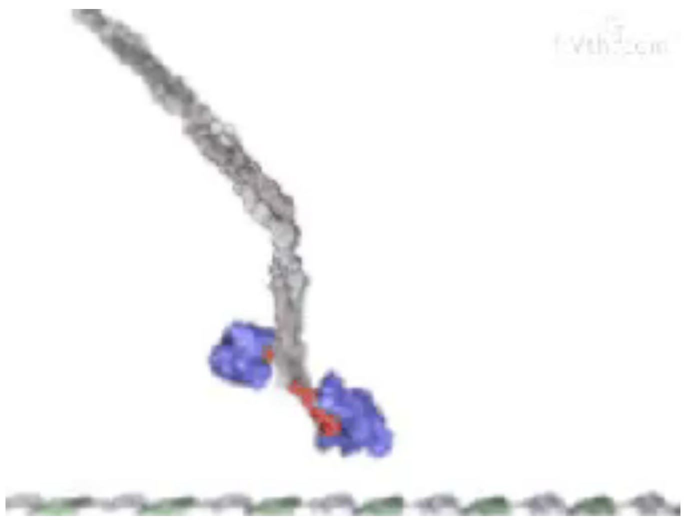
$$\frac{\rho_F(\Delta s_t)}{\rho_R(-\Delta s_t)} = e^{\Delta s_t / k_B}$$

and integral fluctuation theorem

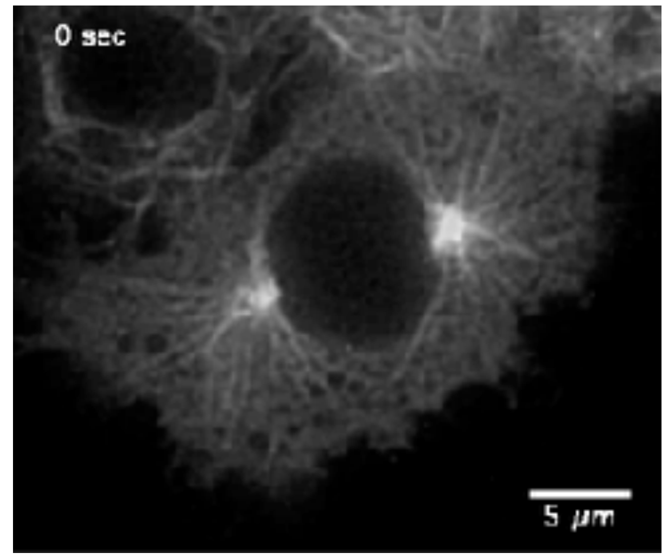
$$\langle e^{-\Delta s_t / k_B} \rangle = 1$$

related to Jarzynsky equality

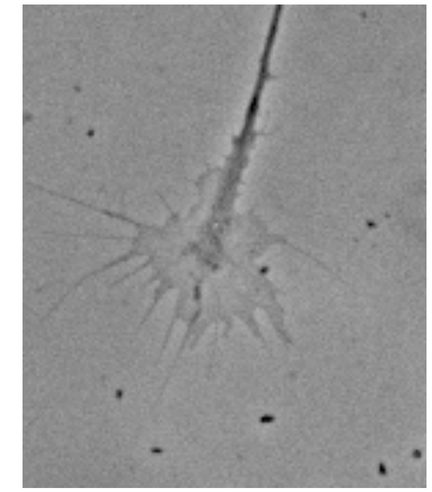
# active Brownian motion



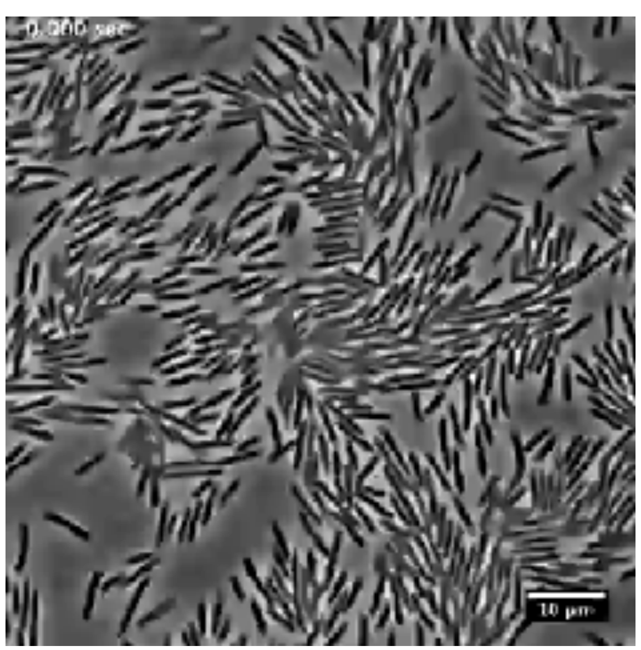
motor proteins



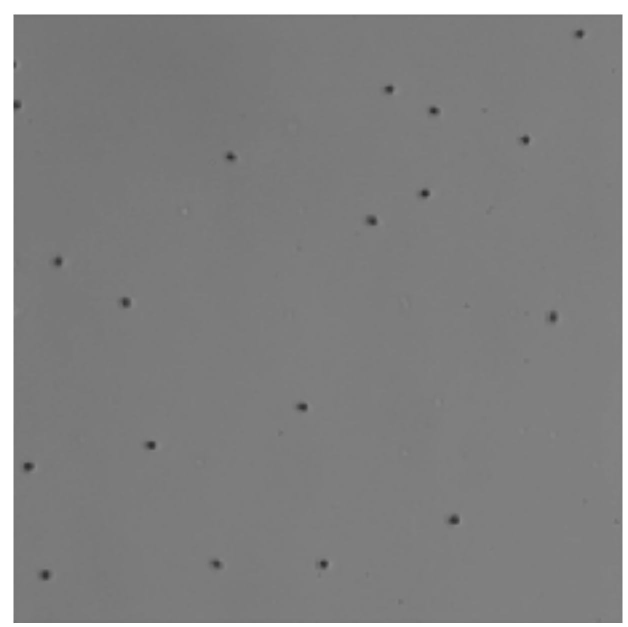

cell division : tubulin



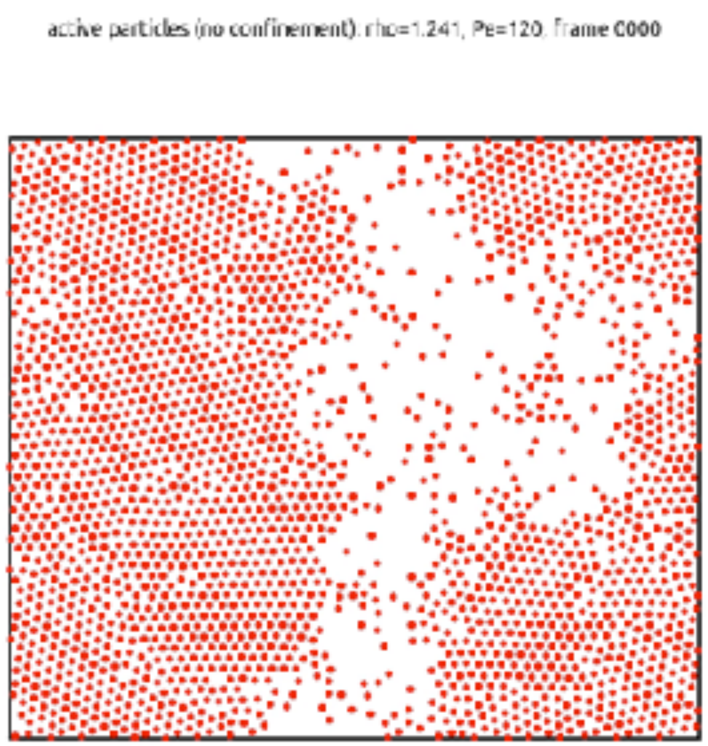
neural growth cone




E coli swarm



active colloids



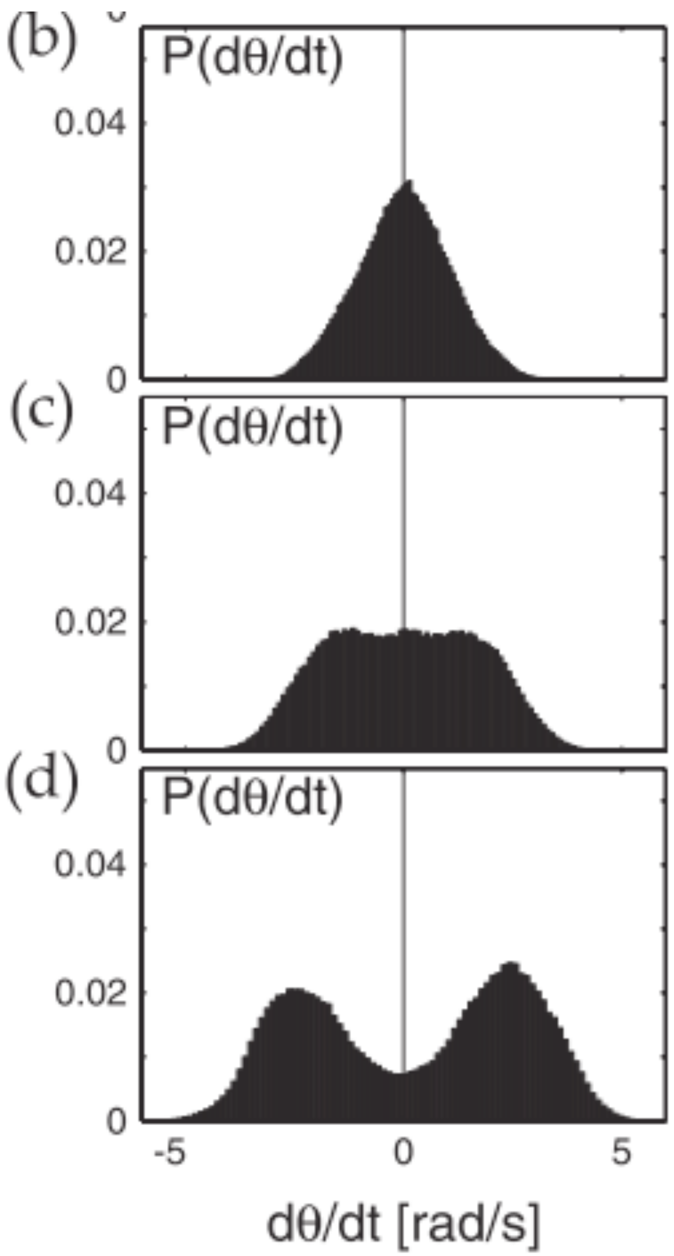

simulations

# outline

- models : active force $F(v)$, Rayleigh-Helmholtz, energy depot
- Langevin equation → fluctuation theorem,
  modified fluctuation-dissipation relation
- simulation results

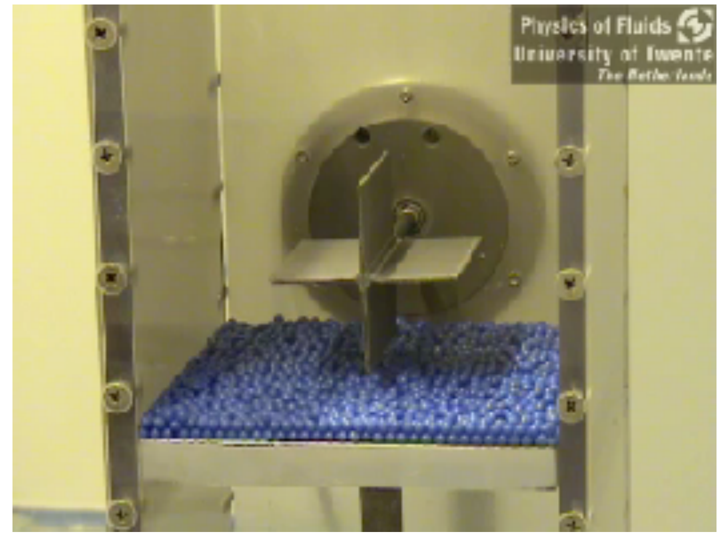
- *Chandrima Ganguly, DC, Phys. Rev. E (2013)*
- *DC, Phys. Rev. E (2014)*
- *DC, Phys. Rev. E (2016)*

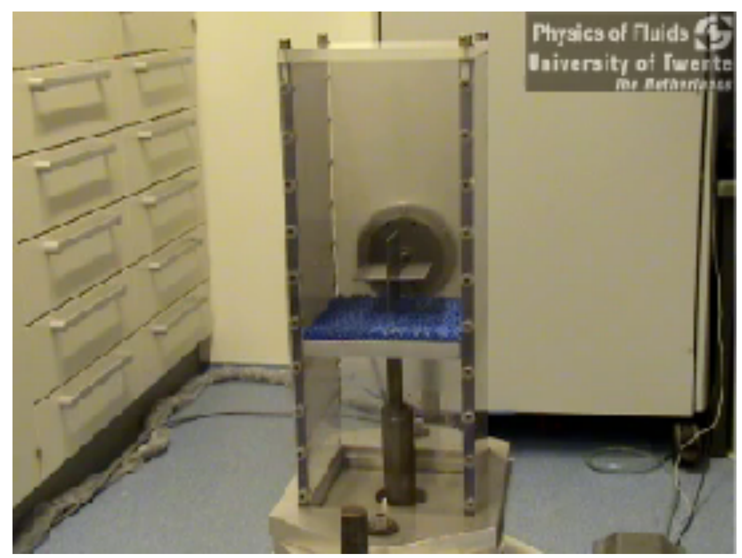
# example: granular ratchet



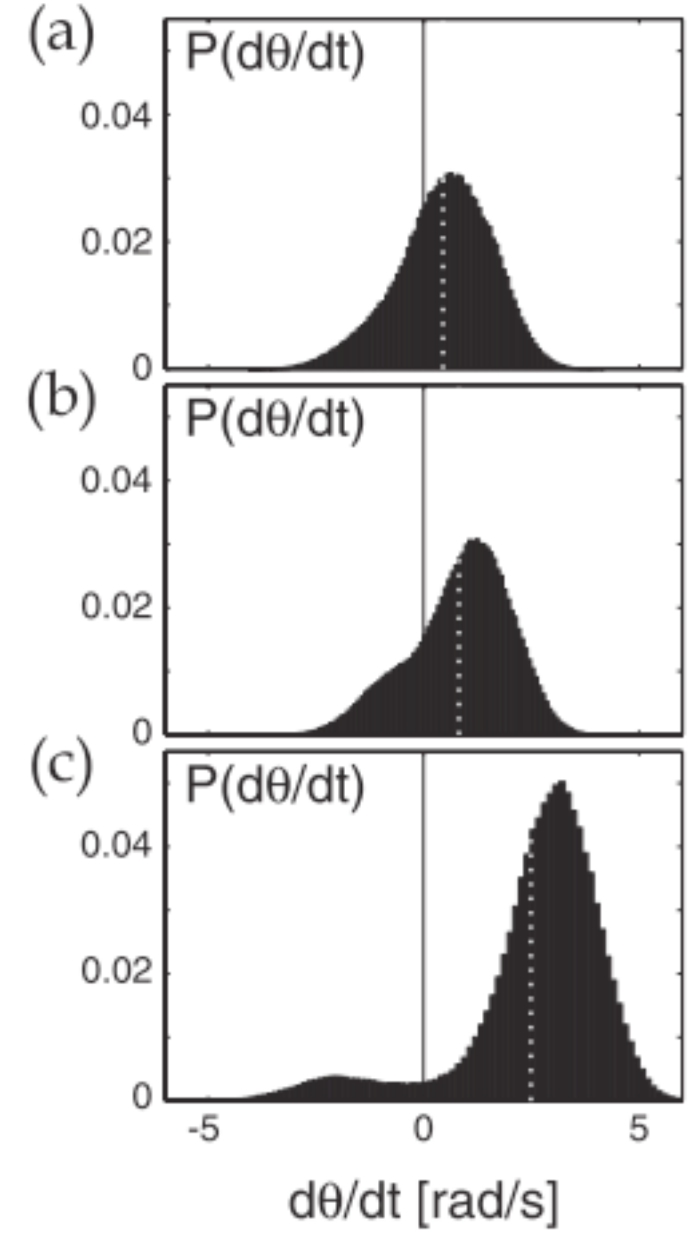

symmetric

even




Devraj van der Meer, PRL (2010)
(Uni Twente)

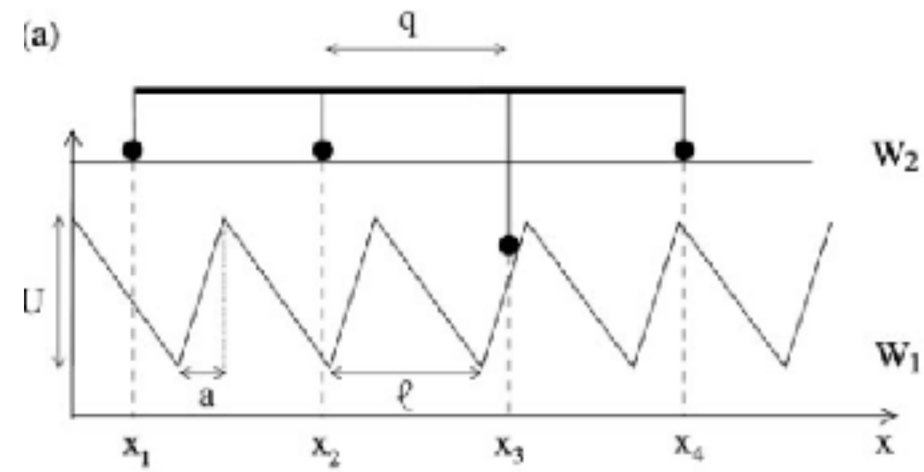


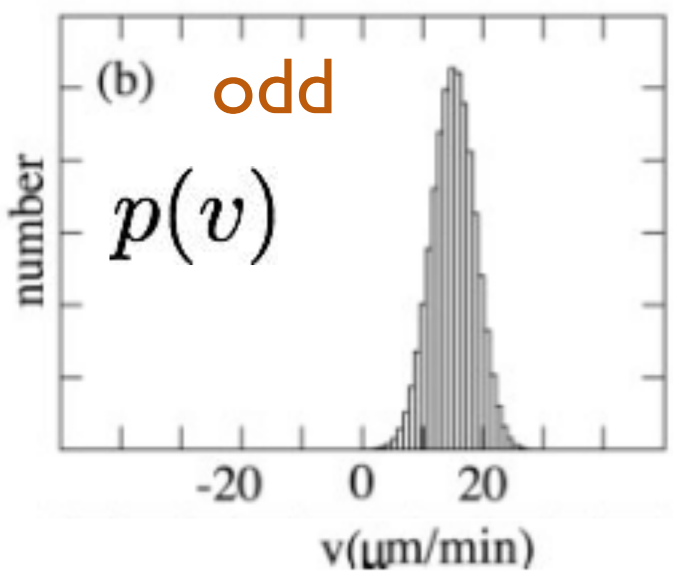

asymmetric

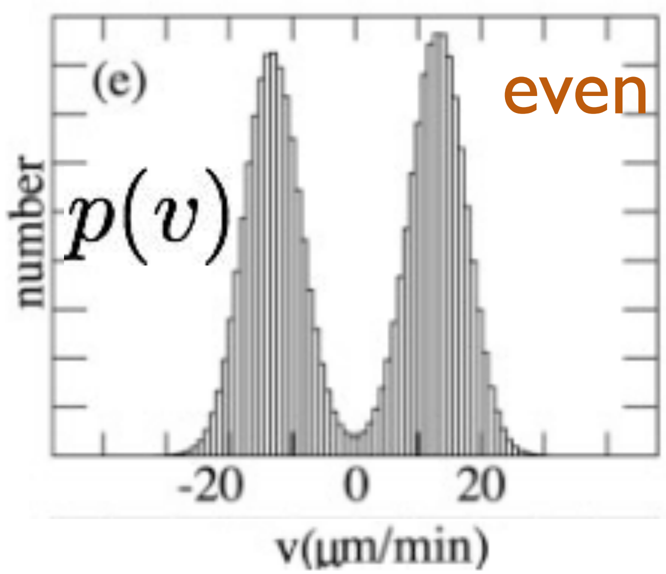
odd

# microtubule: bidirectional motion

- directed motors : kinesin,  ncd
- undirected motors :  nk11




asymmetric ratchet
kinesin, ncd

symmetric ratchet     nk11
bimodal distribution of velocity

Badoual,  Jülicher, Prost,  pnas 2002
(*mpi-pks, dresden + inst. Curie, paris*)

# ... Rayleigh-Helmholtz

bimodal velocity distribution : $p(v) \sim \exp(-\phi(v))$

$$\phi(v) = -\frac{a}{2}v^2 + \frac{b}{4}v^4$$ even

effective velocity dependent force :

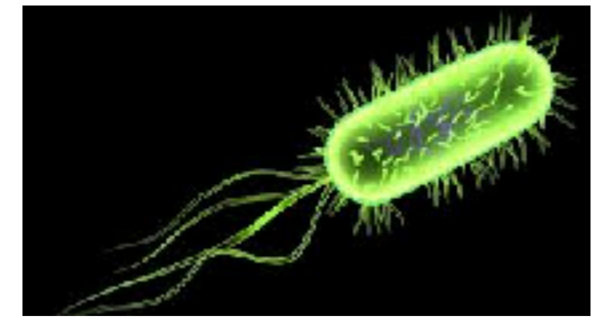
$$F(v) = -\phi'(v) = av - bv^3$$

$$\dot{v} = -\gamma v + \eta(t) + F(v)$$ Rayleigh-Helmholtz model

Lutz Schimansky-Geier
(Humboldt uni, berlin)

# energy depot model

## bacterial motility



- nutrient intake, metabolism, and motion

$$\frac{de(t)}{dt} = q(\mathbf{r}) - ce(t) - h(\mathbf{v})e(t)$$

- simple ansatz $q(\mathbf{r}) = q_0,\ h(\mathbf{v}) = d_2\, v^2$
- power to mechanical d.o.f. $F(v).v = e(t)\, d_2\, v^2$
- force $F(v) = e(t)\, d_2\, v$ steady state : $e_0 = \dfrac{q_0}{c + d_2\, v^2}$
- use $F(v) = \dfrac{q_0 d_2\, v}{c + d_2 v^2}$ in equation of motion

Frank Schweitzer (eth zurich),
*prl*(1998), *epjb* (2011)

# stochastic thermodynamics

Langevin dynamics + self propulsion $F(v)$

$$\dot{x} = v$$
$$m\dot{v} = -\gamma v + \eta + F(v) - \frac{\partial U(x)}{\partial x} + f(t)$$

$\int dt v. \quad \Rightarrow$

$$\delta E = \delta W + \delta q$$

energy conservation

$E = \frac{1}{2} m v^2 + U(x)$

$\delta W = f.\delta x$ work on system

$$\delta q = \delta Q + \delta Q_m$$

$\delta Q = \int dt v.(-\gamma v + \eta)$

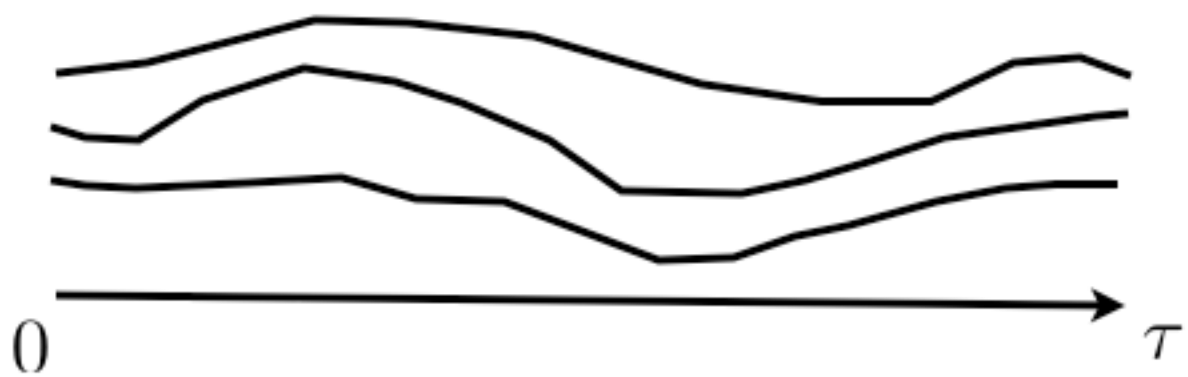
energy from reservoir

$\delta Q_m = \int dt v.F(v)$

energy from self propulsion force

$\delta s_r \neq -\delta q/T$ *Clausius form ?*

# fluctuation theorem -1




- evolution through path $\quad X = \{x(t), v(t), f(t)\}$
- probability of path

$$P_+ \propto \exp\left[-\frac{1}{4D_0}\int_0^\tau dt \left(m\dot{v} - g(v) + \frac{\partial U}{\partial x} - f(t)\right)^2\right]$$

with $\quad g(v) = -\gamma v + F(v)$

$\eta(t)$ Gaussian noise $\quad \langle \eta(t)\eta(0)\rangle = 2D_0\delta(t)$

# fluctuation theorem - 2


time reversed path $X^\dagger = \{x(\tau - t), -v(\tau - t), f(\tau - t)\}$

$$P_- \propto \exp\left[-\frac{1}{4D_0}\int_0^\tau dt\left(m\dot{v} + g(v) + \frac{\partial U}{\partial x} - f(t)\right)^2\right]$$

reversing protocol $f(t)$

# fluctuation theorem -3

ratio :

$$\frac{\mathcal{P}_+}{\mathcal{P}_-} = \exp\left[-\beta\left(\Delta q + \Delta Q_{em} + \frac{1}{\gamma}\Delta\phi\right)\right]$$

where,

$$\Delta Q_{em} = (1/\gamma)(\int^{\tau} dt F(v)(f - \partial_x U))\,, \quad F(v) = -\phi'(v)$$

$$\boxed{\frac{P_f(X)}{P_r(X^\dagger)} = \frac{\pi_i \mathcal{P}_+}{\pi_f \mathcal{P}_-} = e^{\Delta s_t / k_b}}$$

$$s = -k_B \ln \pi$$

$$\Delta s_r = -\frac{1}{T}\left(\Delta q + \Delta Q_{em} + \frac{m}{\gamma}\Delta\phi\right)$$

$$\Delta s_r \neq -\frac{\Delta q}{T}$$

$$\Delta s_t = \Delta s + \Delta s_r$$

# summary

integral fluctuation theorem

$$\langle e^{-\Delta s_t/k_B} \rangle = \int \mathcal{D}[X] \frac{P_r(X^\dagger)}{P_f(X)} P_f(X) = \int \mathcal{D}[X^\dagger] P_r(X^\dagger) = 1.$$

detailed fluctuation theorem (steady state)

$$\frac{\rho_f(\Delta s_t)}{\rho_r(-\Delta s_t)} = e^{\Delta s_t/k_B}.$$

$$s = -k_B \ln \pi$$

$$\Delta s_r = -\frac{1}{T}\left(\Delta q + \Delta Q_{em} + \frac{m}{\gamma}\Delta\phi\right)$$

$$F(v) = -\partial_v \phi(v)$$

Chandrima Ganguly, DC, *Phys Rev E* (2013)

# in ***absence*** of activity

set, $F(v) = 0 \quad \Rightarrow \Delta Q_m = 0,\ \Delta Q_{em} = 0,\ \Delta \phi = 0$

implies

$$\ln \frac{\rho_f(\Delta s_t)}{\rho_r(-\Delta s_t)} = \frac{\Delta s_t}{k_B}$$

with

$$\Delta s_t = \Delta s - \frac{\Delta E - \Delta W}{T}$$

$$\langle e^{-\Delta s_t / k_B} \rangle = 1 \qquad \Rightarrow \qquad \langle e^{-\beta \Delta W_d} \rangle = 1$$

Jarzynski equality with dissipated work

$$\Delta W_d = \Delta W - \Delta F$$

# ABP: breaking of detailed balance

- $$\frac{\partial P(x,v)}{\partial t} = -\frac{\partial}{\partial x}[vP(x,v)] + \frac{\partial}{\partial v}\{[F(v)+U'(x)]P(x,v)\} + \gamma T \frac{\partial^2}{\partial v^2}P(x,v) = -\boldsymbol{\nabla}\cdot\boldsymbol{J}^{rev} - \boldsymbol{\nabla}\cdot\boldsymbol{J}^{irr}$$

where, $\boldsymbol{\nabla} = (\partial_x, \partial_v)$ and $\boldsymbol{J}^{rev} = \begin{pmatrix} vP(x,v) \\ -U'P(x,v) \end{pmatrix}$

$$\boldsymbol{J}^{irr} = \begin{pmatrix} 0 \\ -F(v)P(x,v) - \gamma T\partial_v P(x,v) \end{pmatrix}.$$

- ness $\boldsymbol{\nabla}\cdot(\boldsymbol{J}^{rev} + \boldsymbol{J}^{irr}) = 0.$

- detailed balance:

$$\boldsymbol{J}^{irr} = 0 \quad \Rightarrow \quad \partial_v P(x,v) = -\frac{F(v)}{\gamma T}P(x,v).$$

$$\boldsymbol{\nabla}\cdot\boldsymbol{J}^{rev} = 0, \quad \Rightarrow \quad P(x,v) = p(v)e^{-\frac{U(x)}{\gamma T}\frac{F(v)}{v}}$$

# non-eqm steady state

last two steps $\Rightarrow$ $$\frac{p'(v)}{p(v)} = \frac{U(x)}{\gamma T}\frac{F'(v)v - F(v)}{v^2} - \frac{F(v)}{\gamma T}$$

true if first term = 0

$U(x) = 0$ or $F'(v)v - F(v) = 0$ $\Rightarrow$ $F(v) \propto v.$

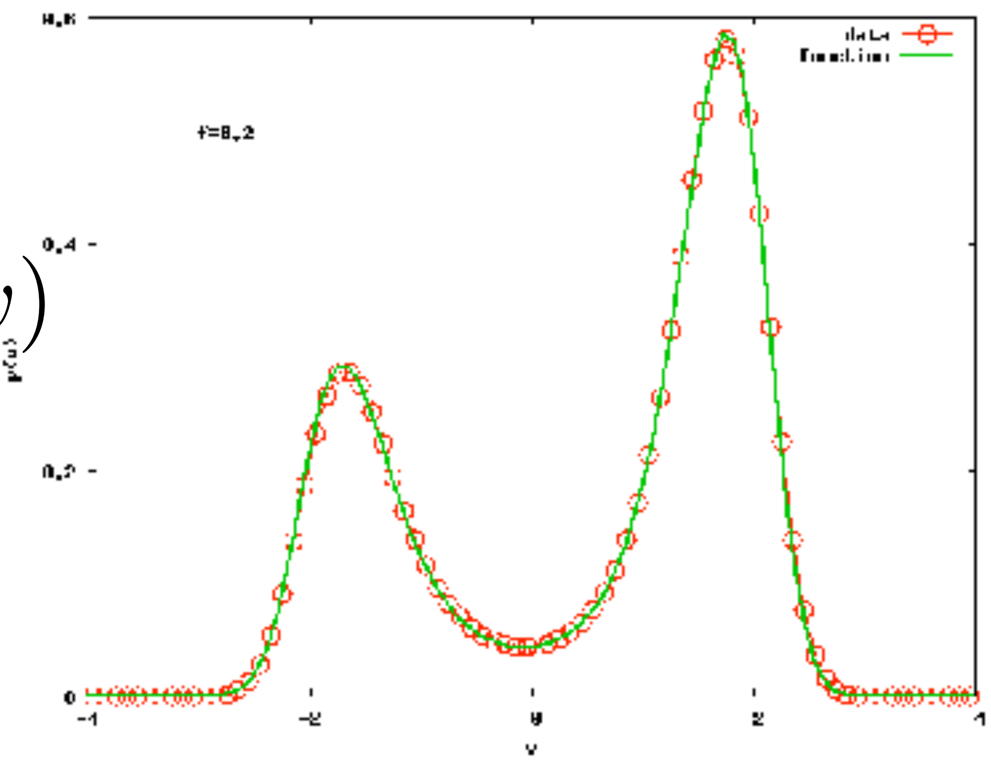
else non-equilibrium ➡ entropy production

either force or potential trap

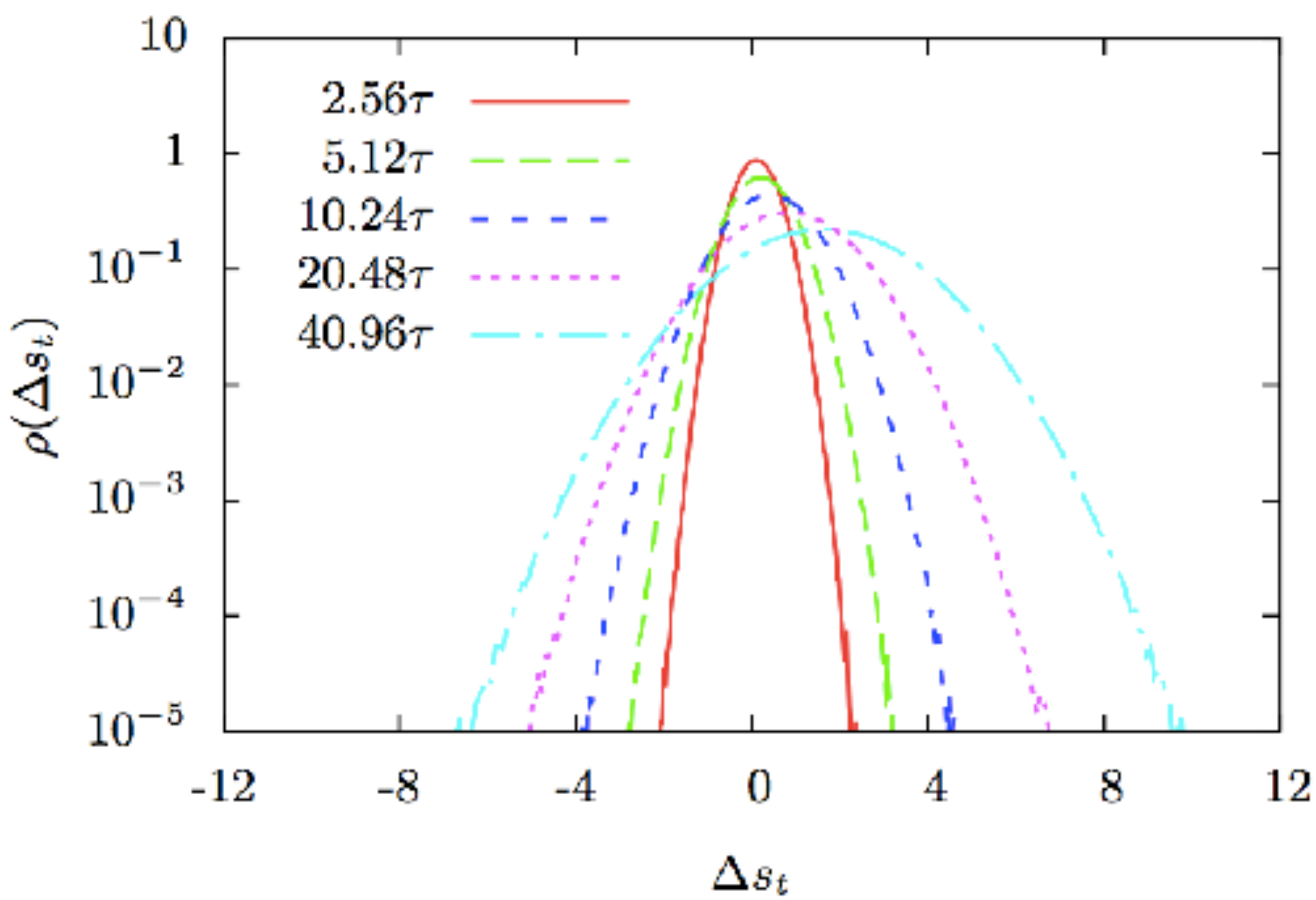
# ness entropy production

molecular dynamics with force $f = 0.2$

$p(v)$



$$p_s(v) = N \exp\left[-\frac{1}{D_0}\{\gamma v^2/2 - fv + \phi(v)\}\right]$$



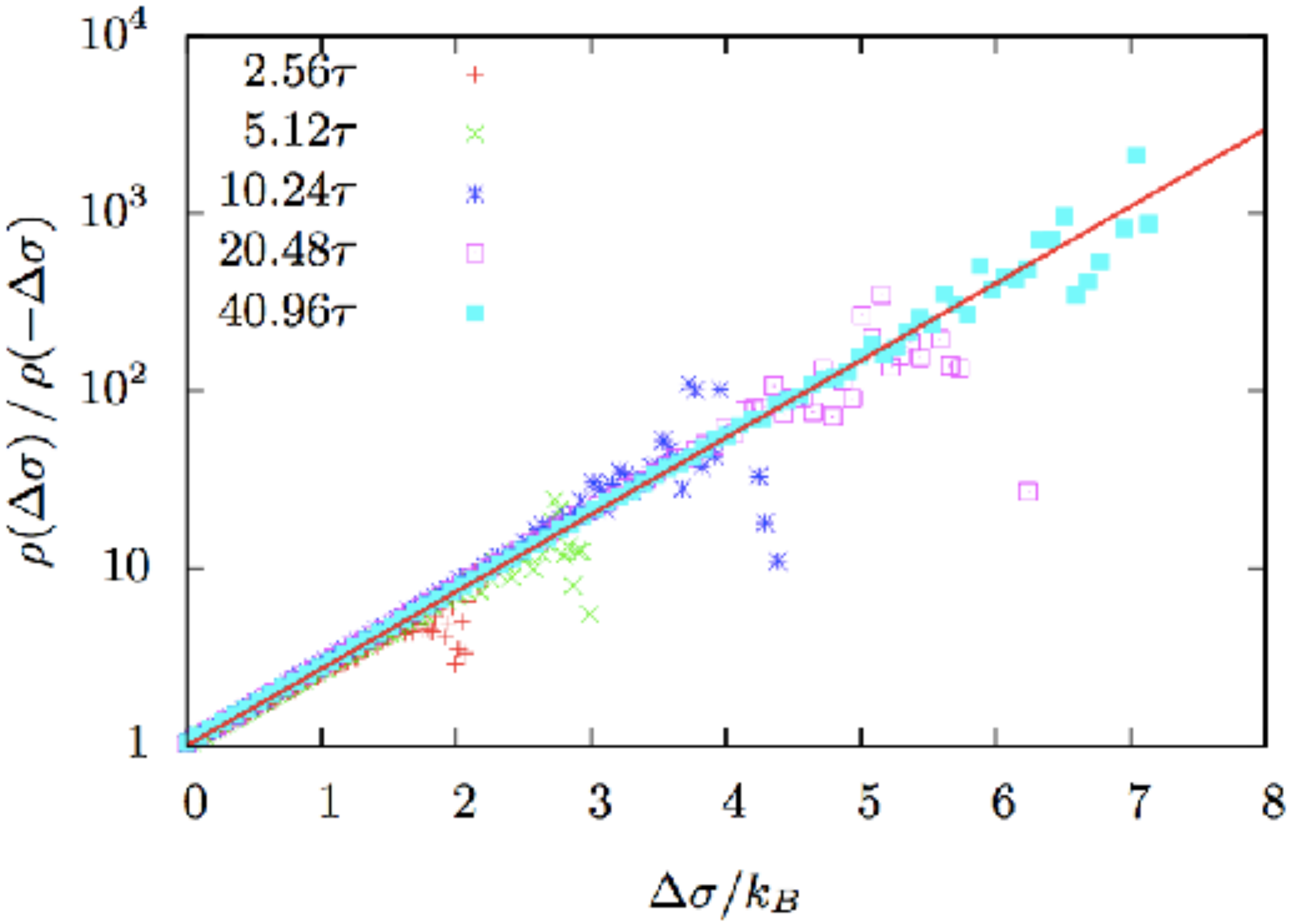

$$\frac{\Delta s_t}{k_B} = -\frac{f}{D_0}\left[(v_f - v_i) + \int^{\tau} dt F(v)\right] + \beta f(x_f - x_i)$$

**DC**, *Phys. Rev. E* (2014)

# detailed fluctuation theorem

molecular dynamics: $f = 0.2$

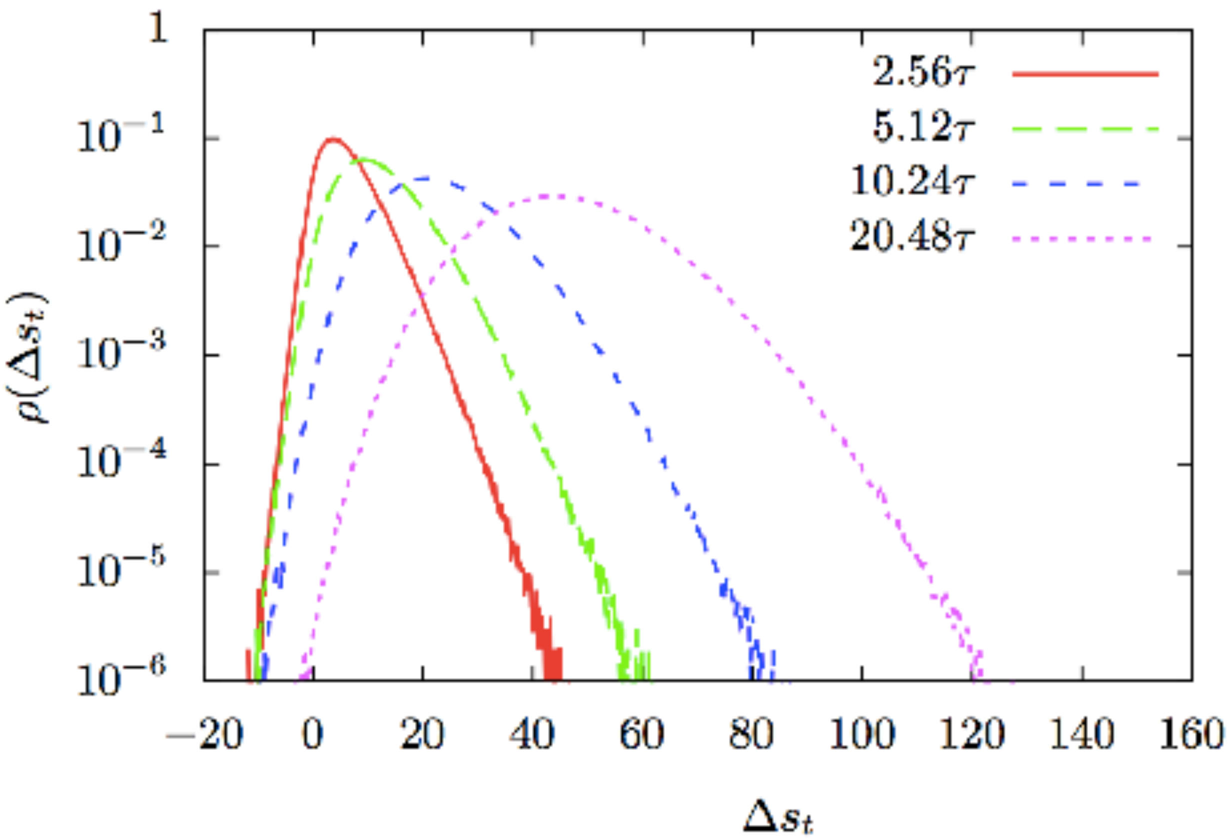
$$\frac{\rho(\Delta s_t)}{\rho(-\Delta s_t)} = e^{\Delta s_t / k_B}$$

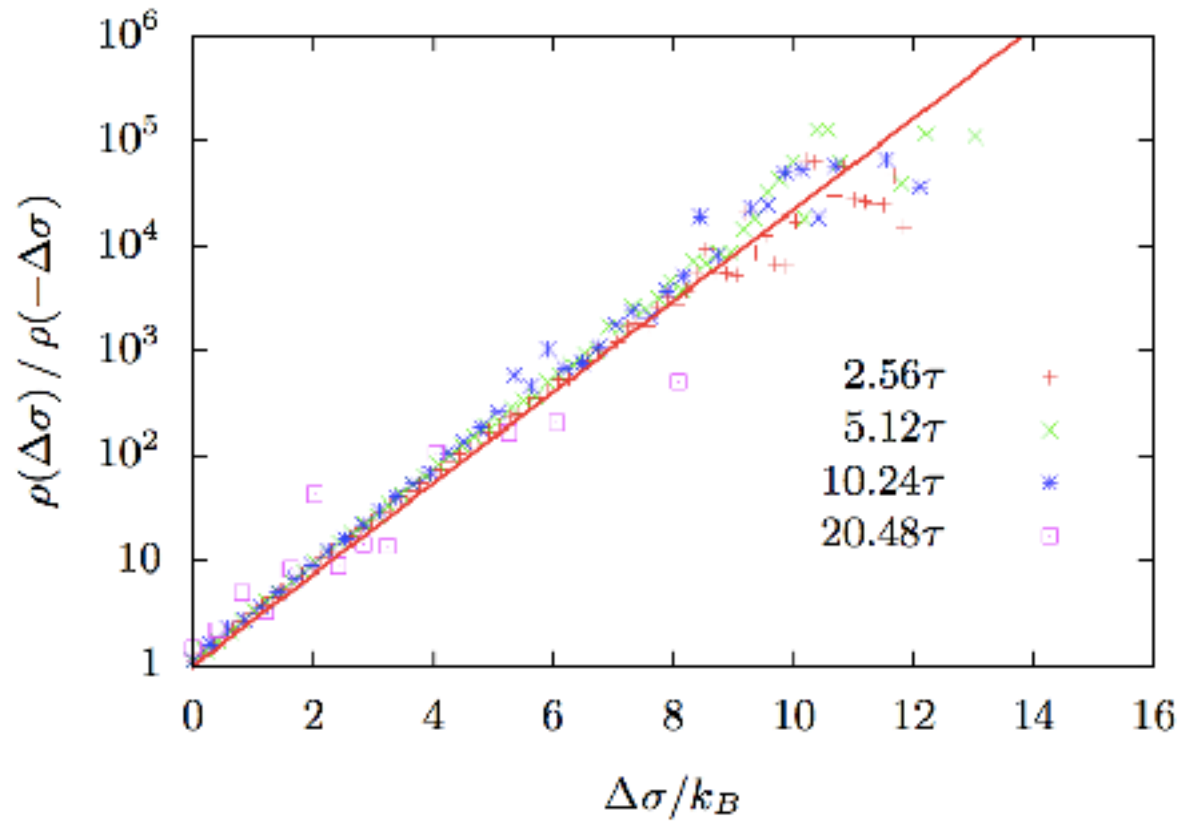



**DC**, *Phys. Rev. E* (2014)

# ness of RH in harmonic trap

with potential : $$U(x) = \frac{1}{2}kx^2$$




no external force.
harmonic trap breaks time reversal symmetry

**DC**, *Phys. Rev. E* (2014)

# mfdr for spp

response function $$R_A(t-t') = \left\langle \frac{\delta A[\eta]}{\delta \eta(t')} \right\rangle = \frac{1}{2D_0} \langle A(t)\eta(t') \rangle$$

treating noise as force

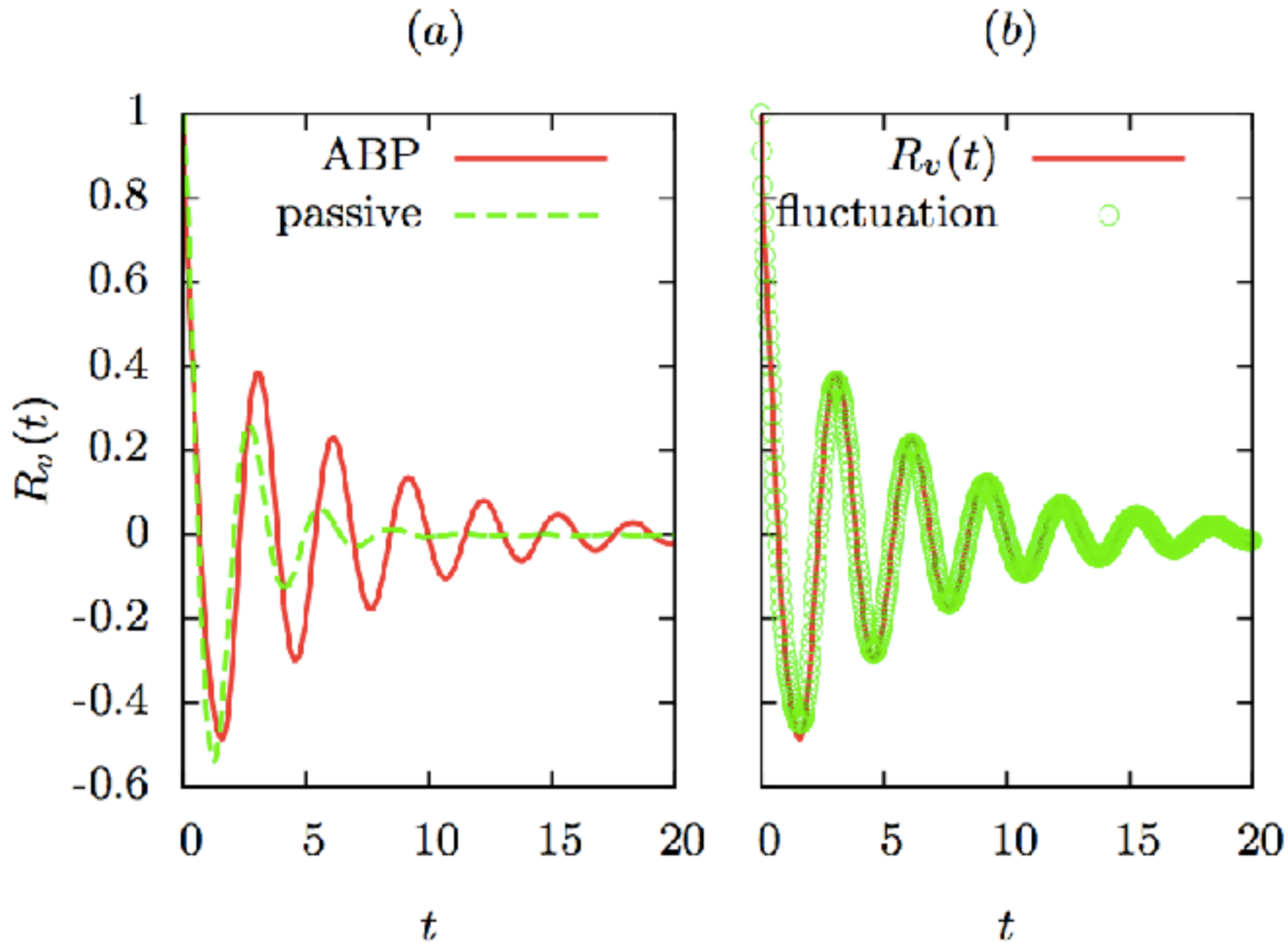
ABP in Harmonic trap

$$R_v(t) = -\frac{1}{2D_0} [\, \langle g[v(t)]v(0) \rangle + \langle v(t)g[v(0)] \rangle \,]$$

eqm: $g(v) = -\gamma v$ ➡ $R_v(t) = \beta \langle v(t)v(0) \rangle$

**DC**, *Phys. Rev. E* (2014)

# mfdr : RH in harmonic trap




**DC**, *Phys. Rev. E* (2014)

# odd and even functions of velocity

$$\dot{x} = v$$

$$\dot{v} = -\gamma v + \eta(t) + [\xi(v) + \zeta(v)] - \partial_x U + f(t)$$

$$\xi(-v) = \xi(v), \quad \zeta(-v) = -\zeta(v)$$

use Fokker-Planck equation to obtain entropy production

$$\partial_t P(x,v) = -\nabla.(\mathbf{j}_r + \mathbf{j}_d) \ , \quad \nabla \equiv (\partial_x, \partial_v)$$

with reversible current $\quad \mathbf{j}_r = \{vP, [f(t) - \partial_x U + \xi(v)]P\}$

dissipative current $\quad \mathbf{j}_d = \{0, [-\gamma v + \zeta(v)]P - D_0 \partial_v P\}$

**DC**, *Phys. Rev. E* (2016)

# entropy production

$$\frac{dS}{dt} = -k_B \int dx\, dv\, \ln P\, \frac{\partial P}{\partial t} = k_B \int dx\, dv\, \ln P\, [\nabla \cdot (\mathbf{j}_r + \mathbf{j}_d)].$$

first part

$$\int dx\, dv\, \ln P\, \nabla \cdot \mathbf{j}_r = \int dx\, dv\, P\, \nabla \cdot (\mathbf{j}_r / P) = \langle \partial_v \xi(v) \rangle$$

and, total EP

$$\dot{S}_t = \dot{S} + \dot{S}_r = k_B \int dx\, dv \frac{j_d^2}{P\, D_0} \geqslant 0$$

with

$$\frac{1}{k_B} \dot{S}_r = -\langle \partial_v \xi(v) \rangle + \frac{1}{D_0} \int dx\, dv\, j_d\, g(v).$$

and scalar

$$j_d = [-\gamma v + \zeta(v)] P - D_0 \partial_v P$$

# stochastic entropy production

undo two step averaging over

- phase space probability $P(x, v, t)$
- stochastic trajectories

$$\langle \dot{v} | x, v, t \rangle = j_v / P = [-\partial_x U + f(t) + \xi(v)] + j_d / P$$

to get
$$\frac{1}{k_B} \dot{s}_r = -\partial_v \xi(v) + \frac{-\gamma v + \zeta(v)}{D_0} [-\gamma v + \eta(t) + \zeta(v)]$$

$$\boxed{\dot{s}_r = -\frac{\dot{Q}}{T} - \frac{\zeta(v) v}{T} - \frac{\dot{\psi}(v)}{\gamma T} - \frac{\dot{Q}_{em}}{T} - k_B \, \partial_v \xi(v)}$$

with
$$\gamma \dot{Q}_{em} = \zeta(v)[f(t) - \partial_x U + \xi(v)], \quad \zeta(v) = -\partial_v \psi(v)$$

# fluctuation theorem

using forward and reverse trajectories

- $\mathcal{P}_r/\mathcal{P}_f = \exp(-\Delta s_t/k_B),$ $\qquad \dfrac{\rho(\Delta s_t)}{\rho(-\Delta s_t)} = e^{\Delta s_t/k_B},$

with $\Delta s_t = \int^\tau dt\,[\dot{s} + \dot{s}_r]$

use $\zeta(v) = av - cv^3$ $,\xi(v) = b\,v^2$

total entropy production

$$\Delta s_t = -\frac{1}{T}\left[\Delta\left(\frac{b}{3\gamma}v^3\right) + \int^{\tau_0} dt\{\zeta(v) - v\}\xi(v)\right] - \int^{\tau_0} dt\, k_B \partial_v \xi(v).$$

ness in absence of external potential or force

# distributions

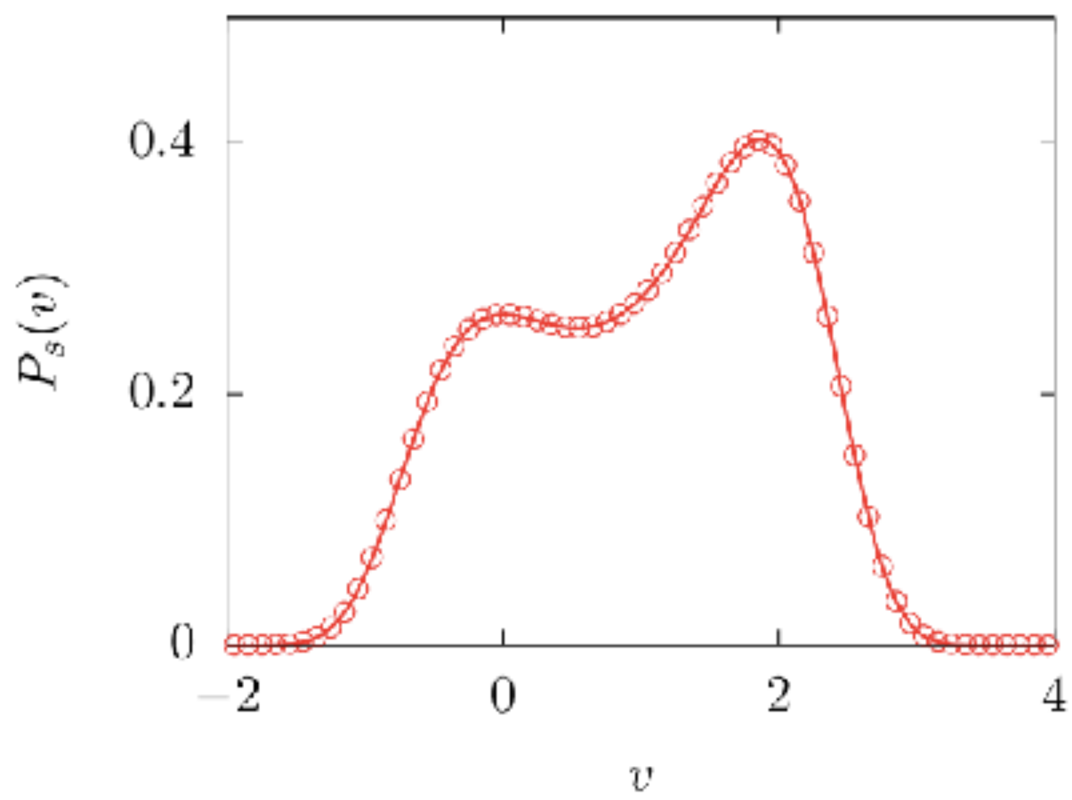



FIG. 1. Steady state probability distribution obtained from simulation (points), compared against the line drawn using the analytic form $P_s(v) = \mathcal{N} \exp[-\chi(v)/D_0]$, with $\chi(v) = \frac{1}{2}(a+\gamma)v^2 - \frac{b}{3}v^3 + \frac{c}{4}v^4$, where $a = 0$, $\gamma = 1$, $b = 2.4$, $c = 1$, and $D_0 = 1$.

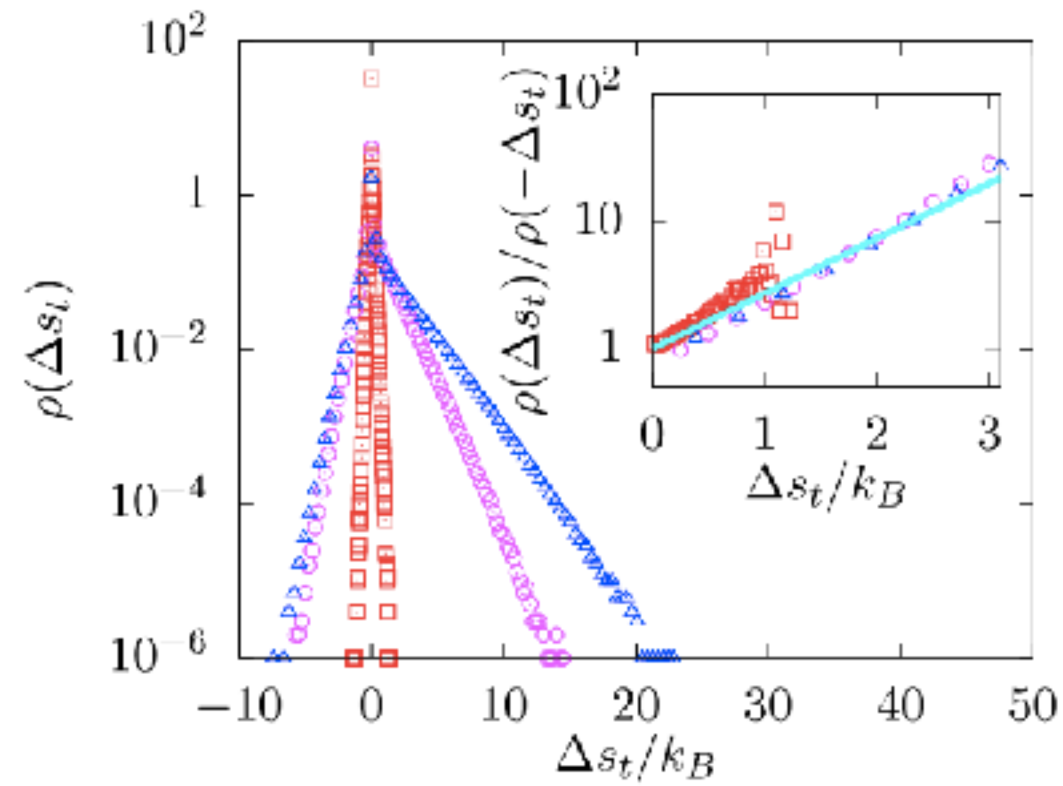



FIG. 2. Probability distribution of entropy production $\Delta s_t$ over time span $\tau_0 = 16$ (□), 64 (○), 128 (△) $\delta t$ plotted in linear-log scale.

**DC**, *Phys. Rev. E* (2016)

# stochastic energy depot

$$\dot{v} = -\gamma v + \eta_v(t) + \frac{\nu(x,v)e(t)}{v} \quad , \quad \dot{e}(t) = \dot{q}_e(x) - r_m e(t) - \nu(x,v)e(t) + \eta_e(t)$$

using the Fokker-Planck equation

$$\dot{s}_r = \nu_o - \partial_v\left(\frac{e\nu_o}{v}\right) + \frac{1}{D_e}(\dot{q}_e - r_m e - \nu_e e)(\dot{e} + e\nu_o) + \frac{1}{D_v}\left(-\gamma v + \frac{e\nu_e}{v}\right)\left[\dot{v} - \frac{e\nu_o}{v}\right]$$

where, odd and even terms are $\nu_0(x,v), \ \nu_e(x,v)$

corresponding total entropy production obeys detailed fluctuation theorem

*ongoing work, Priyo S. Pal & DC*

# conclusion

- fluctuation theorems for stochastic dynamics of self propelled particles
- self propulsion leads to *non-Clausius terms* in entropy production
- modified fluctuation-dissipation relation at ness