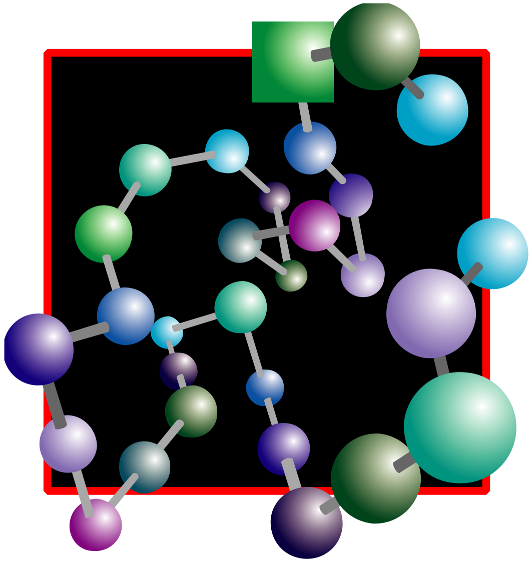
From Sisyphus to Boltzmann: an example of repulsive depletion interaction

Rutgers 119 Statistical Mechanics Meeting
May 6-8, 2018

J.-F.Joanny,
ESPCI



Cato Sandford
NYU

Alexander Grosberg
Department of Physics & Center for Soft Matter Research,
New York University

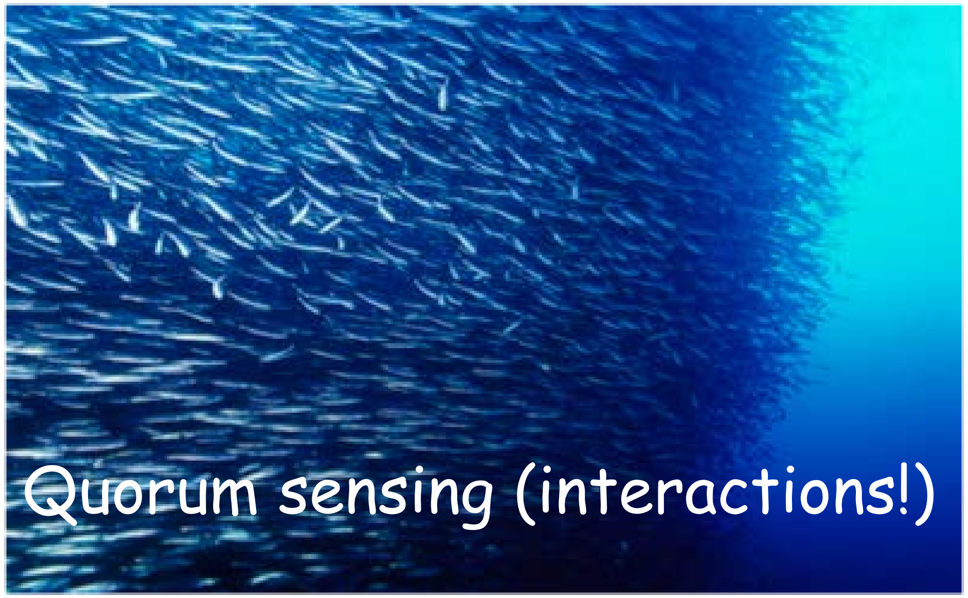
While depletion interaction, e.g., between two plates in an equilibrium system (such as a colloidal solution) is an attraction, we show how colloids driven by a colored Ornstein-Uhlenbeck noise may leave to the counter-intuitive opposite effect. This is due to the accumulation of lackadaisical particles in the gap between plates. The underlying physical effect is the difference between white noise drive, which sets particle energy fluctuations of order kT (Boltzmann limit), and colored noise drive with long persistence time, which controls particle propulsion ("pushing") force (Sisyphus limit).

Zeroes of Rieman ζ-function?

74, 76, 80, 99, 106, 111, 119…

Analogies

what I will not consider in this talk

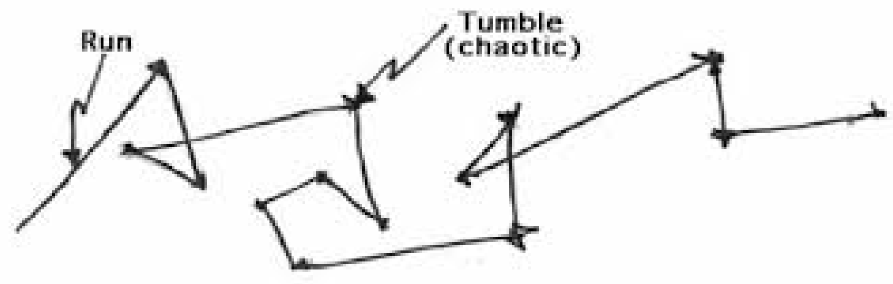


I will consider single particle (ideal gas) physics only

This image is not related to the subject of the talk, but very cute…

Random images from the internet

How microbes move: Run-and-Tumble

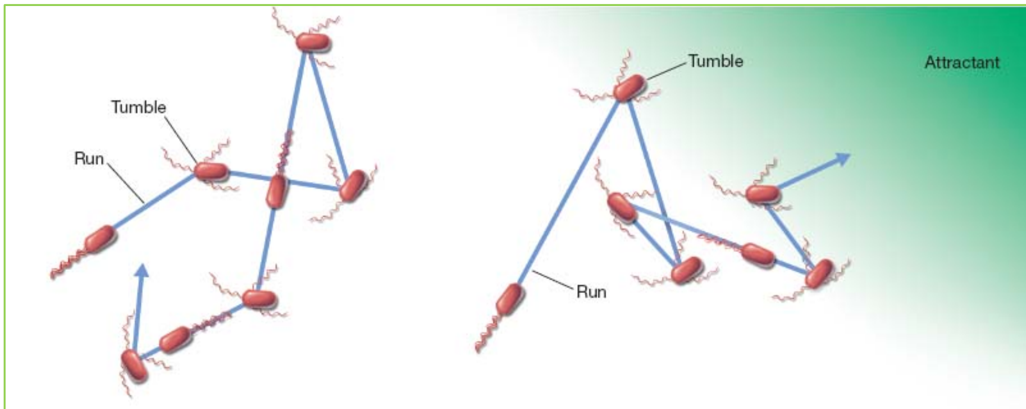


"Run-tumble" paradigm for taxis
Berg and Brown, Nature, (1972)

From afar, it looks like what they do is nothing but a random walk…

Osmotic pressure?

Depletion interaction?



(a) No attractant present: Random movement (b) Attractant present: Directed movement

Michael T. Madigan, John M. Martinko, Kelly S. Bender, Daniel H. Buckley, David A. Stahl, Thomas Brock
Brock Biology of Microorganisms (14th Edition)

Single particle phenomenon 1:

distribution of bacteria in a structure with a funnel wall

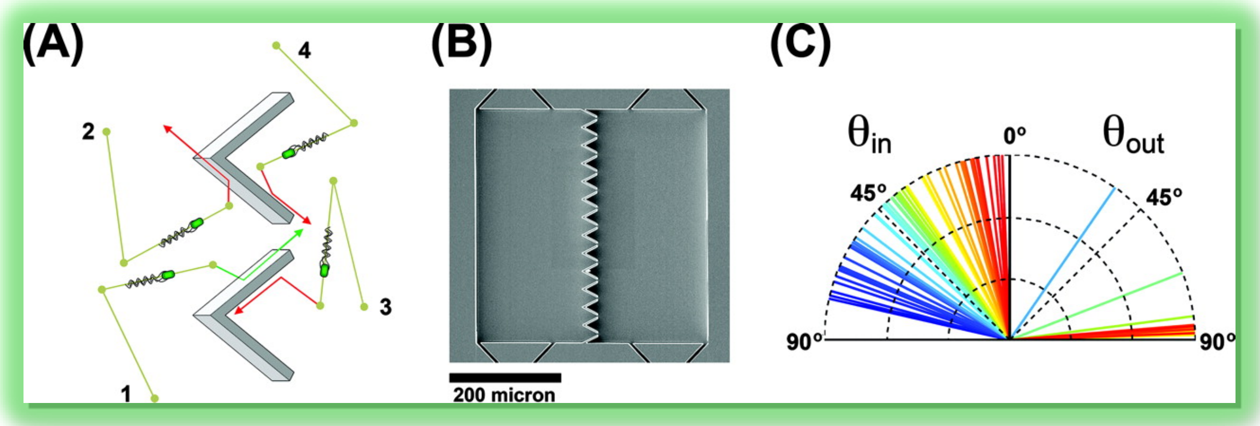


Figure 1

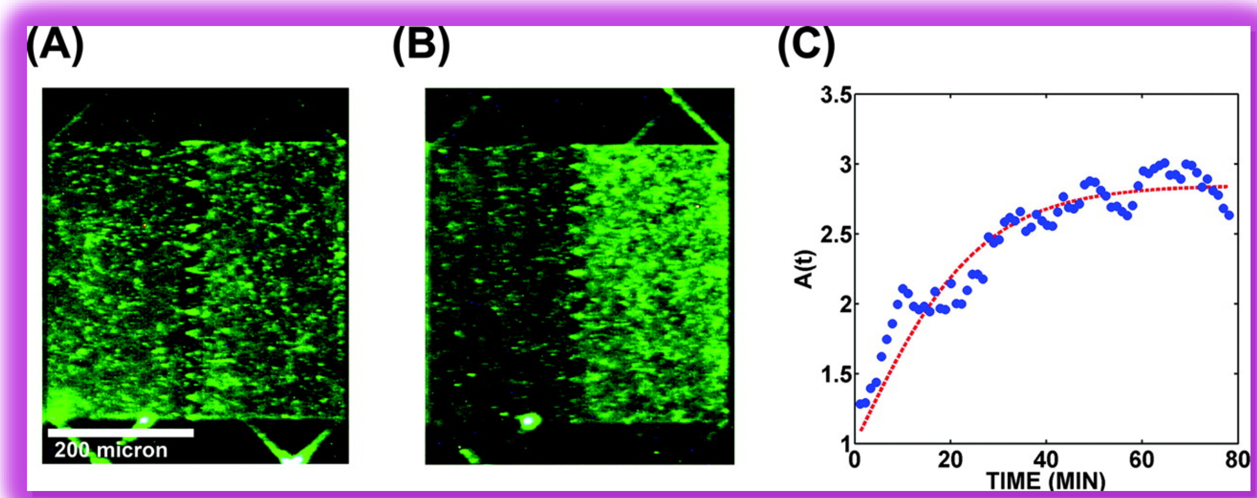


Figure 2

Peter Galajda, Juan Keymer, Paul Chaikin, and Robert Austin "A Wall of Funnels Concentrates Swimming Bacteria" J. Bacteriol. 2007; v. 189 p. 8704-8707

Journal of Bacteriology

Single particle phenomenon 2

Bacterial ratchet motors

R. Di Leonardo[a,1], L. Angelani[a], D. Dell'Arciprete[b], G. Ruocco[b], V. Iebba[c], S. Schippa[c], M. P. Conte[c], F. Mecarini[d,e], F. De Angelis[d,e], and E. Di Fabrizio[d,e]

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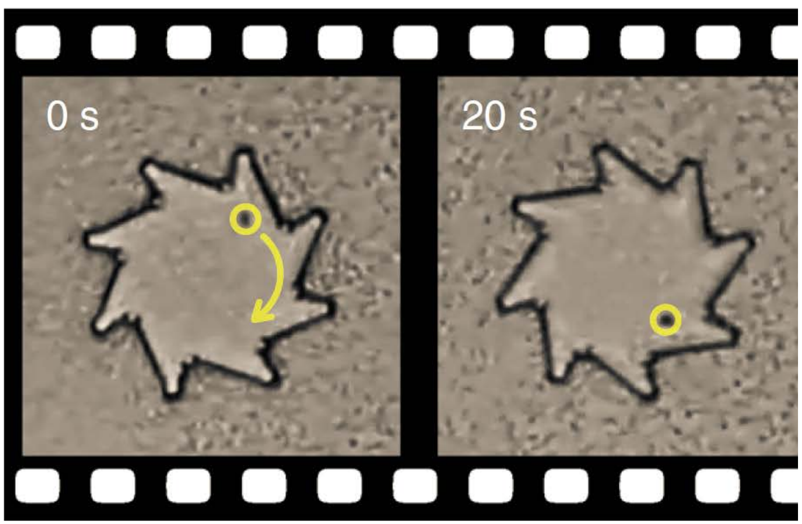
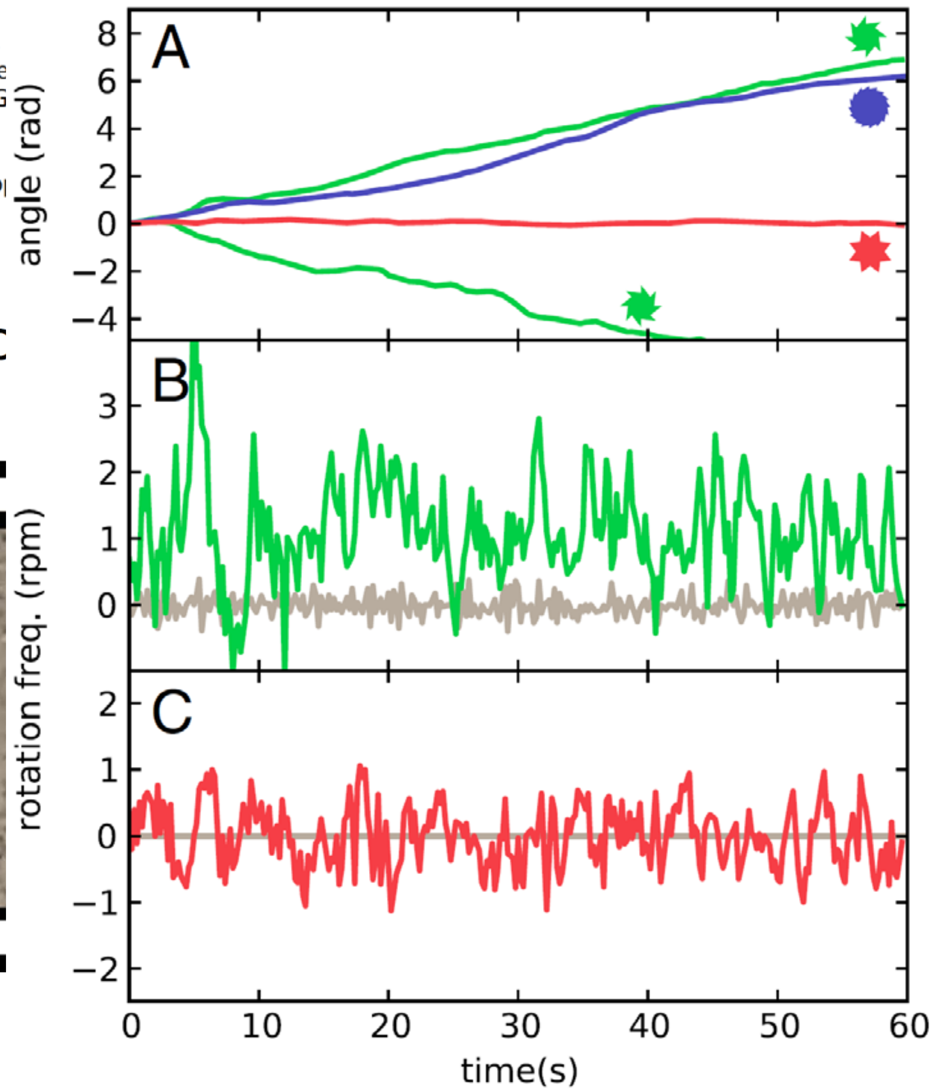
[d]Nanobioscience Department, Italian Institute of Technology, I-16163, G
Università della Magna Graecia, I-88100, Catanzaro, Italy

Edited by Howard C. Berg, Harvard University, Cambridge, MA, and ap

PNAS | **May 25, 2010** | vo





Many papers...

PHYSICAL REVIEW FLUIDS **2**, 043103 (2017)

Hot particles attract in a cold bath

Hidenori Tanaka,[*] Alpha A. Lee,[†] and Michael P. Brenner[‡]

THE JOURNAL OF CHEMICAL PHYSICS **141**, 044903 (2014)

Unusual swelling of a polymer in a bacterial bath

A. Kaiser[a)] and H. Löwen

THE JOURNAL OF CHEMICAL PHYSICS **141**, 194901 (2014)

The role of particle shape in active depletion

J. Harder,[1,a)] S. A. Mallory,[1,a)] C. Tung,[1,a)] C. Valeriani,[2] and A. Cacciuto[1,b)]

Soft Matter

PAPER

CrossMark
click for updates

Cite this: Soft Matter, 2016, 12, 7136

The nonequilibrium glassy dynamics of self-propelled particles†

Elijah Flenner,[a] Grzegorz Szamel*[ab] and Ludovic Berthier*[b]

Journal of Statistical Mechanics: Theory and Experiment
An IOP and SISSA journal

PAPER: Classical statistical mechanics, equilibrium and non-equilibrium

2017, 043203

Steady-state distributions of ideal active Brownian particles under confinement and forcing

Caleb G Wagner, Michael F Hagan and Aparna Baskaran

PHYSICAL REVIEW E **90**, 012111 (2014)

Self-propelled particle in an external potential: Existence of an effective temperature

Grzegorz Szamel

PRL **108**, 168301 (2012) PHYSICAL REVIEW LETTERS week ending 20 APRIL 2012

Crystallization in a Dense Suspension of Self-Propelled Particles

Julian Bialké, Thomas Speck, and Hartmut Löwen

Model

Ornstein-Uhlenbeck

$$\zeta \dot{x} = f(x) + \eta(t)$$

External force f(x), assumed potential

$$\langle \eta(t)\eta(t') \rangle = \frac{T\zeta}{\tau} e^{-|t-t'|/\tau}$$

Colored driving noise violates
Fluctuation-Dissipation theorem

Mathematical trick: pretend there is hidden white noise source ξ(t):

$$\zeta \dot{x} = f(x) + \eta(t)$$
$$\tau \dot{\eta} = -\eta + \xi(t)$$

$$\langle \xi(t)\xi(t') \rangle = 2T\zeta\delta(t-t')$$

- η is propulsion force
- overall power in η the same as in ξ
- This trick is known, it is not our invention

From Langevin to Fokker-Planck

$$\zeta \dot{x} = f(x) + \eta(t)$$
$$\tau \dot{\eta} = -\eta + \xi(t)$$

Drift in η

$$\partial_t \rho = -\frac{1}{\zeta}\partial_x \left[(\eta + f(x))\,\rho \right] + \frac{1}{\tau}\partial_\eta \left[\eta\rho \right] + \frac{\zeta T}{\tau^2}\partial_\eta^2 \left[\rho \right]$$

Drift in x

Diffusion in η

No diffusion in x!!!

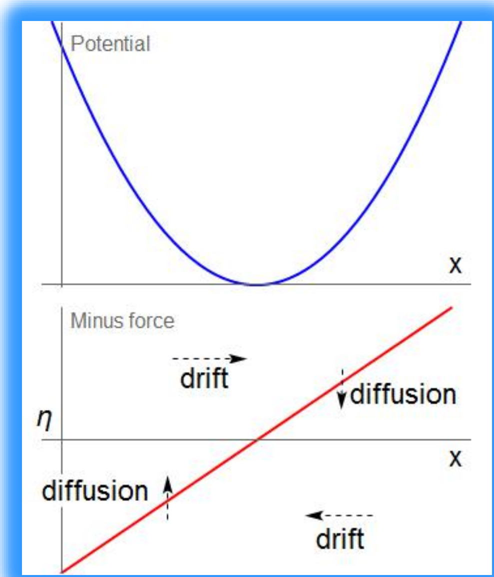
Exactly solvable model

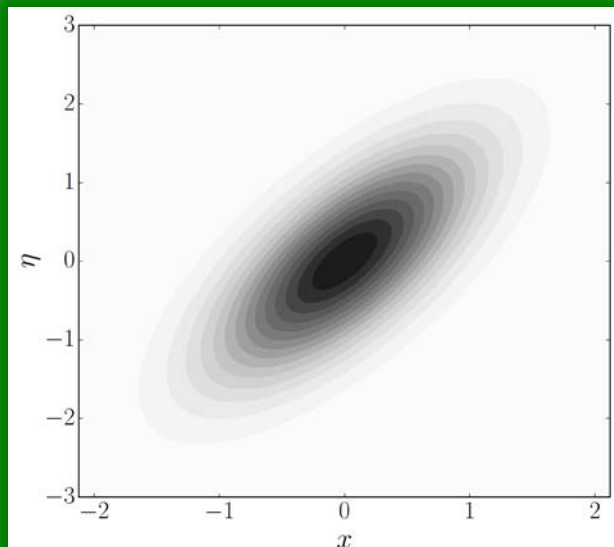
"harmonic oscillator"

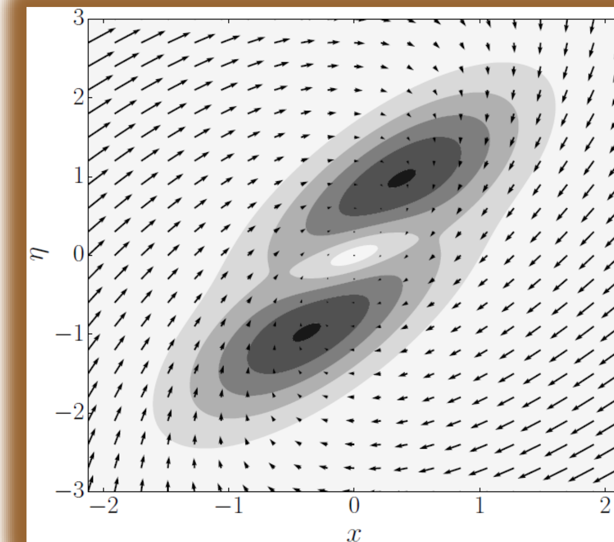
$$U = kx^2/2$$

$$\zeta \dot{x} = -kx + \eta(t)$$
$$\tau \dot{\eta} = -\eta + \xi(t)$$

$$\rho(x,\eta) \propto \exp\left[-\frac{k}{2T}\left(\frac{k\tau}{\zeta}+1\right)\left[x^2 + \frac{k\tau}{\zeta}\left(\frac{\eta}{k}-x\right)^2\right]\right]$$







PHYSICAL REVIEW E **87**, 062130 (2013)

Two-temperature Langevin dynamics in a parabolic potential

Victor Dotsenko,[1,2] Anna Maciołek,[3,4,5] Oleg Vasilyev,[3,4] and Gleb Oshanin[1]

PHYSICAL REVIEW E **90**, 012111 (2014)

Self-propelled particle in an external potential: Existence of an effective temperature

Grzegorz Szamel

Subtlety: time reversal signature of η

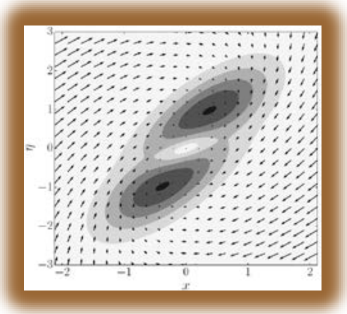
$$\boxed{\zeta \dot{x} = f(x) + \eta(t)}$$

$$\boxed{\dot{x} = \frac{1}{\zeta} f(x) + \tilde{\eta}(t)}$$

η is …

… propulsion force.

Loopy probability currents do indicate lack of equilibrium



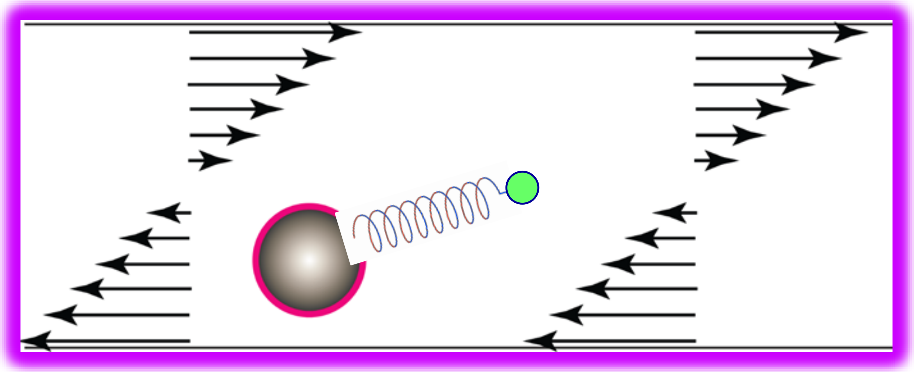
… swimming speed.

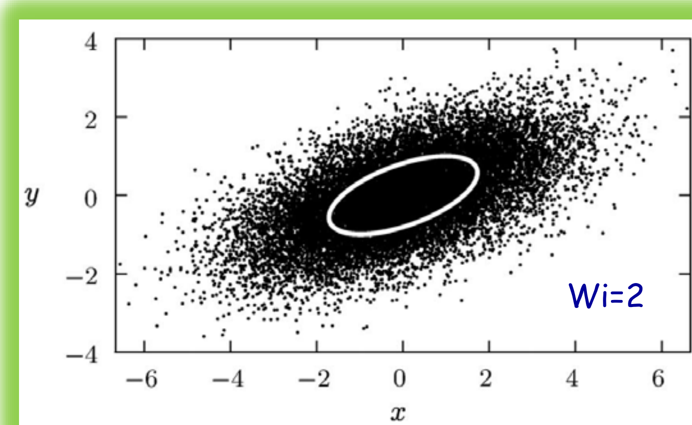
Loopy probability currents do not indicate deviations from equilibrium

Do not rush to integrate η out!!!

See on this also recent paper by C.Marchetti

Similarity and difference with shear flow





$$\zeta_x \dot{x} = -k_x x + \gamma y + \xi_x(t)$$
$$\zeta_y \dot{y} = -k_y y + \xi_y(t)$$

Main difference:
diffusion in x

$$\zeta \dot{x} = -kx + \eta(t)$$
$$\tau \dot{\eta} = -\eta + \xi(t)$$

PHYSICAL REVIEW E **81**, 041124 (2010)

Dynamics of a trapped Brownian particle in shear flows

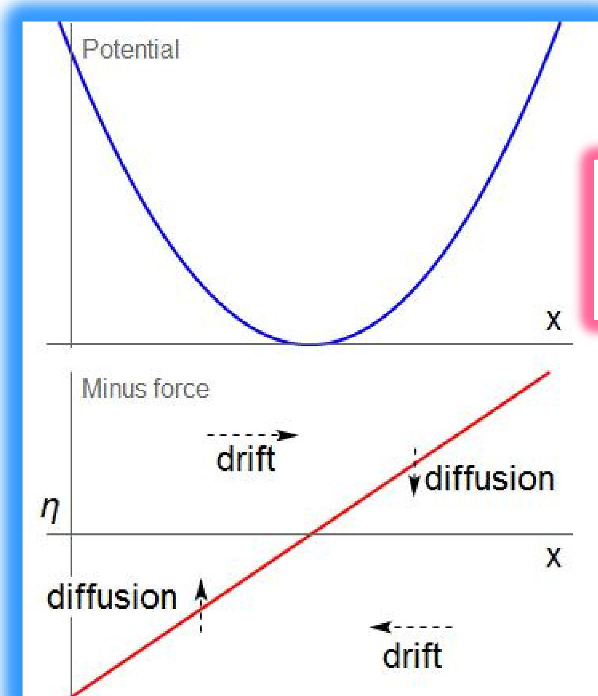
Lukas Holzer,[1] Jochen Bammert,[1] Roland Rzehak,[2] and Walter Zimmermann[1]

Boltzmann limit vs Sisyphus limit

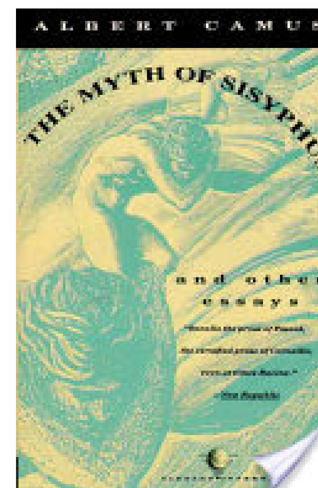
energy control vs. force control

$$\zeta \dot{x} = -kx + \eta(t)$$
$$\tau \dot{\eta} = -\eta + \xi(t)$$

$$\rho(x,\eta) \propto \exp\left[-\frac{k}{2T}\left(\frac{k\tau}{\zeta}+1\right)\left[x^2 + \frac{k\tau}{\zeta}\left(\frac{\eta}{k}-x\right)^2\right]\right]$$



$$\ell_{\mathrm{OUP}} = \frac{\sqrt{T/k}}{\sqrt{\frac{k\tau}{\zeta}+1}}$$



Boltzmann $\tau \to 0$:

$$U(x) = \frac{1}{2}T \Longrightarrow kx^2 = T$$

Sisyphus, $\tau \gg \zeta/k$:

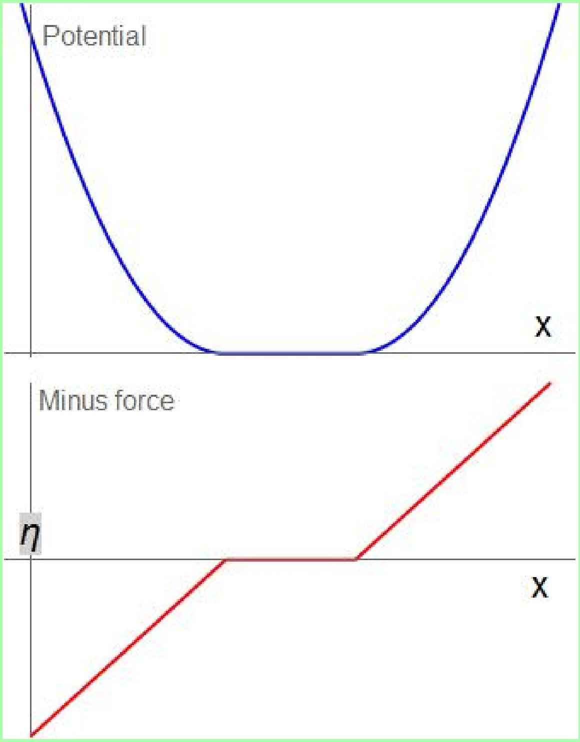
$$f(x) = \sqrt{\langle \eta^2 \rangle} \Longrightarrow kx = \sqrt{T\zeta/\tau}$$

Pressure

$$f_i(\vec{x}) = -\langle \eta_i \rangle (\vec{x}),$$
$$f_j(\vec{x}) n(\vec{x}) = \frac{\tau}{\zeta} \partial_{x_i} \left[\left(\langle \eta_i \eta_j \rangle - \langle \eta_i \rangle \langle \eta_j \rangle \right) n(\vec{x}) \right]$$

$$P = - \int_{\text{bottom of wall}}^{\text{top of wall}} f(x) n(x) \, \mathrm{d}x,$$

$$P = \frac{\tau}{\zeta} \left(\left[\langle \delta \eta_x^2 \rangle n(x) \right]_{\text{bottom}} - \left[\langle \delta \eta_x^2 \rangle n(x) \right]_{\text{top}} \right)$$



Pressure: comparison with equilibrium system

Non-potential field

$$f_i(\vec{x}) = -\langle \eta_i \rangle (\vec{x}),$$

$$f_j(\vec{x})n(\vec{x}) = \frac{T}{\zeta}\partial_{x_i}\left[\left(\langle \eta_i \eta_j \rangle - \langle \eta_i \rangle \langle \eta_j \rangle\right) n(\vec{x})\right]$$

memory

$$P = -\int_{\text{bottom of wall}}^{\text{top of wall}} f(x)n(x)\,\mathrm{d}x,$$

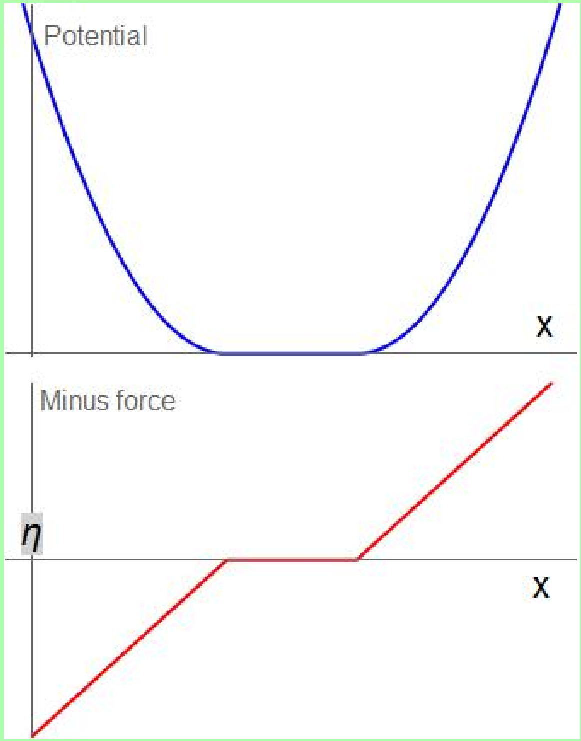
equilibrium

$$u(\vec{r}) + \mu(n(\vec{r})) = \text{const}$$

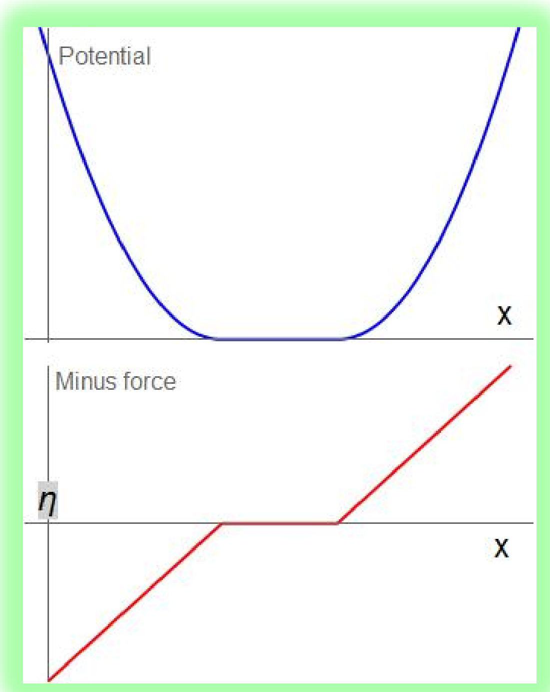
$$-\vec{f}(\vec{r}) + \frac{\partial \mu}{\partial n}\vec{\nabla} n = 0$$

$$n(\vec{r})\vec{f}(\vec{r}) = n\frac{\partial \mu}{\partial n}\vec{\nabla} n = \frac{\partial p}{\partial n}\vec{\nabla} n = \vec{\nabla} p(n)$$

Potential field

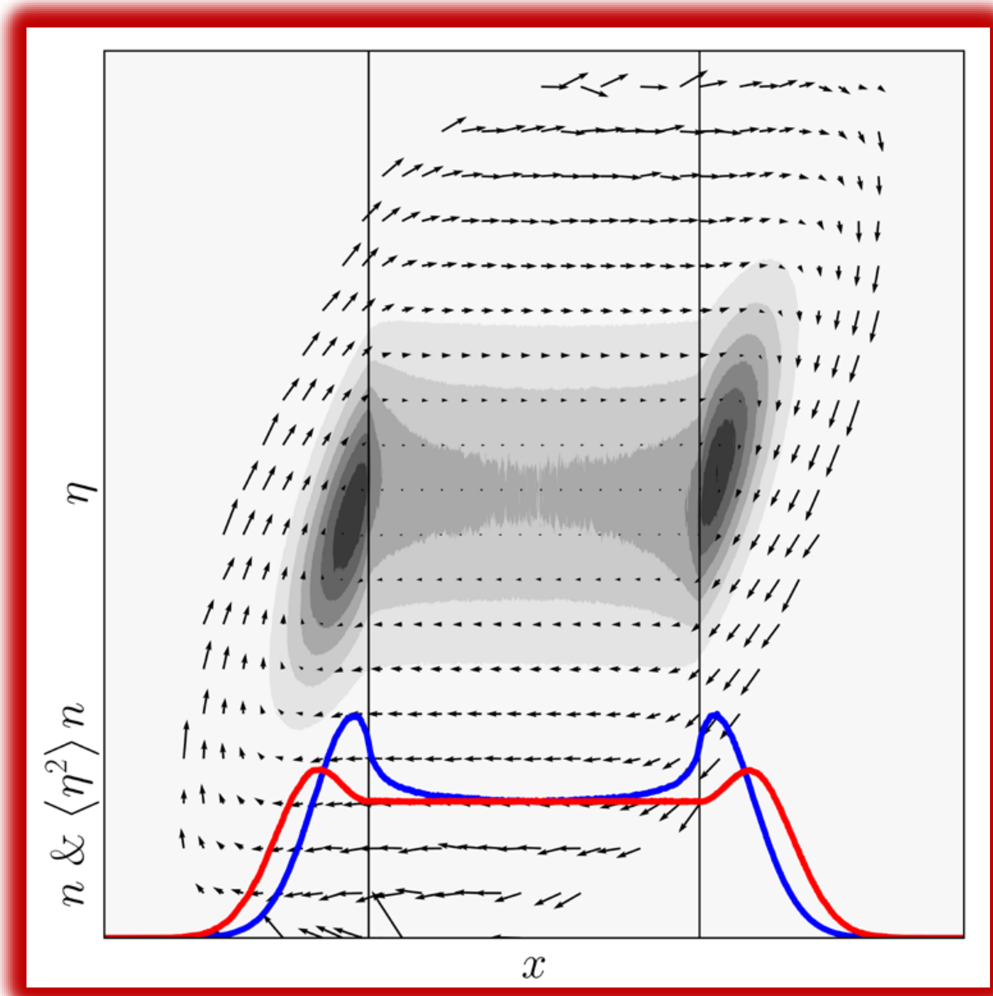


Flat bottom model

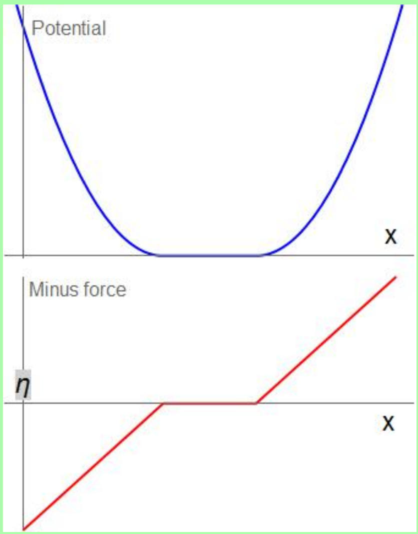


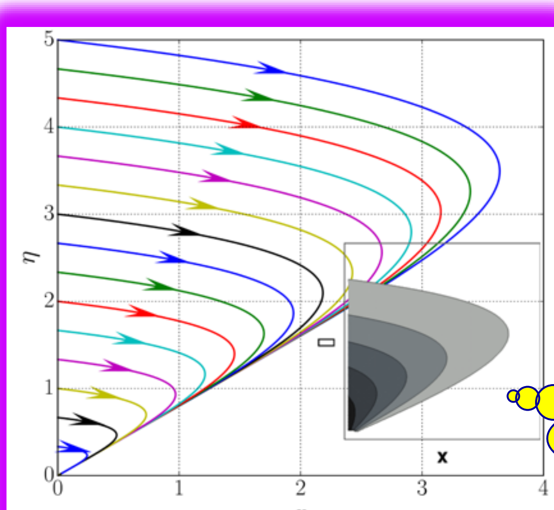
Theorem: in a "bulk"

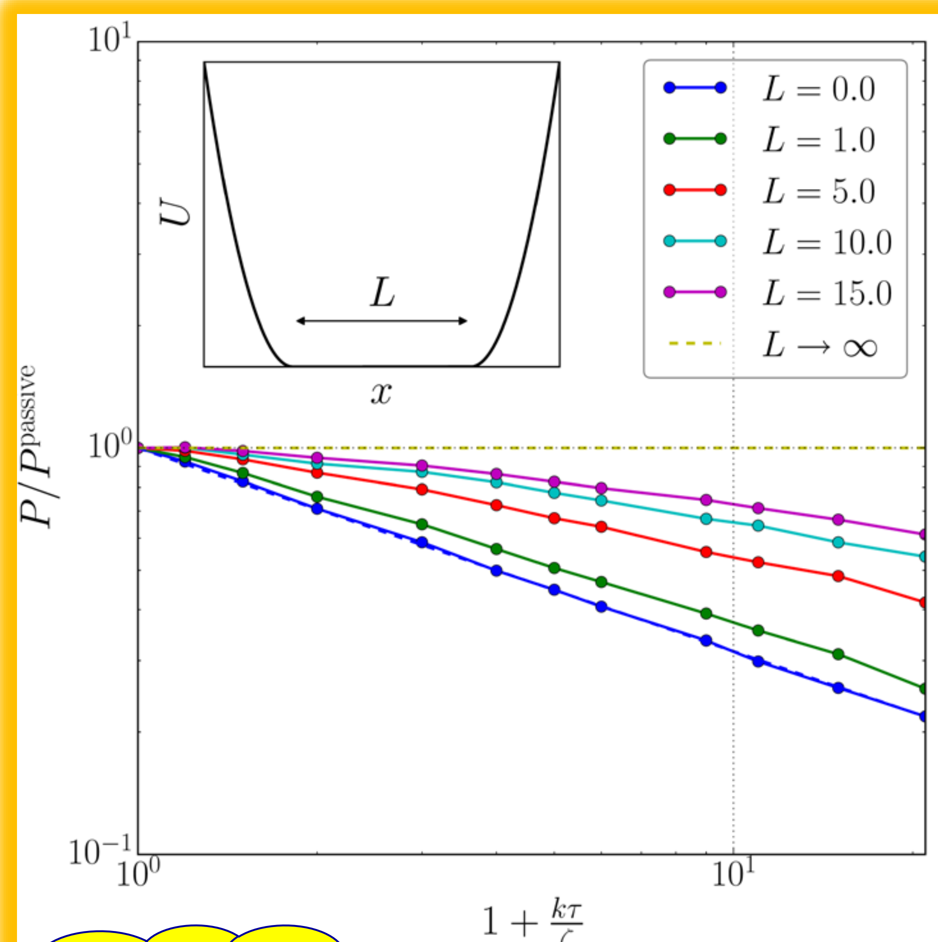
$$\left\langle \delta\eta^2 \right\rangle (x) n(x) = \text{const}$$



Particles in the narrow gap are "lackadaisical"



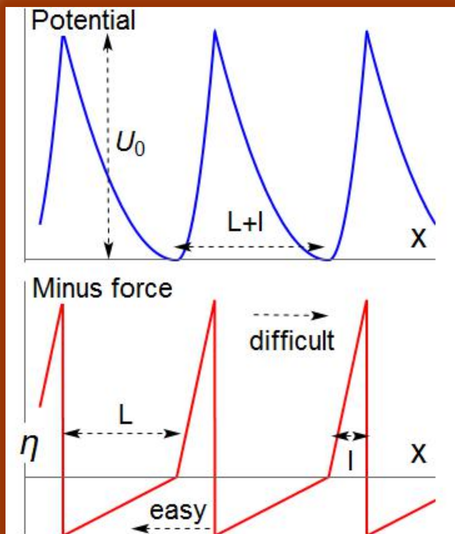


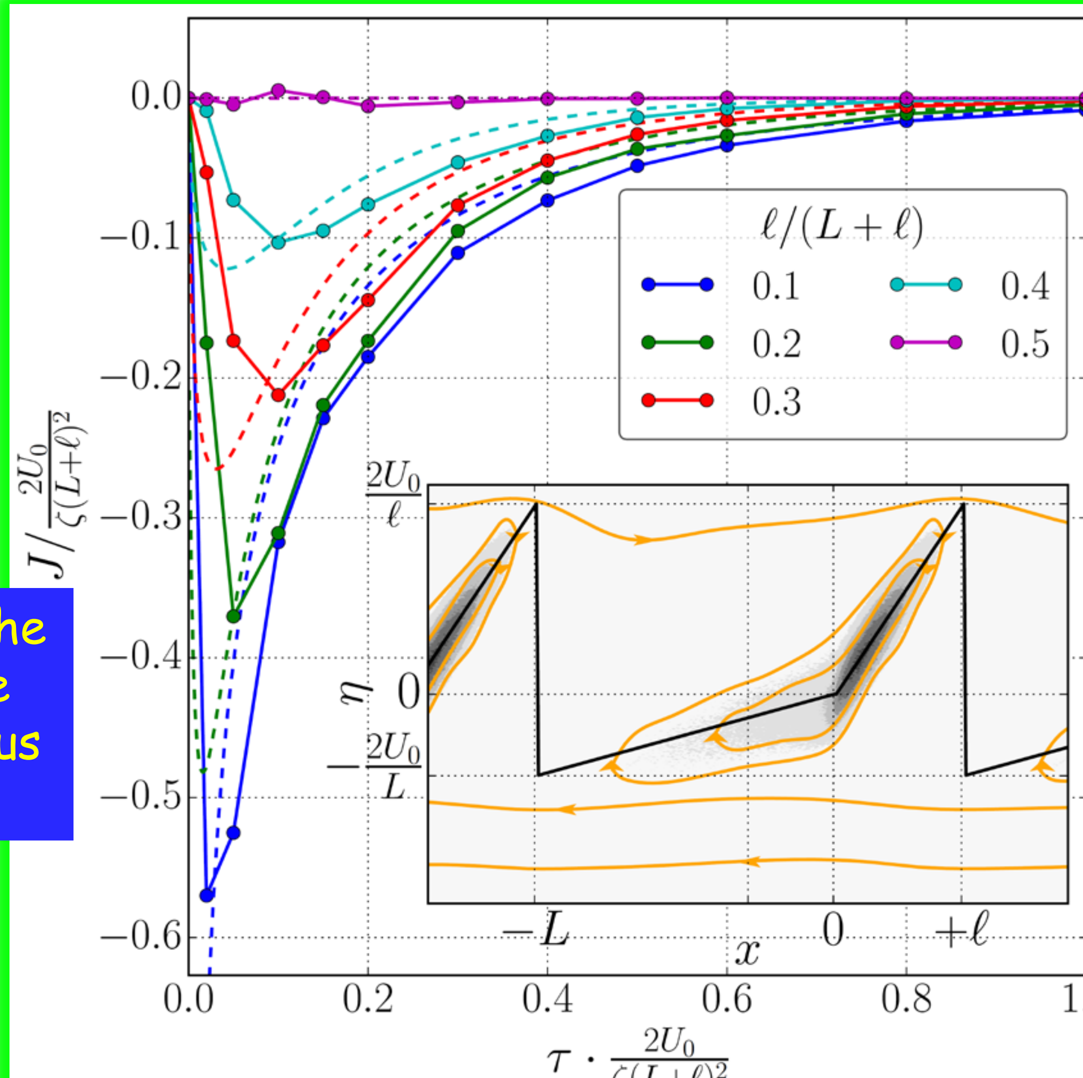


If we neglect diffusion altogether

Narrow bulk reduces pressure

Asymmetrical potential generates flow

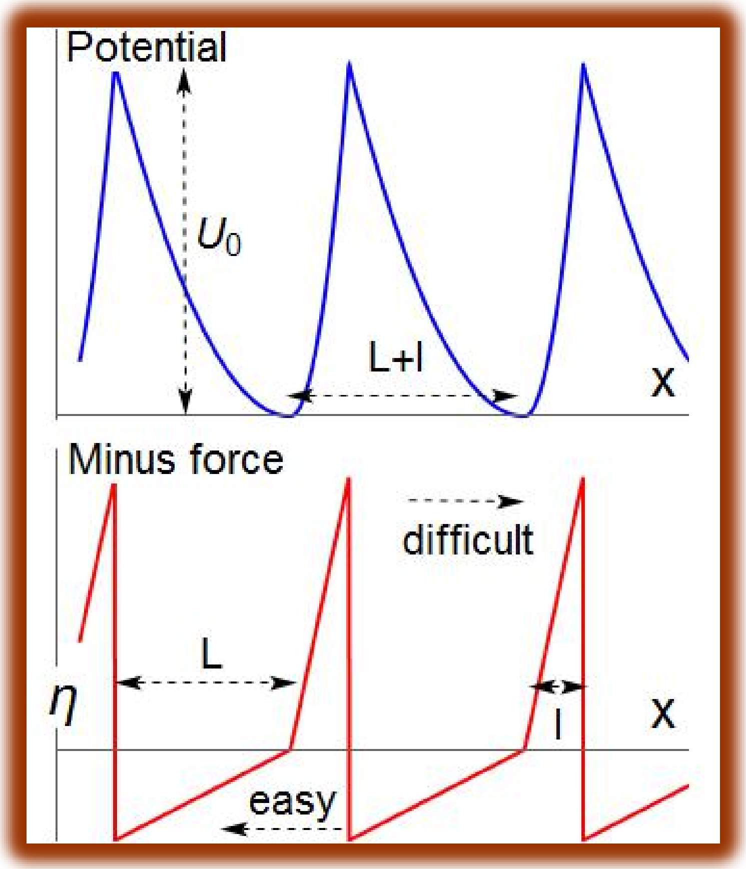




Although energy barriers are the same in both directions, force barriers are relevant in Sisyphus limit, and they are different

Similar to: M. O. Magnasco, Forced Thermal Ratchets, Phys. Rev. Lett. **71**, 1477 (1993).

Solvable model of a pump

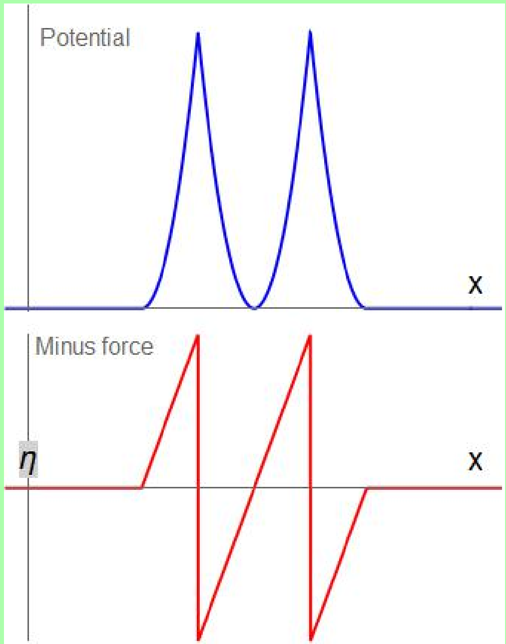


$$\rho(x,\eta) \approx \begin{cases} A\, p_K(x,\eta) & \text{for} \quad -L < x < 0 \\ a\, p_k(x,\eta) & \text{for} \quad 0 < x < \ell \end{cases}$$

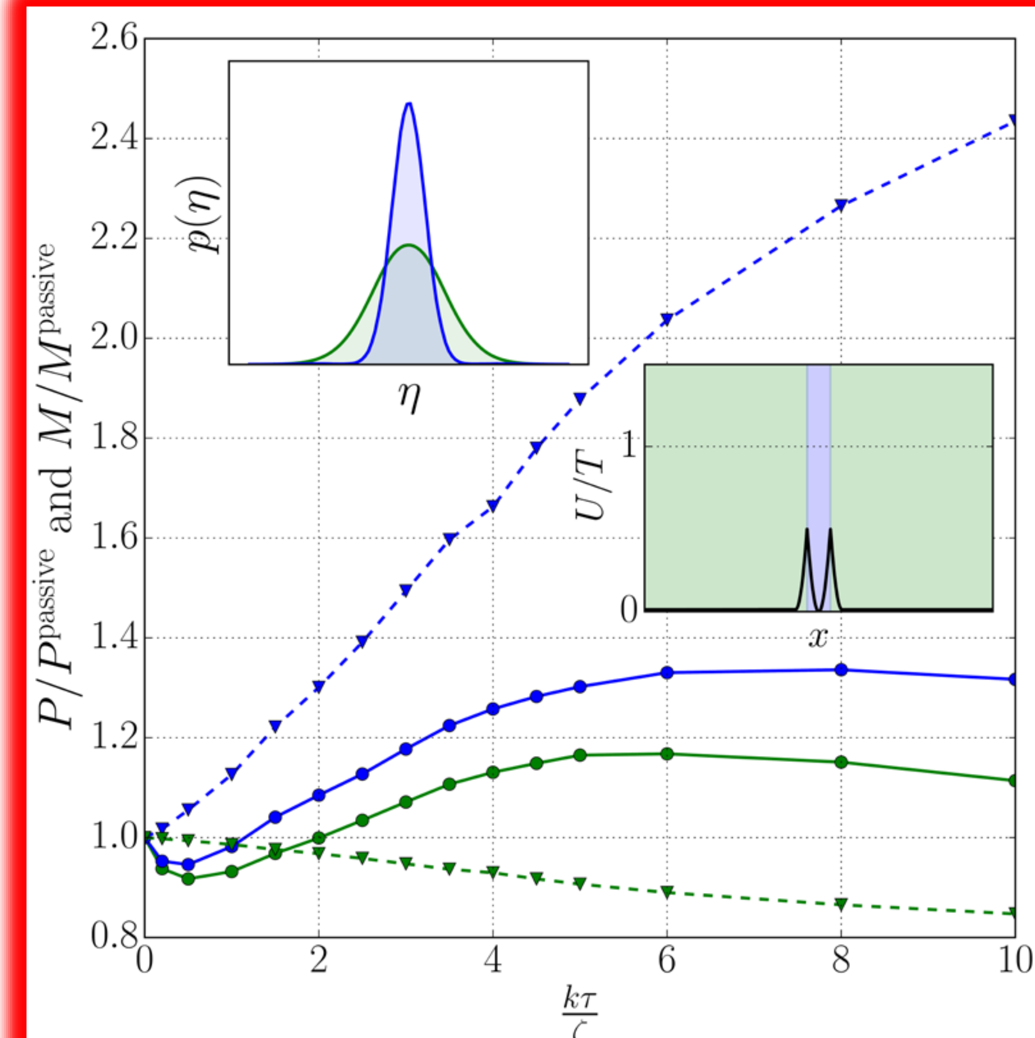
$$J = a \int_{k\ell}^{\infty} p_k(x=\ell,\eta)\frac{\eta - k\ell}{\zeta}\,\mathrm{d}\eta + \\ + A\int_{-\infty}^{-KL} p_K(x=L,\eta)\frac{\eta + KL}{\zeta}\,\mathrm{d}\eta$$

Although energy barriers LEFT and RIGHT are the same in Sisyphus limit FORCE barriers are different....

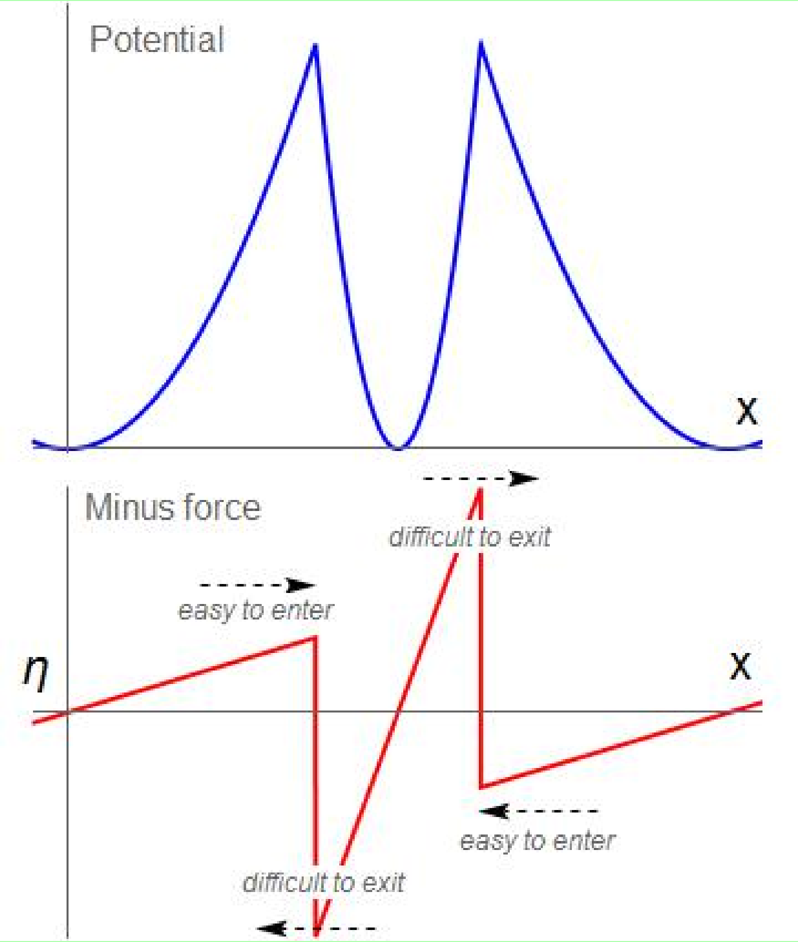
Narrowly spaced barriers repel



Particles in the gap are lackadaisical, but there are many of them



Solvable model of repulsive depletion



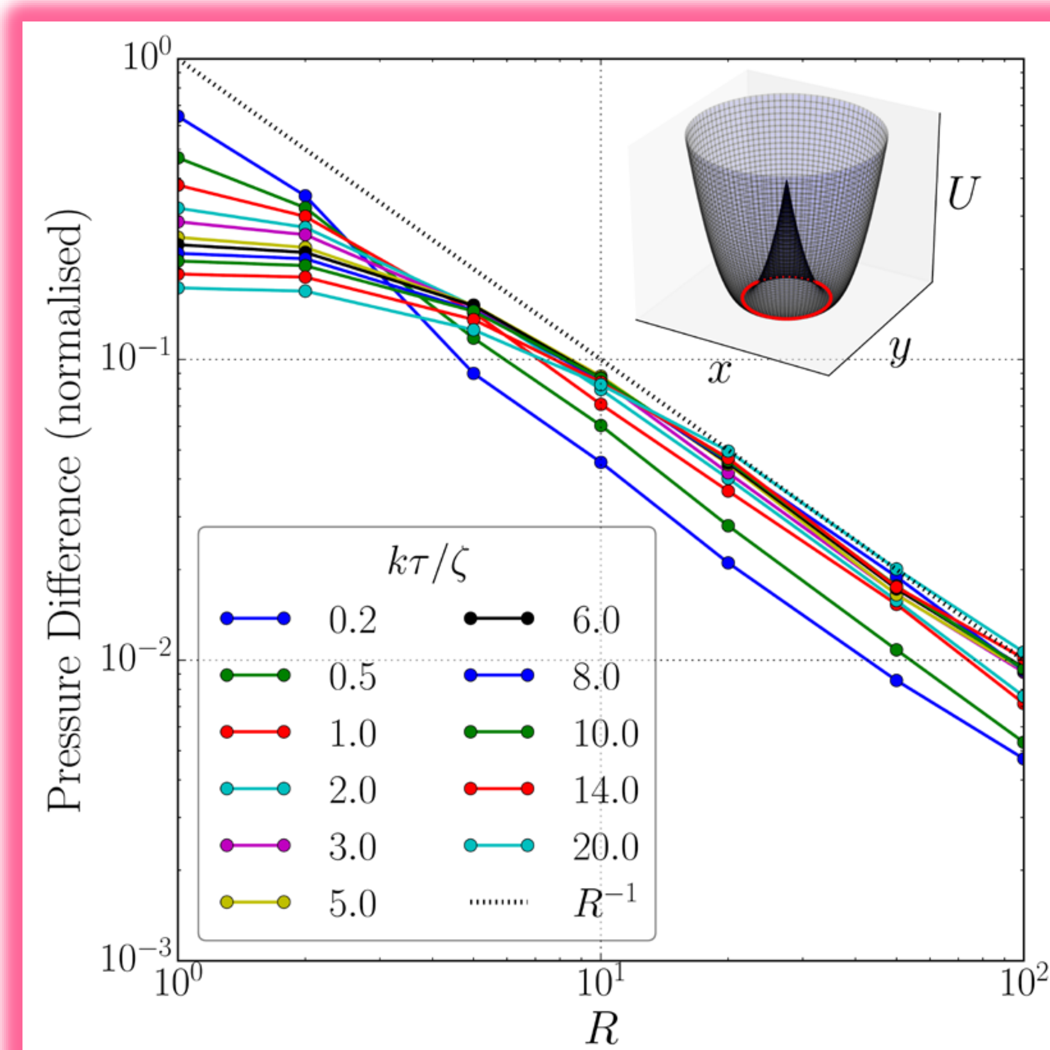
$$\rho(x,\eta) \approx \begin{cases} A\, p_K(x,\eta) & \text{for} \quad -L < x < 0 \\ a\, p_k(x,\eta) & \text{for} \quad 0 < x < \ell \end{cases}$$

$$J = a \int_{k\ell}^{\infty} p_k(x=\ell,\eta) \frac{\eta - k\ell}{\zeta} \, \mathrm{d}\eta + \\ + A \int_{-\infty}^{-KL} p_K(x=L,\eta) \frac{\eta + KL}{\zeta} \, \mathrm{d}\eta$$

Although energy barriers IN and OUT are the same in Sisyphus limit FORCE barriers are different....

Laplace pressure?

It does look like Laplace pressure, because it is ~1/R (inevitable result of expansion), but there is no surface tension



Conclusions

$$\zeta\dot{x} = f(x) + \eta(t)$$
$$\tau\dot{\eta} = -\eta + \xi(t)$$