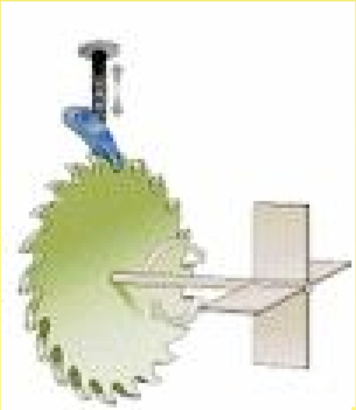
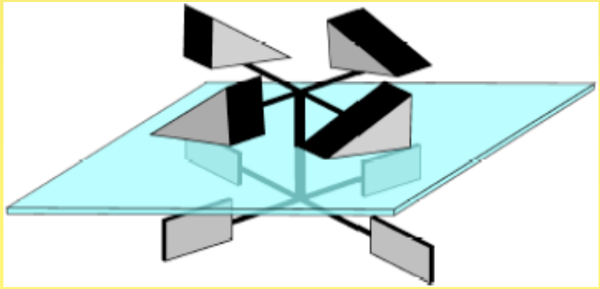
From Brownian motors to Brownian refrigerators





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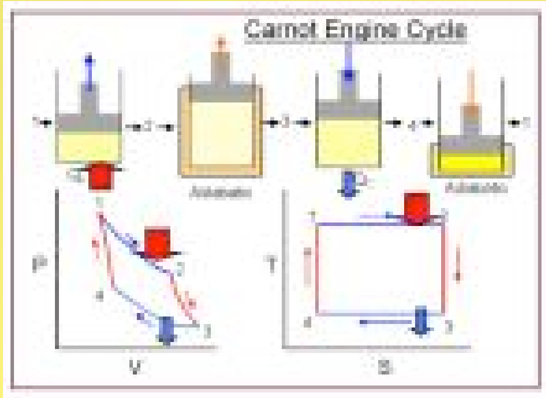
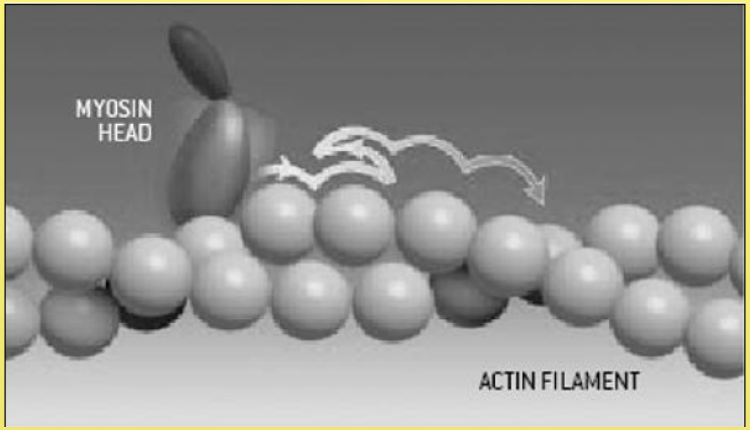


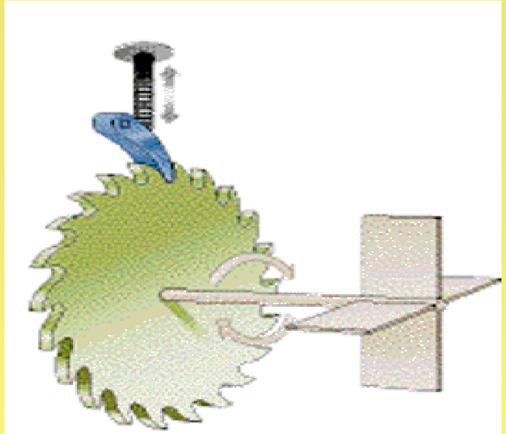
$$\eta = \frac{W}{Q} \leq 1 - \frac{T_1}{T_0}.$$

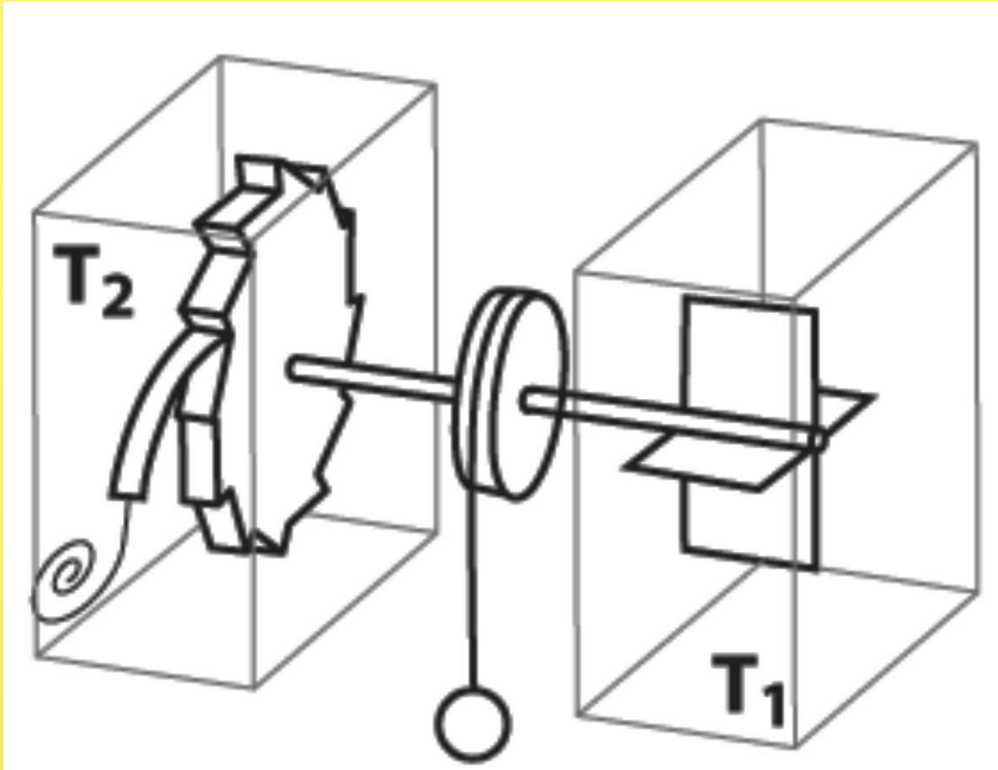
Equality reached for reversible process
Zero overall entropy production

Brownian motor?



Feynman
Caltech 1961



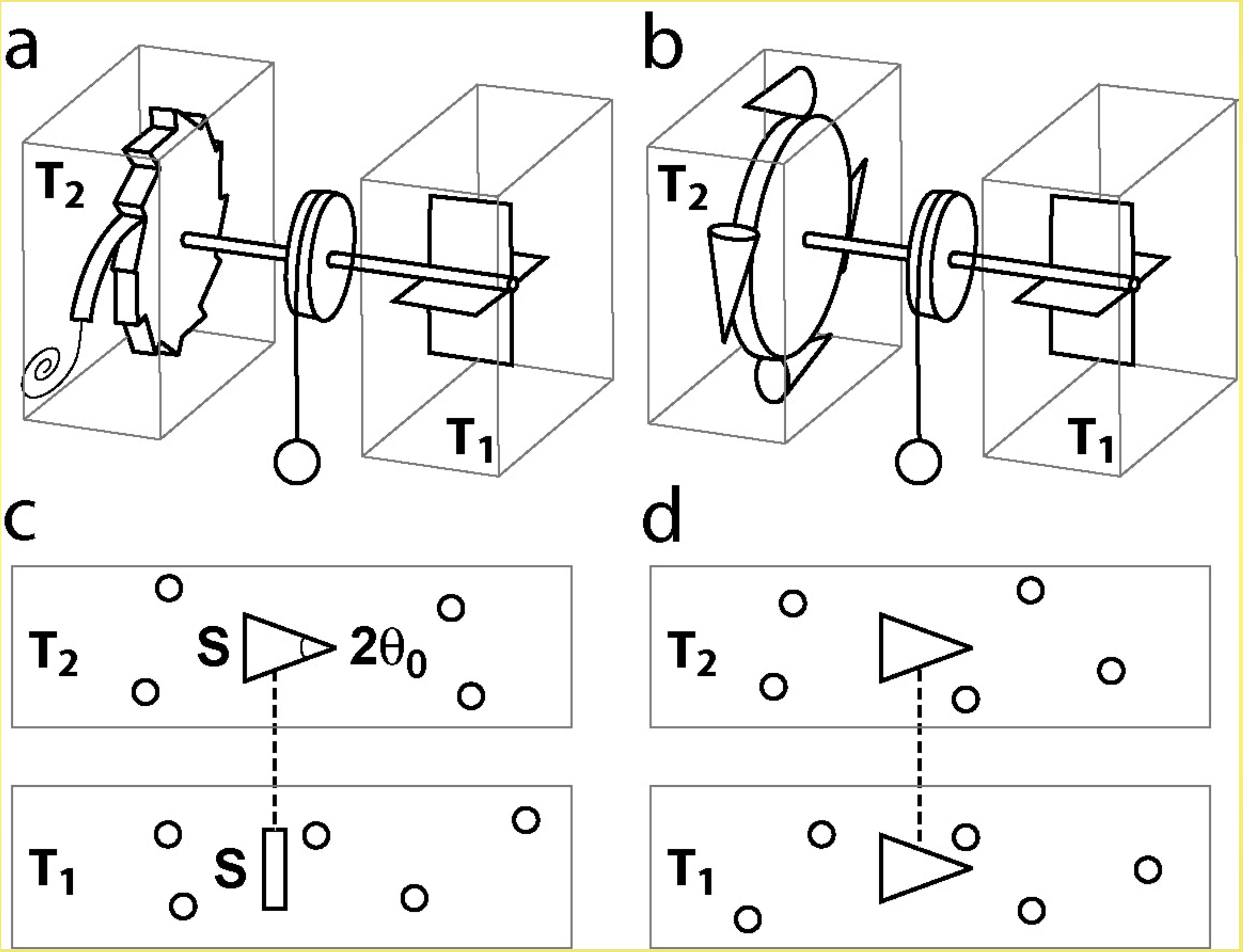


Boltzmann distribution

⇕

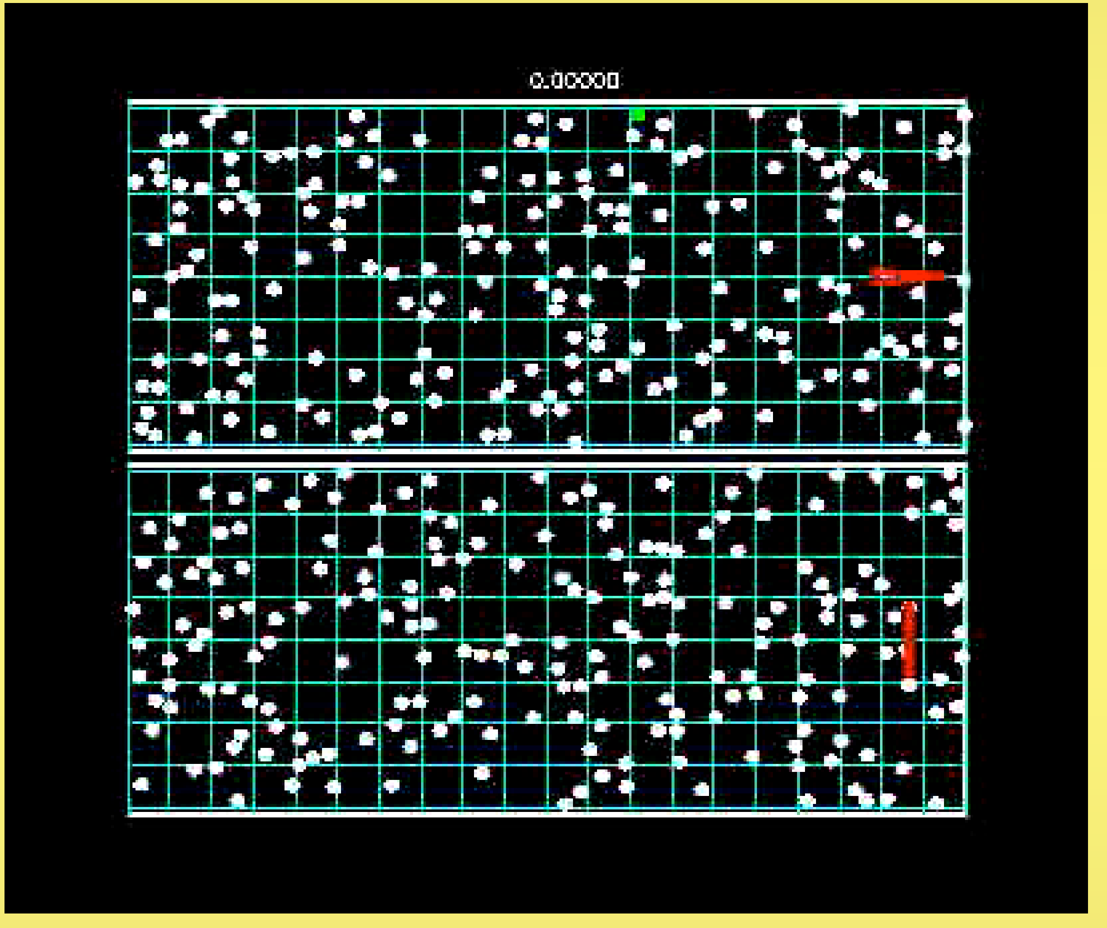
Carnot efficiency

Simplifying the Smoluchowski-Feynman ratchet

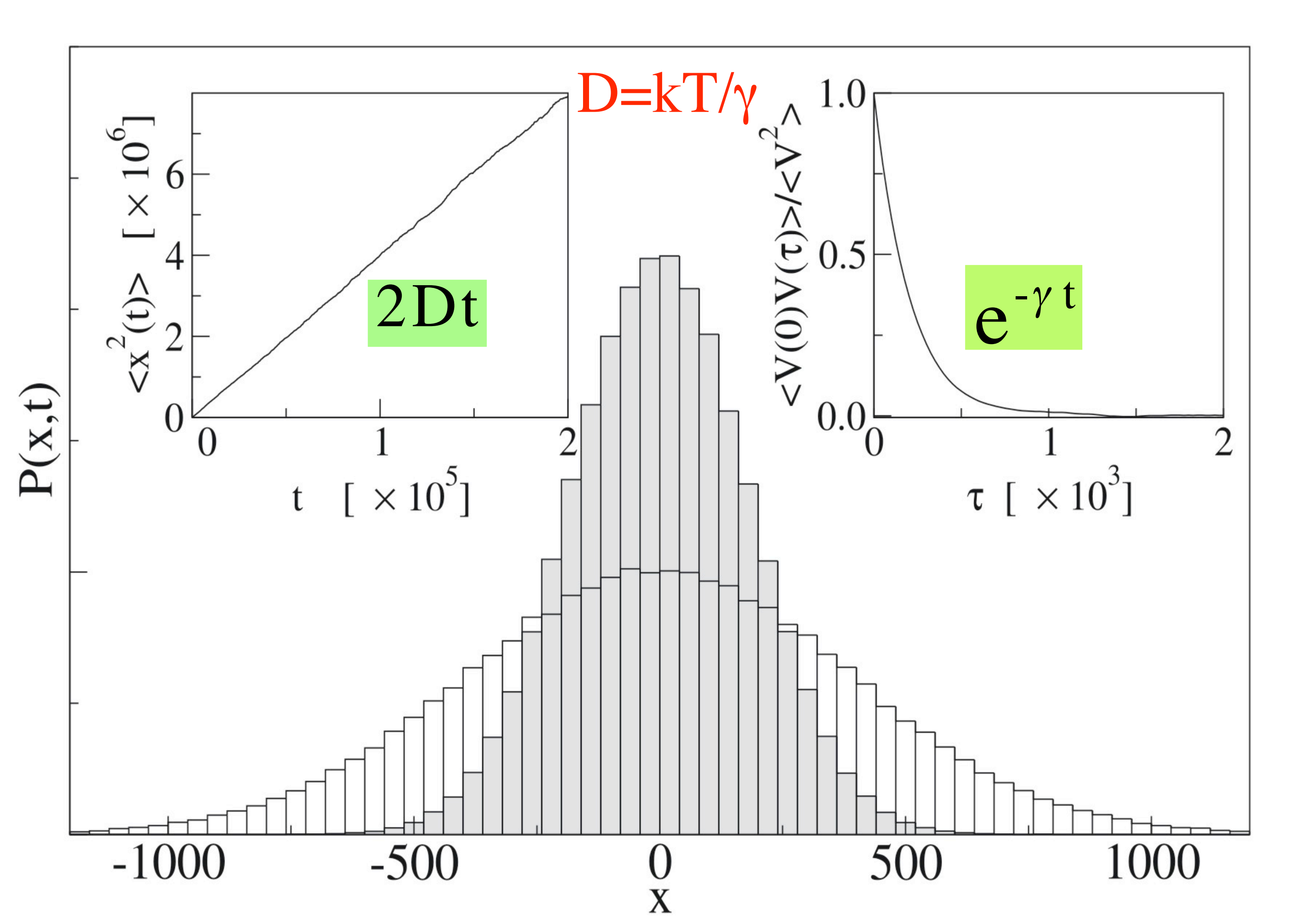


Triangulita Triangula

Triangulita molecular dynamics

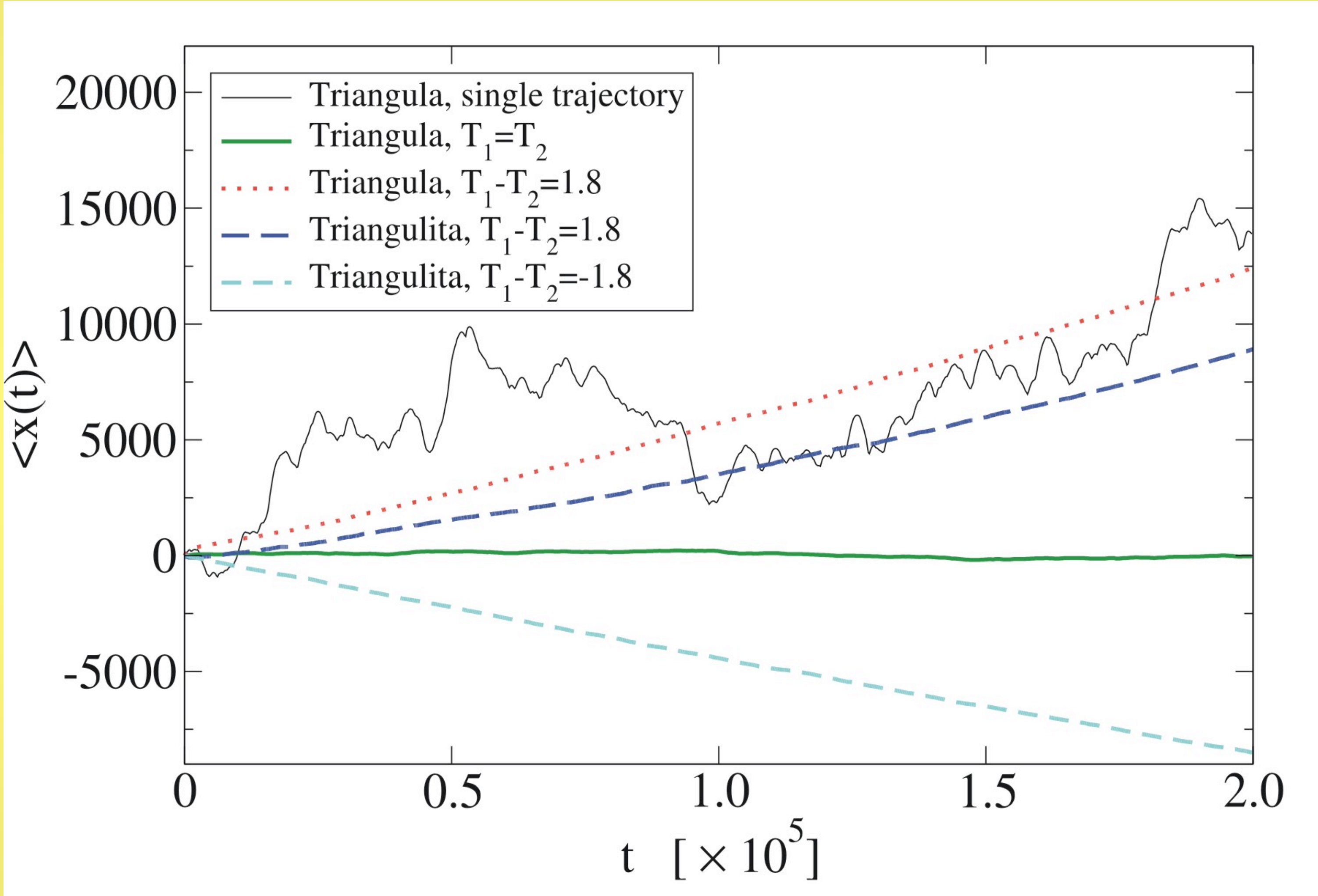


Triangula at equilibrium (T_1=T_2)



Unbiased Brownian motion

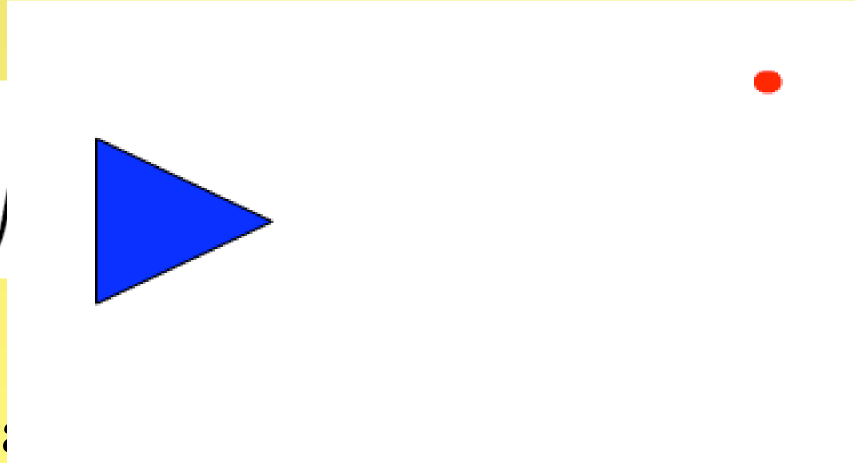
Triangula and Triangulita away from equilibrium ($T_1 \neq T_2$)



Average systematic drift: Brownian motor

Theory: Boltmann-Master equation

$$\frac{\partial P(V,t)}{\partial t} = \int \; \ldots \; V'|V)P(V,t)\Big]$$



Tr… …ory

$$W(V|V') = \sum_i \int_0^{2\pi} d\theta \, S_i F_i(\theta) \int_{-\infty}^{+\infty} dv'_x \int_{-\infty}^{+\infty} dv'_y \rho_i \phi_i(v'_x, v'_y)$$
$$\times (\vec{V}' - \vec{v}') \cdot \hat{e}_\perp \Theta \left[(\vec{V}' - \vec{v}') \cdot \hat{e}_\perp \right]$$
$$\times \delta \left[V - V' - \frac{2 \frac{m}{M} \sin^2\theta}{1 + \frac{m}{M}\sin^2\theta} \left(v'_x - v'_y \cot\theta - V' \right) \right]$$

Exact perturbative solution of steady state in terms of √ m/M

Lowest order: linear Langevin equation

$$\frac{\partial P(V,t)}{\partial t} = \int dV' \left[W(V|V')P(V',t) - W(V'|V)P(V,t) \right]$$

Van Kampen N G
Stochastic Processes in Physics and Chemistry

$\Downarrow$ Lowest order term in expansion

$$M\partial_t V = -(\gamma_1 + \gamma_2)V + \sqrt{2\gamma_1 k_B T_1}\,\xi_1(t) + \sqrt{2\gamma_2 k_B T_2}\,\xi_2(t)$$

$$\langle \xi_i(t)\xi_j(t') \rangle = \delta(t-t')\delta_{i,j}$$

$$\gamma_i = 4\rho_i L_i \sqrt{\frac{k_B T_i m}{2\pi}} \int_0^{2\pi} d\theta F_i(\theta) \sin^2\theta.$$

P(V)
Maxwellian
<V>=0

$$T_{eff} = \frac{\gamma_1 T_1 + \gamma_2 T_2}{\gamma_1 + \gamma_2}$$

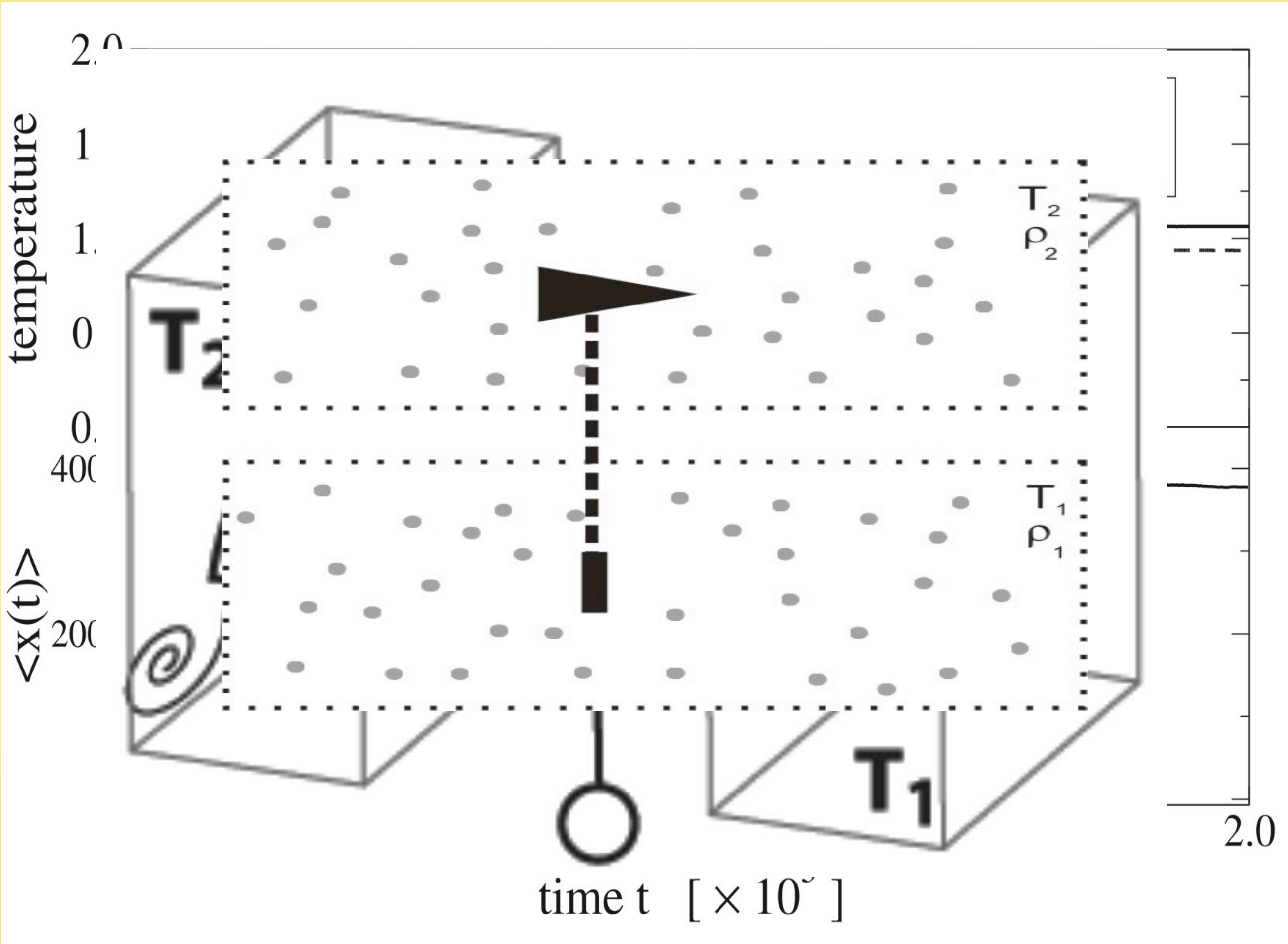
Heat conduction $\Downarrow$

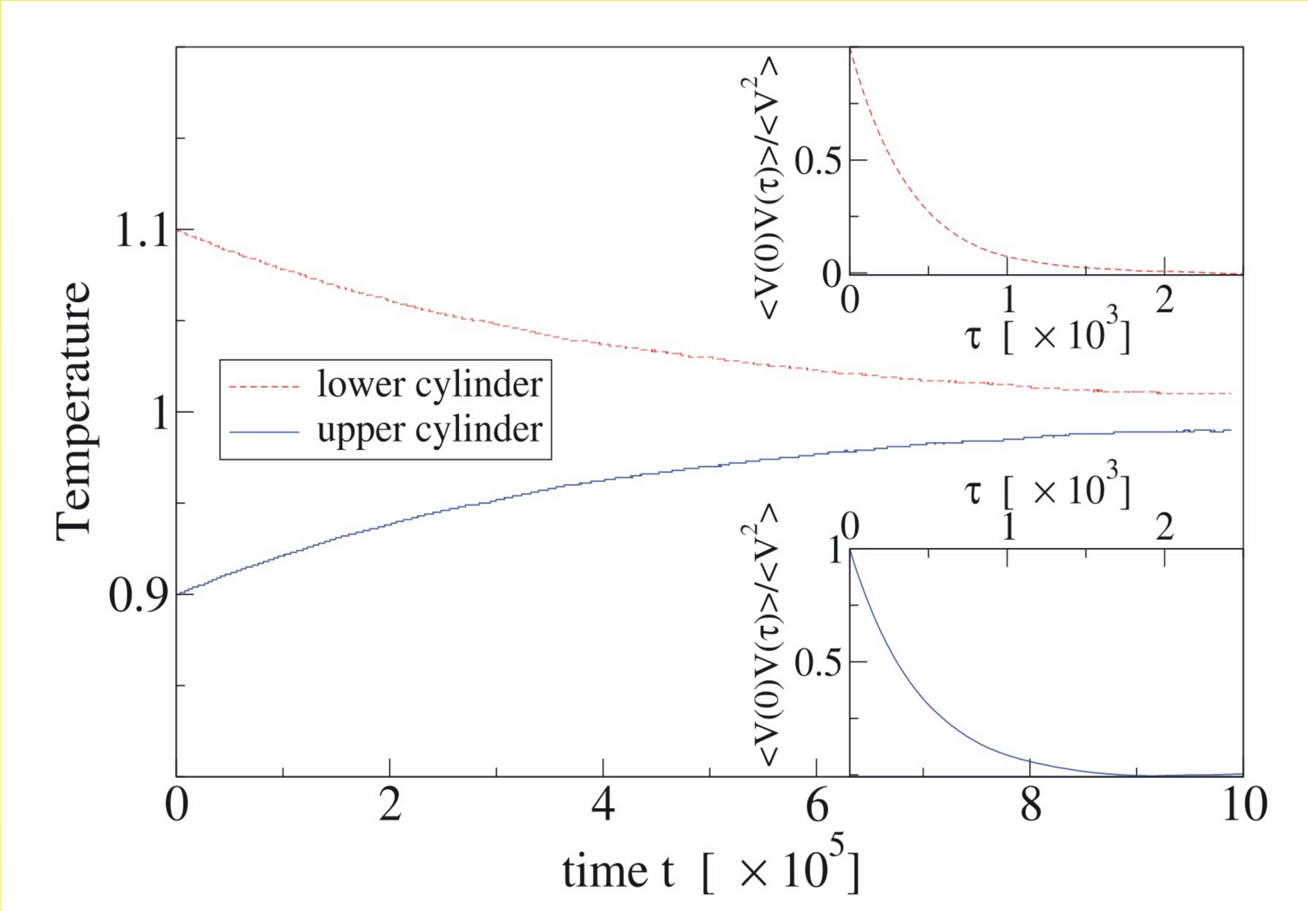
Fourier law

Parrondo J M R and Espagnol P
1996 *Am. J. Phys.* **64** 1125

$$Q_{1\to 2} = \kappa(T_1 - T_2), \qquad \kappa = \frac{k_B \gamma_1 \gamma_2}{M(\gamma_1 + \gamma_2)}$$

Heat conduction: source and demise of motion





$\kappa = 1.24 \times 10^{-3}$

$\kappa = 1.13 \times 10^{-3}$

theory

MD

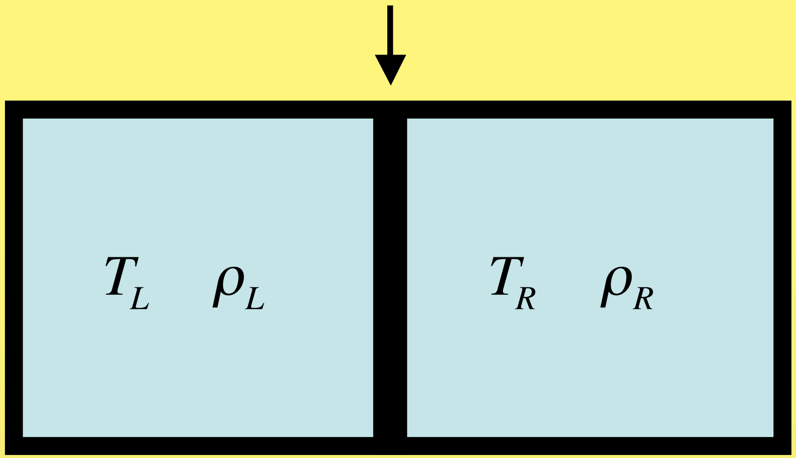
$$Q_{1\to 2} = \kappa(T_1 - T_2), \qquad \kappa = \frac{k_B \gamma_1 \gamma_2}{M(\gamma_1 + \gamma_2)}$$

The "adiabatic" piston: And yet it moves

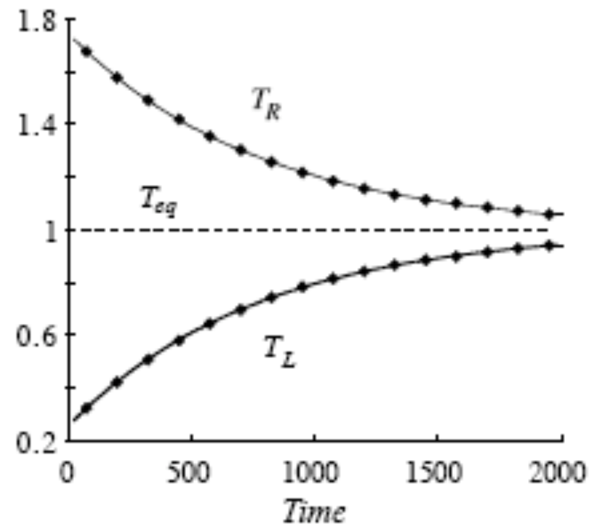
E. Kestemont[1], C. Van den Broeck[2] and M. Malek Mansour[1]

Europhys. Lett., 49 (2), pp. 143–149 (2000)

adiabatic piston



$$T_L \;\rho_L = T_R \;\rho_R$$



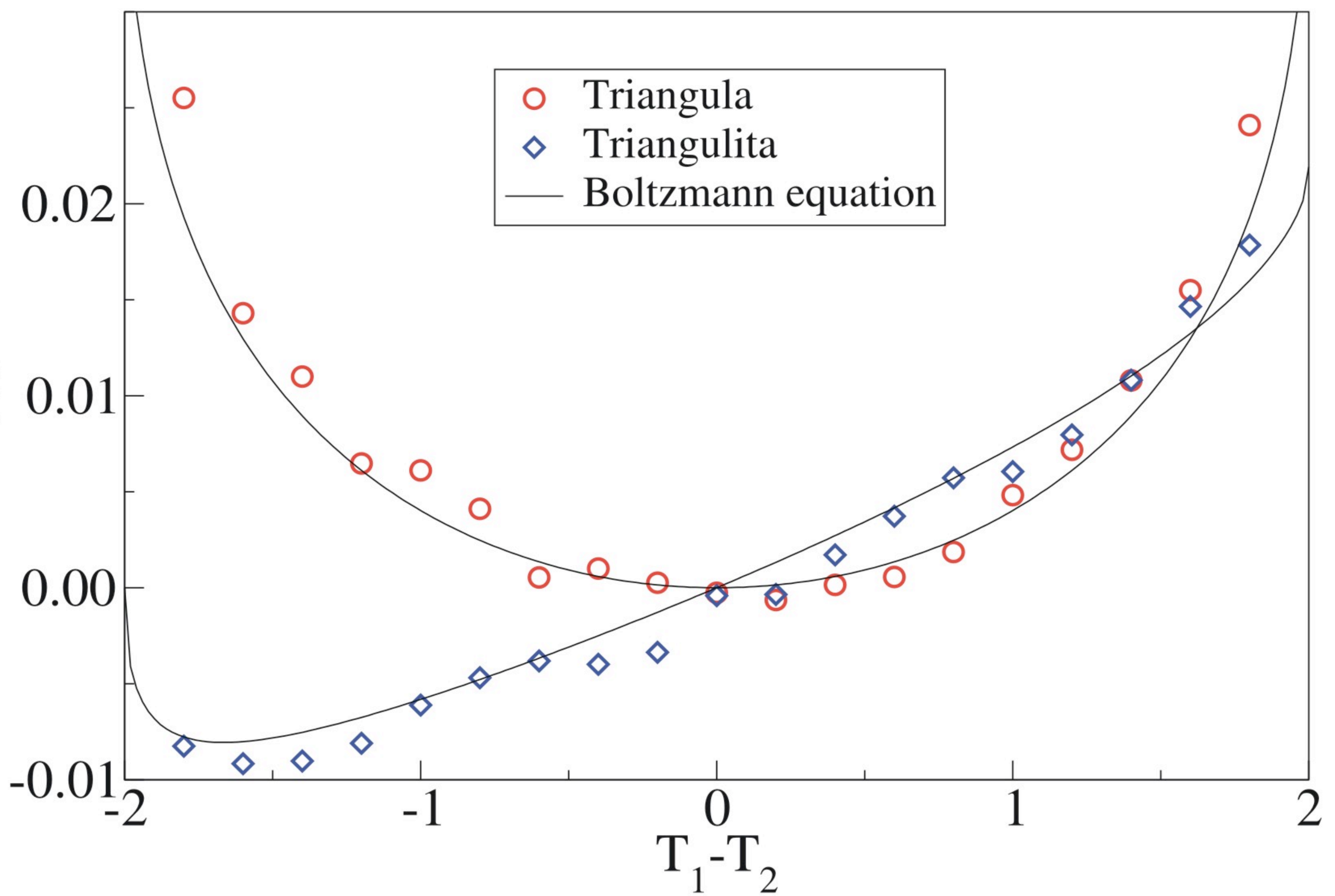
Next order: nonlinear non-Gaussian effects

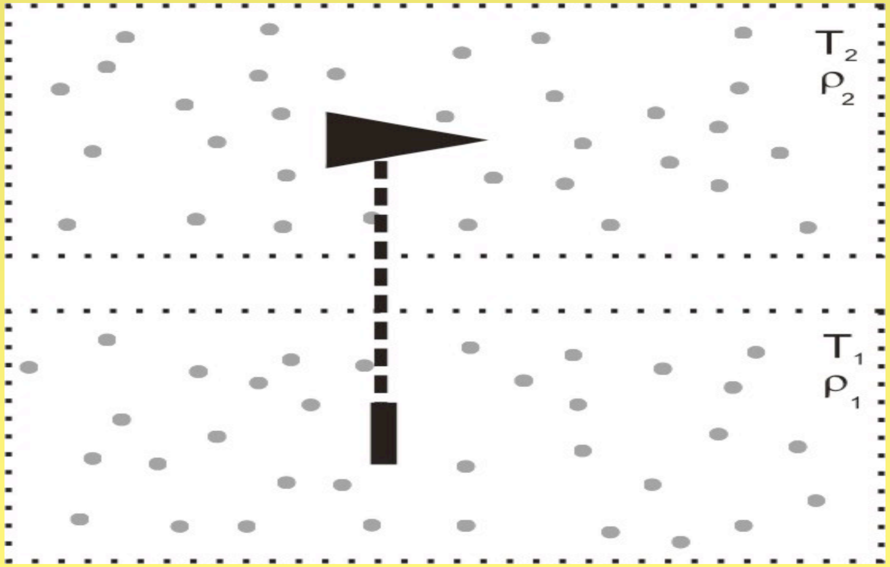
$$\langle V \rangle_{\mathrm{Triangula}} = \rho_1 \rho_2 (1 - \sin\theta_0) \frac{\sqrt{2\pi k_B m}}{4M} \frac{(T_1 - T_2)(\sqrt{T_1} - \sqrt{T_2})}{\left[\rho_1\sqrt{T_1} + \rho_2\sqrt{T_2}\right]^2}.$$

$$\langle V \rangle_{\mathrm{Triangulita}} = \rho_1 \rho_2 (1 - \sin^2\theta_0) \frac{\sqrt{2\pi k_B m}}{2M} \times \frac{(T_1 - T_2)\sqrt{T_1}}{[2\rho_1\sqrt{T_1} + \rho_2\sqrt{T_2}(1 + \sin\theta_0)]^2}.$$

Speed zero at equilibrium ($T_1 = T_2$) or symmetry ($\theta_0 = \pi/2$)
Speed ~ 1/M : Brownian motor
Maximum speed for maximum asymmetry (θ_0 -> 0)
Thermal speed $\sqrt{kT/M}$
Triangula: speed always positive
Triangulita: speed reversal at equilibrium

Comparison MD - theory: temperature difference





Friction

$$\gamma_i = 4\rho_i L_i \sqrt{\frac{k_B T_i m}{2\pi}} \int_0^{2\pi} d\theta F_i(\theta) \sin^2\theta.$$

Heat conduction

$$Q_{1\to 2} = \kappa(T_1 - T_2), \qquad \kappa = \frac{k_B \gamma_1 \gamma_2}{M(\gamma_1 + \gamma_2)}$$

Brownian motor

$$\langle V\rangle = \sqrt{\frac{m}{M}}\sqrt{\frac{\pi k_B T_{\text{eff}}}{8M}} \frac{\sum_i S_i\rho_i\left(\frac{T_i}{T_{\text{eff}}} - 1\right)\int_0^{2\pi} d\theta F_i(\theta)\sin^3\theta}{\sum_i S_i\rho_i\sqrt{\frac{T_i}{T_{\text{eff}}}}\int_0^{2\pi} d\theta F_i(\theta)\sin^2(\theta)}$$

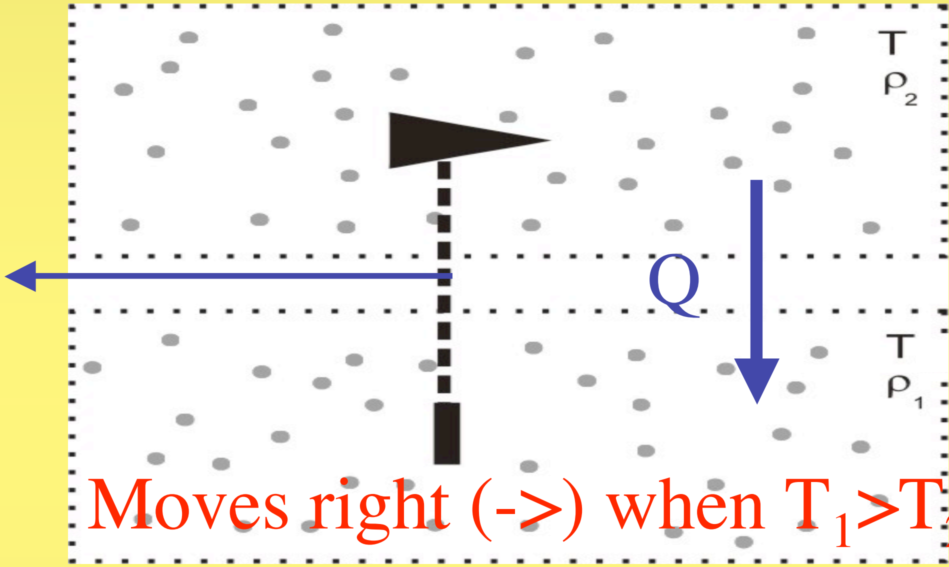
Brownian refrigerator ?!

Equilibrium

$T_1=T_2=T$

Apply force F

Effect?



Moves right (->) when $T_1>T_2$

Le Chatelier: an action on a system at equilibrium induces processes that attenuate or counteract the original perturbation.

Implication Q ~ F !

Onsager symmetry **force X_1**

Dissipation (~F^2)

$J_1 =$

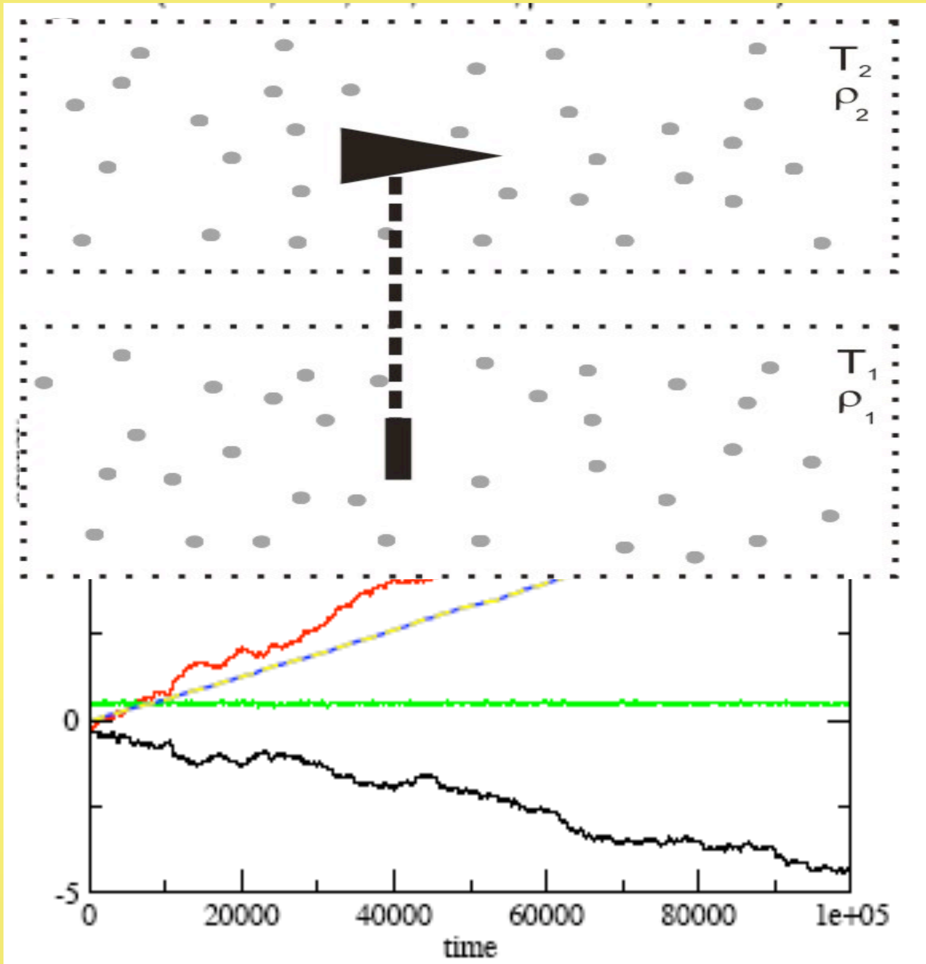
T-gradient –> particle flux

$X_2 = \Delta T / T^2$ $J_1 = \dot{x}$

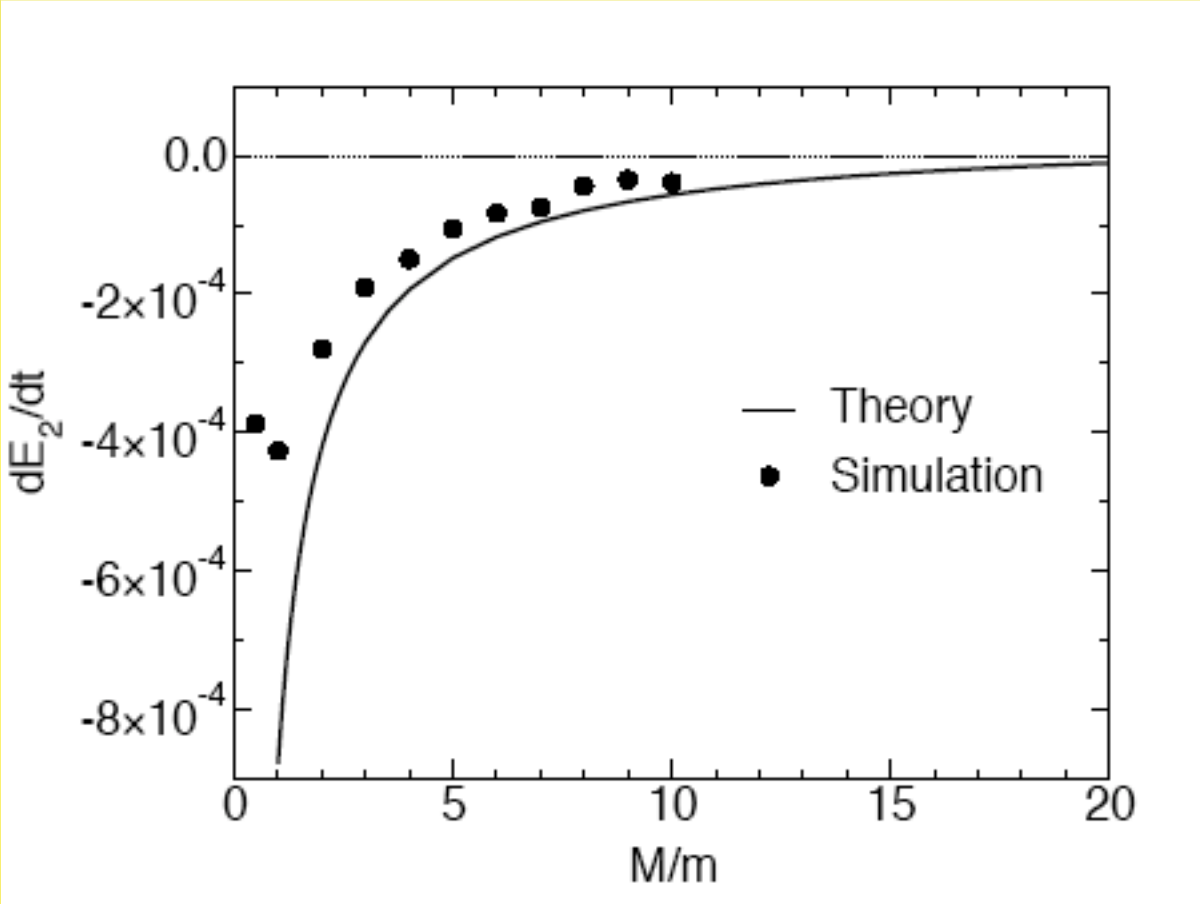
$$L_{12} = L_{21}.$$

Force –> heat flux

$X_1 = F/T$ $J_2 = \dot{Q}$



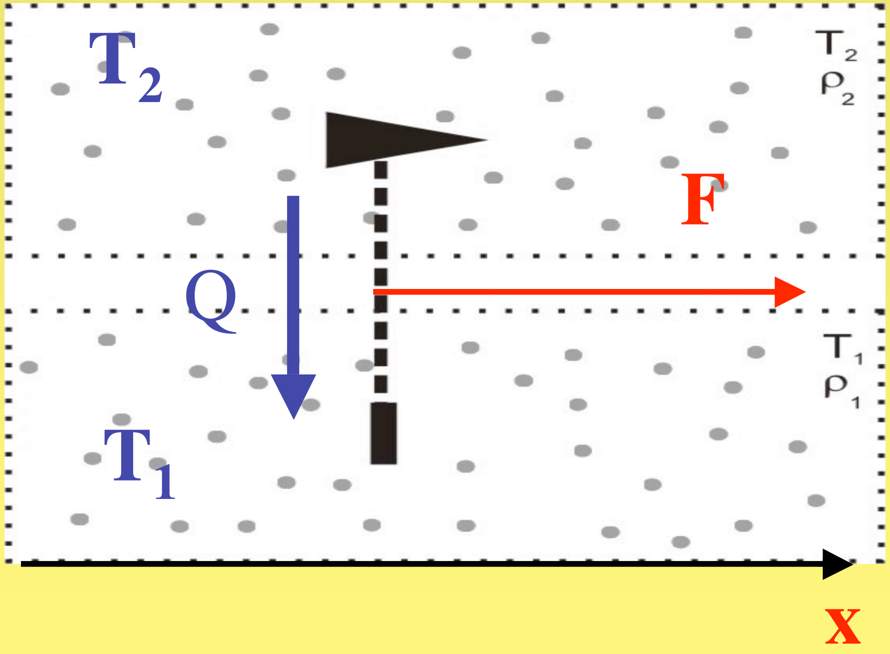
heat flux


0.0
-2×10^-4
-4×10^-4
-6×10^-4
-8×10^-4
dE2/dt
0
5
10
15
20
M/m
Theory
Simulation

$$dU = TdS \quad (V,N,...\mathrm{constant})$$

$$dS_1 = \frac{dU_1}{T_1} = \frac{dQ + F_1\,dx}{T_1}$$

$$dS_2 = \frac{dU_2}{T_2} = \frac{-dQ + F_2\,dx}{T_2}$$



$$dS = \left(\frac{1}{T_1} - \frac{1}{T_2}\right)dQ + \left(\frac{F_1}{T_1} + \frac{F_2}{T_2}\right)dx$$

$$\frac{dS}{dt} = \frac{\Delta T}{T^2}\frac{dQ}{dt} + \frac{F_1 + F_2}{T}\frac{dx}{dt}$$

$$\frac{dS}{dt} = \sum L_{ij} X_i X_j \geq 0$$

$$\frac{dS}{dt} = X_2 J_2 + X_1 J_1$$

$$X_2 = \Delta T / T^2$$

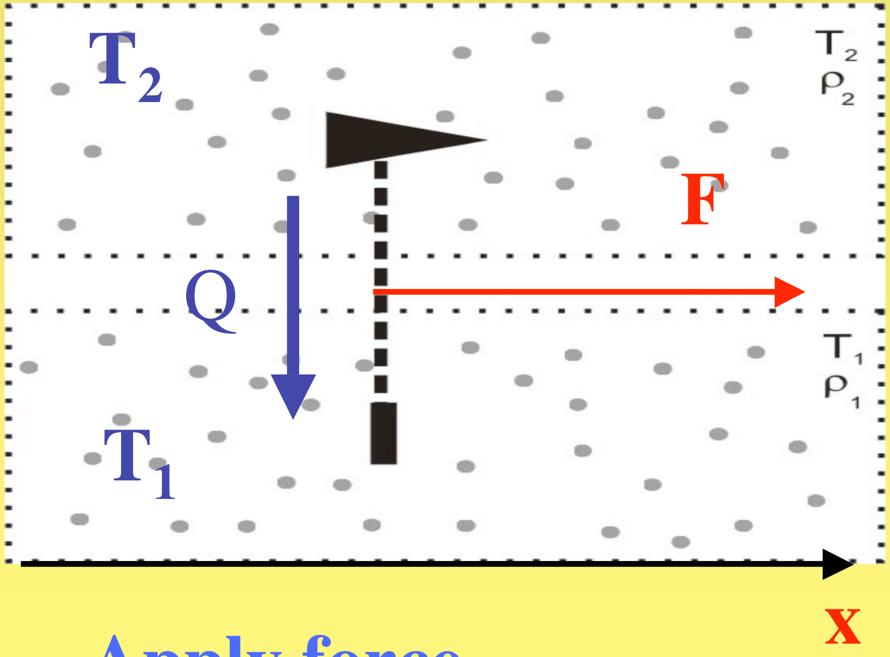
$$J_2 = \dot{Q}$$

$$X_1 = F/T$$

$$J_1 = \dot{x}$$

$$J_1 = L_{11}X_1 + L_{12}X_2$$

$$J_2 = L_{21}X_1 + L_{22}X_2.$$



Apply force

Friction

Refrigeration

Apply T gradient

Brownian motor

Heat conduction

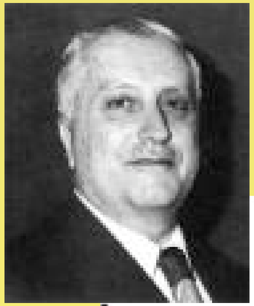
$$J_1 = L_{11}X_1 + L_{12}X_2$$
$$J_2 = L_{21}X_1 + L_{22}X_2.$$

$X_1 = F/T$ $X_2 = \Delta T/T^2$

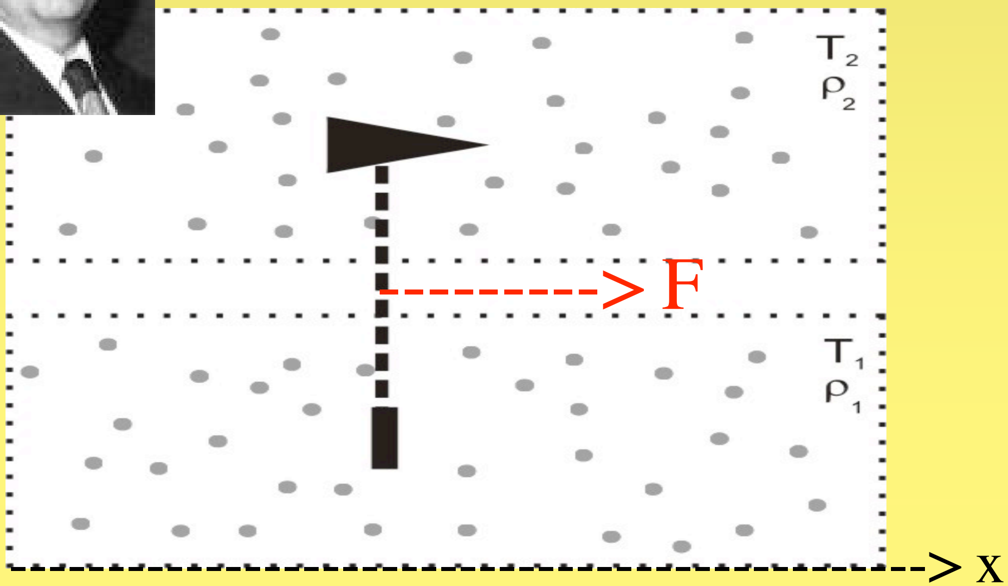
$$L_{11} = \frac{T}{\gamma},\quad L_{22} = \frac{k_B \gamma_1 \gamma_2 T^2}{M\gamma}.$$

$$L_{12} = \rho_1\rho_2(1 - \sin^2\theta_0) \times \sqrt{\frac{m}{M}}\sqrt{\frac{\pi k_B}{2M}}\frac{T^{3/2}}{[2\rho_1 + \rho_2(1+\sin\theta_0)]^2}.$$

$$\gamma_1 = 8\rho_1 L\sqrt{\frac{k_B T m}{2\pi}},\qquad \gamma_2 = 4\rho_2 L\sqrt{\frac{k_B T m}{2\pi}}(1+\sin\theta_0),$$



Linear irreversible thermodynamics



$X_1 = F/T \qquad J_1 = \dot{x}$

$X_2 = \Delta T/T^2 \qquad J_2 = \dot{Q}$

$\dot{W} = -F\dot{x} = -J_1 X_1 T$

$$\begin{aligned} J_1 &= L_{11}X_1 + L_{12}X_2 \\ J_2 &= L_{21}X_1 + L_{22}X_2. \end{aligned}$$

$d_iS/dt = J_1X_1 + J_2X_2 \geq 0$

$L_{11} \geq 0 \qquad L_{22} \geq 0$

$L_{11}L_{22} - L_{12}L_{21} \geq 0.$

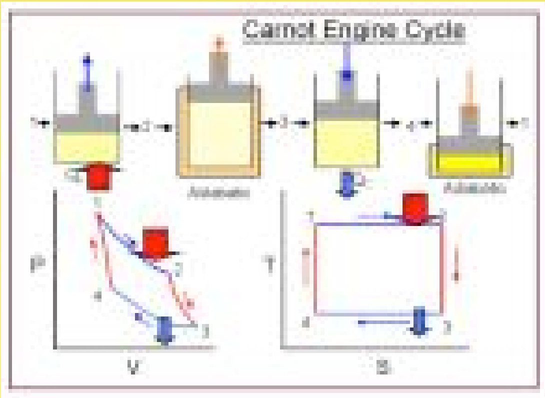
$$\eta = \frac{\dot{W}}{\dot{Q}} = -\frac{\Delta T}{T}\frac{J_1X_1}{J_2X_2} = \frac{\Delta T}{T}\left(-\frac{L_{11}}{L_{21}}\kappa\right)\frac{\kappa + L_{12}/L_{11}}{\kappa + L_{22}/L_{21}}$$

$\kappa = X_1/X_2$

Determinant Onsager matrix zero for $L_{12}/L_{11}=L_{22}/L_{21}$:

Both fluxes zero for stopping force: $-L_{11}/L_{21}\ \kappa = 1$!

Zero entropy production: Carnot efficiency $\eta=\Delta T/T$!



Best partner: $L_{12}/L_{11}=L_{22}/L_{21}$

Does the F-S ratchet have this property?

No

Can one make such a machine?

Yes (effusion, biological motors)

DISCUSSION

Feynman ratchet is unnecessarily complicated
Fully microscopic mechanical model
Hard disk molecular dynamics: only round-off error
Theory: perturbation in m/M, but exact, no adjustable parameters

Brownian motor moving at the speed of sound
Onsager symmetry: refrigerator dominant for small forcing
Full Onsager matrix

Efficiency: Carnot not achieved but in principle possible
Architectural constraint: strong coupling $L_{11}L_{22} = L_{12}L_{21}$

Curzon Ahlborn law for efficiency at maximum power:
also strong coupling $L_{11}L_{22} = L_{12}L_{21}$

Brownian motor

C. Van den Broeck, R. Kawai and P. Meurs, Phys Rev Lett **93**, 090601 (2004)

P. Meurs, C. Van den Broeck and A, Garcia, Phys Rev **E70**, 051109 (2004)

C. Van den Broeck, P. Meurs and R. Kawai, New J Phys **7**, 10 (2005)

Thermodynamic efficiency

C. Van den Broeck, Phys Rev Lett **95**, 190602 (2005)

C. Van den Broeck, Adv Chem Phys 135, 189 (2007)

Brownian refrigerator

C. Van den Broeck and R. Kawai, Phys Rev Lett **96**, 210601 (2006)