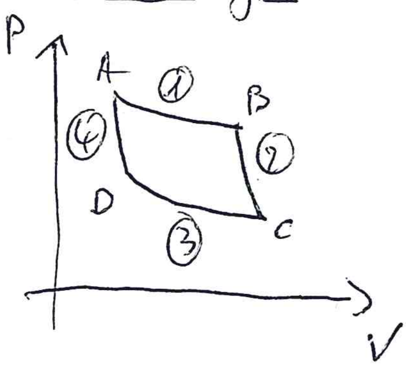
Chapter V: Thermal Ratchet and Stochastic Motors

If equilibrium is contagious and if equilibrated systems cannot break time-reversal symmetry, how can one create a motor? How can one produce a non-zero mean, directed motion?

I) No isothermal motor: the Carnot cycle

Reversible cycle



A→B: The system spontaneously expand (produce work). We inject heat to maintain T_H ⇒ isothermal expansion

B→C: Isolate the engine and let the expansion continue: adiabatic cooling, isentropic expansion.

C→D: isothermal compression (produce heat) at T_c

D→A: adiabatic, isentropic compression.

1st principle of thermodynamics: $dU = TdS - pdV$

$$\int_{cycle} dU = 0 = \underbrace{\int TdS}_{\text{Heat } Q} - \underbrace{\int pdV}_{\text{Work}} \Rightarrow \text{Work} = \int_{1} TdS + \overbrace{\int_{2} TdS}^{=0} + \int_{3} TdS + \overbrace{\int_{4} TdS}^{=0}$$

since $\Delta Q = 0$

1. $Q_H = T_H (S_B - S_A)$
2. $Q_c = T_c (S_D - S_c) = T_c (S_A - S_B)$

$\Big\}$ $W = (T_H - T_c)(S_B - S_A) > 0$ (Engine)

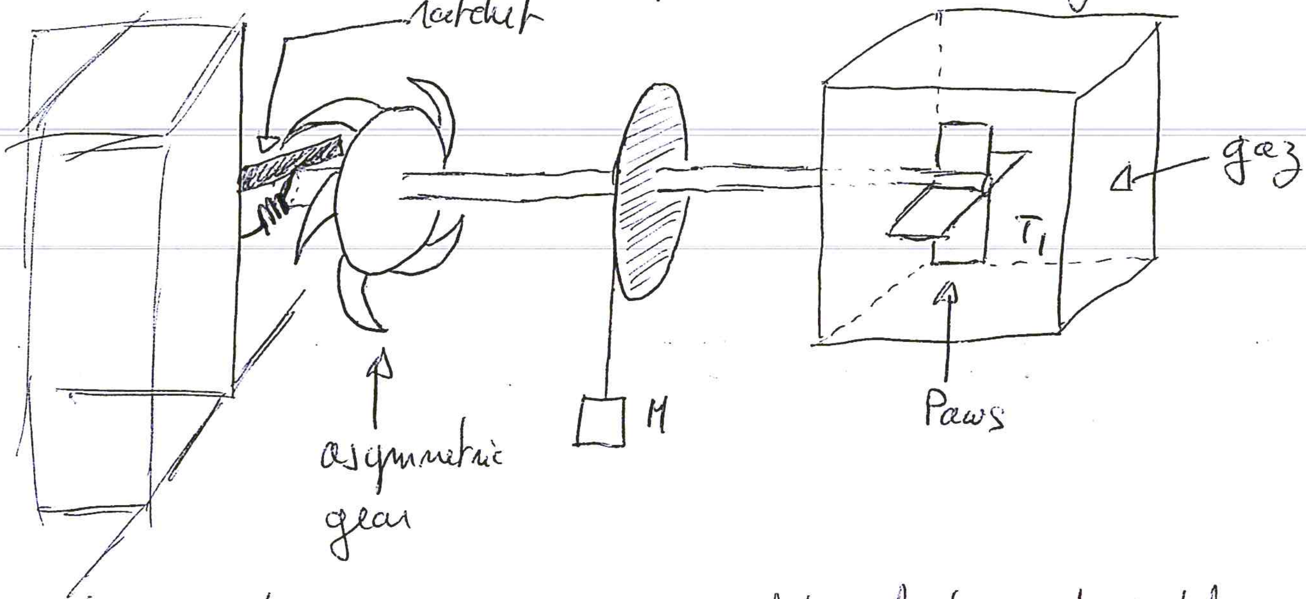
Cost: $Q_H > 0$ Efficiency $\frac{W}{Q_H} = 1 - \frac{T_c}{T_H}$; $T_c \to T_H$; $\eta \to 0$

⇒ Cannot extract work out of a single temperature engine at thermodynamic level (macroscopic world).

Maybe the fluctuations can help?

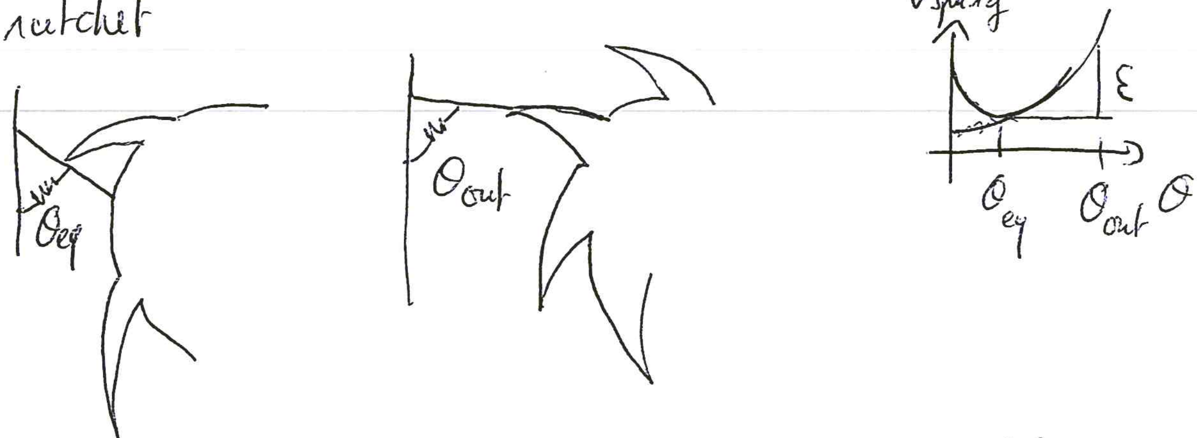
II Thermal ratchets

. Smoluchowsky, Phys. Z. 13, 1069 (1912)
. R.P. Feynman, Mecanics, Chap 46, lectures on Physics



Idee: The gear can easily rotate clockwise but the ratchet prevents counter-clockwise rotations. Fluctuations of the paws are thus rectified and the gear rotate in one direction, lifting the mass $M \to$ motor.

Where is the catch? To make the wheel rotate $\to$ need to lift the ratchet



$\Rightarrow$ Increase of energy ε. If there is no dissipation, the ratchet bounce and the wheel can rotate in both directions. If there is dissipation

$\boxed{10.4}$ then heat is produced and the ratchet a spring acquires a temperature T_1. Then the probability of a fluctuation of the paw that makes the spring spread is $P_{paw} \propto e^{-\frac{\varepsilon}{k_B T_1}}$ but the probability that the spring spontaneously opens up is also $P_{spring} \propto e^{-\frac{\varepsilon}{k_B T_1}}$

$\Rightarrow$ no motion except if $T_{spring} \neq T_{paw}$.

[Parrondo, Español, Am. J. Phys. 64, 1125 (1996)]

Conclusion: No motion out of equilibrium fluctuations

Need to break two symmetries:

- space $(x \to -x)$, asymmetric potential is ok.
- time $(t \to -t) \to$ need out of equilibrium dynamics $\Rightarrow$ need a steady-state flux in configuration space.

Several different strategies:

① Non-isothermal systems (2 different temperatures, energy flux)

② Two-state systems with transition rates between states that drive the system out of equilibrium (cf molecular motors)

③ Break FDT with temporal correlations

$$\dot p = -\int_{-\infty}^{t} ds\, \gamma(t-s)\, p(s) - V'(x(t)) + \sqrt{2k_BT}\,\eta(t)$$

with $\langle \eta(t)\eta(t')\rangle = \gamma(t-t') \to$ equilibrium

$\neq \gamma(t-t') \to$ not necessarily $\to$ motion?

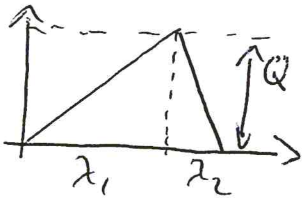
Conversely $\dot p = -\gamma p - V'(x) + \sqrt{2k_BT}\,\eta(t)$ with $\langle \eta(t)\eta(t')\rangle \neq \delta(t-t')$
$= \gamma(t-t')$

$\to$ may drive the system out of equilibrium.

III Fluctuating forces [Magnasco, Phys. Rev. Lett. 71, 1477 (1993)]

$\lambda = \lambda_1 + \lambda_2$

$\Delta = \lambda_1 - \lambda_2$

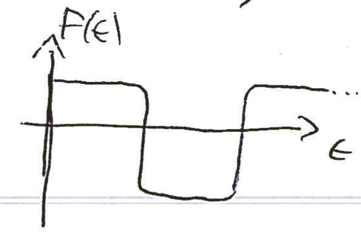


$\dot{x} = -\partial_x V(x) + \xi(t) + F(t)$

$\xi(t)$ GWN $\langle \xi \rangle = 0$; $\langle \xi(t)\xi(t')\rangle = \delta(t-t')2k$

$F(t)$ a fluctuating force of zero mean

Periodic boundary conditions.



(A) Constant F

FPE $\partial_t P = kT\partial_{xx}P + \partial_x(V'P - FP) = -\partial_x J$; $J = -kT\partial_x P + FP - V'P$

Steady-state $\Rightarrow$ constant $J \Rightarrow$ $\partial_x P = \beta[F - V']P - \beta J$ (1)

homogeneous solution $P_H(x) = \alpha\, e^{\beta[Fx - V(x)]}$

Look for $P_s(x) = \alpha(x)\, e^{\beta[Fx - V(x)]}$; (1) $\Rightarrow$ $\alpha'(x) = -\beta J\, e^{-\beta[Fx - V(x)]}$

$$\boxed{P(x) = P(0)\, e^{\beta[Fx - V(x)]} - \beta J \int_0^x du\, e^{-\beta[V(x) - Fx]}\, e^{\beta[V(u) - Fu]}}$$

$x \le \lambda_1$; $V(0) = 0$; $V(\lambda_1) = Q \Rightarrow V(x) = \frac{Qx}{\lambda_1}$

$\lambda_1 \le x \le \lambda$; $V(\lambda_1) = Q$; $V(\lambda) = 0 \Rightarrow V(x) = \frac{\lambda - x}{\lambda_2} Q$

Need to fix J and $P(0) \Rightarrow$ $P(\lambda) = P(0)$ and $\int_0^1 dx\, P(x) = 1$

Periodicity: $P(\lambda) = P(0)$

$$P(0) = P(0)\, e^{\beta F\lambda} - \beta J e^{\beta F\lambda} \int_0^\lambda du\, e^{\beta[V(u) - Fu]}$$

$$P(0)(1 - e^{\beta F\lambda}) = -\beta J e^{\beta F\lambda}\left[\int_0^{\lambda_1} du\, e^{\beta(\frac{Q}{\lambda_1} - F)u} + \int_{\lambda_1}^{\lambda} du\, e^{\beta\frac{\lambda Q}{\lambda_2} - \beta(F + \frac{Q}{\lambda_2})u}\right]$$

$$= -\beta J e^{\beta F\lambda}\left\{\frac{e^{\beta(\frac{Q}{\lambda_1} - F)\lambda_1} - 1}{\beta(\frac{Q}{\lambda_1} - F)} + e^{\beta\frac{\lambda Q}{\lambda_2}}\, \frac{e^{-\beta(F + \frac{Q}{\lambda_2})\lambda} - e^{-\beta(F + \frac{Q}{\lambda_2})\lambda_1}}{-\beta(F + \frac{Q}{\lambda_2})}\right\}$$

$$= -J\left\{\lambda_1 \frac{e^{\beta(Q + \lambda_1 F)} - e^{\beta\lambda F}}{Q - \lambda_1 F} - \lambda_2 \frac{1 - e^{\beta\lambda_2 F + \beta Q}}{Q + \lambda_2 F}\right\}$$

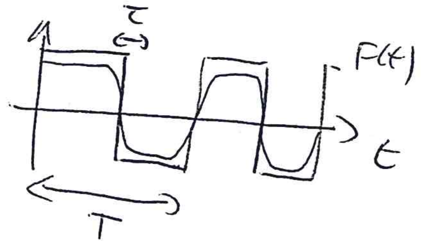
Multiply by $\exp\left[-\frac{\lambda_1+\lambda_2}{2}F\right]$

$$2P(0)\,\mathrm{sh}\left(\frac{\beta\lambda F}{2}\right)=J\left\{\lambda_1\frac{e^{\beta(Q-\frac{\Delta F}{2})}-e^{\beta\frac{\lambda F}{2}}}{Q-\lambda_1 F}+\lambda_2\frac{e^{\beta(Q-\frac{\Delta F}{2})}-e^{-\beta\frac{\lambda F}{2}}}{Q+\lambda_2 F}\right\}$$

$$\Rightarrow \boxed{J=\frac{2P(0)\,\mathrm{sh}\left(\beta\frac{\lambda F}{2}\right)}{\frac{\lambda_1}{Q-\lambda_1 F}\left(e^{\beta(Q-\frac{\Delta F}{2})}-e^{\beta\frac{\lambda F}{2}}\right)+\frac{\lambda_2}{Q+\lambda_2 F}\left(e^{\beta(Q-\frac{\Delta F}{2})}-e^{-\beta\frac{\lambda F}{2}}\right)}}$$

(B) Slowly varying F

$$\overline{J}=\frac{1}{T}\int_0^T J(F(t))\,dt$$



$T \gg$ relaxation time τ $\quad \overline{J}\simeq\frac{1}{2}\left(J(F)+J(-F)\right)$

Q°: under what condition is $\overline{J}\neq 0$?

① $\lambda_1=\lambda_2$, symmetric potential $P_0(-F)=P_0(F)$; $\lambda_1=\lambda_2=\frac{\lambda}{2}$

$J(F)=\frac{N(F)}{D(F)}$; $N(F)$ odd since $\mathrm{sh}(\beta\frac{\lambda F}{2})$ odd

$$D(F,\Delta=0)=\frac{\lambda}{2Q-\lambda F}\left(e^{\beta Q}-e^{\beta\frac{\lambda F}{2}}\right)+\frac{\lambda}{2Q+\lambda F}\left(e^{\beta Q}-e^{-\beta\frac{\lambda F}{2}}\right)$$

$$= f(F) + f(-F) \Rightarrow \text{even}$$

$\Rightarrow J(F)$ is odd and $\overline{J}(F)=0$

② $\lambda_1\neq\lambda_2$ In principle, need to compute $P_0(F)$. (See Magnasco's PRL)

Here, assume F small $P_0(\pm F)\simeq P_0\pm F$, numerator "close" to odd

$\overline{J}\neq 0$ if $D(F)-D(-F)\neq 0$

2019 ② $\lambda_1 \neq \lambda_2$ small Δ.

$$P_0(+\Delta) = P_0(-\Delta) \Rightarrow P_0^0 = P_0^0 + \frac{\Delta^2}{2} P_0''(\Delta=0)$$

$$J = \frac{N(F)}{D(F)} \; ; \; N(F) \simeq 2P_0^0 \, sh(\beta\lambda F/2)$$ odd function of F.

$$D(F) \simeq \underbrace{\frac{\lambda+\Delta}{2Q-\lambda F-\Delta F}} \left(e^{\beta Q}\left(1-\beta\frac{\Delta F}{2}\right) - e^{\beta\frac{\lambda F}{2}} \right) + \frac{\lambda-\Delta}{2Q+\lambda F-\Delta F}\left(e^{\beta Q}\left(1-\beta\frac{\Delta F}{2}\right) - e^{-\beta\frac{\lambda F}{2}} \right)$$

$$D(F) \simeq \frac{(\lambda+\Delta)}{2Q-\lambda F}\left(1+\frac{\Delta F}{2Q-\lambda F}\right)\left(e^{\beta Q} - e^{\beta\frac{\lambda F}{2}} - \beta e^{\beta Q}\frac{\Delta F}{2}\right) + \frac{\lambda-\Delta}{2Q+\lambda F}\left(1+\frac{\Delta F}{2Q+\lambda F}\right)\left(e^{\beta Q} - e^{-\beta\frac{\lambda F}{2}} - \beta e^{\beta Q}\frac{\Delta F}{2}\right)$$

$$\simeq \cancel{\frac{\lambda}{2Q-\lambda F}} N_0(F) + \Delta N_1(F)$$

$$D_0(F) = \frac{\lambda}{2Q-\lambda F}\left(e^{\beta Q} - e^{\beta\frac{\lambda F}{2}}\right) + \frac{\lambda}{2Q+\lambda F}\left(e^{\beta Q} - e^{-\beta\frac{\lambda F}{2}}\right) \equiv f(F) + f(-F)$$

$$D_1(F) = \frac{1}{2Q-\lambda F}\left(e^{\beta Q} - e^{\beta\frac{\lambda F}{2}}\right) - \frac{1}{2Q+\lambda F}\left(e^{\beta Q} - e^{-\beta\frac{\lambda F}{2}}\right)$$

$$+ \frac{\lambda F}{(2Q-\lambda F)^2}\left(e^{\beta Q} - e^{\beta\frac{\lambda F}{2}}\right) - \frac{-\lambda F}{(2Q+\lambda F)^2}\left(e^{\beta Q} - e^{-\beta\frac{\lambda F}{2}}\right)$$

$$- \frac{\beta\lambda F/2}{2Q-\lambda F} e^{\beta Q} + \frac{-\beta\lambda F/2}{2Q+\lambda F} e^{\beta Q}$$

$$= g(F) - g(-F)$$

$$J(F) = \frac{N(F)}{D_0(F)+\Delta D_1(F)} \simeq \frac{N(F)}{D_0(F)}\left(1-\Delta\frac{D_1(F)}{D_0(F)}\right) = \overset{\text{odd}}{\overset{\downarrow}{\frac{N(F)}{D_0(F)}}} - \Delta \overset{\text{even}}{\overset{\downarrow}{\frac{N(F)D_1(F)}{D_0(F)^2}}}$$

$$\bar{J}(F) \simeq -\Delta\frac{N(F)D_1(F)}{D_0(F)^2}$$ $\Rightarrow$ current when $\Delta \neq 0$