Macroscopic Stochastic Thermodynamics (Lecture V)

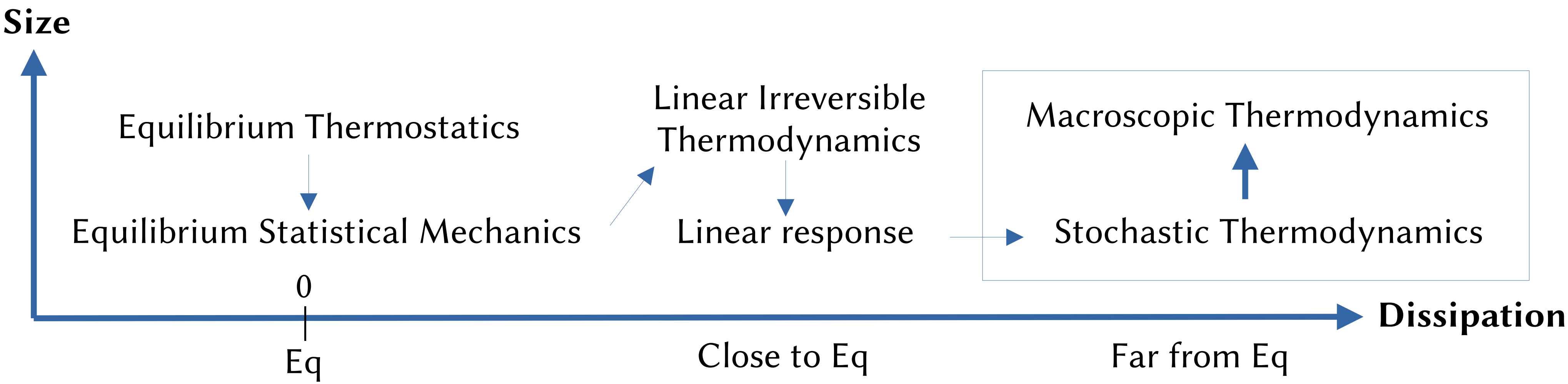
Massimiliano Esposito

RRI, Bangalore, Sep 10, 2024

UNIVERSITÉ DU LUXEMBOURG

Fonds National de la Recherche Luxembourg

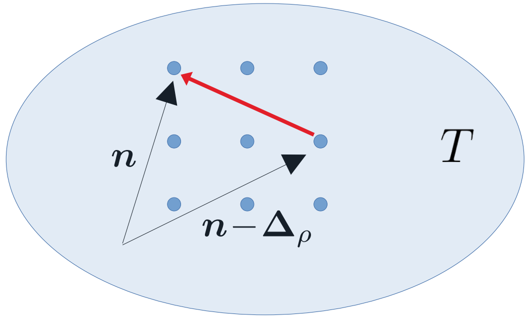
Introduction



Stochastic thermodynamics

Stochastic thermodynamics

$$\partial_t P_t(\boldsymbol{n}) = \sum_\rho \left[\lambda_\rho(\boldsymbol{n}-\boldsymbol{\Delta}_\rho)P_t(\boldsymbol{n}-\boldsymbol{\Delta}_\rho) - \lambda_\rho(\boldsymbol{n})P_t(\boldsymbol{n})\right]$$



Thermodynamic consistency is introduced via the **local detailed balance** condition:

$$\log \frac{\lambda_\rho(\boldsymbol{n})}{\lambda_{-\rho}(\boldsymbol{n}+\boldsymbol{\Delta}_\rho)} = -\frac{1}{k_b T}\left[\Phi(\boldsymbol{n}+\boldsymbol{\Delta}_\rho) - \Phi(\boldsymbol{n}) - W_\rho(\boldsymbol{n})\right]$$

For simplicity: isothermal, autonomous

In general see:

Rao, Esposito, *NJP* **20**, 023007 (2018)

Free energy of the state

$\Phi(\boldsymbol{n}) = E(\boldsymbol{n}) - TS(\boldsymbol{n})$

Nonconservative work

Reservoirs causing the transitions are at equilibrium

1st Law: $d_t\langle E\rangle = \langle \dot{W}\rangle + \langle \dot{Q}\rangle$

2nd Law: $\dot{\Sigma} = d_t S - \frac{\langle \dot{Q}\rangle}{T} = \frac{\langle \dot{W}\rangle - d_t\Phi}{T} \geqslant 0$

Heat $$\langle \dot{Q}\rangle = \sum_{\rho,\boldsymbol{n}} Q_\rho(\boldsymbol{n}) j_\rho(\boldsymbol{n})$$

Work $$\langle \dot{W}\rangle = \sum_{\rho,\boldsymbol{n}} W_\rho(\boldsymbol{n}) j_\rho(\boldsymbol{n})$$

$$j_\rho(\boldsymbol{n}) = \lambda_\rho(\boldsymbol{n}) P_t(\boldsymbol{n})$$

Entropy production $$\dot{\Sigma} = \frac{k_b}{2}\sum_{\rho,\boldsymbol{n}}\left(j_\rho(\boldsymbol{n}) - j_{-\rho}(\boldsymbol{n}+\boldsymbol{\Delta}_\rho)\right)\log\frac{j_\rho(\boldsymbol{n})}{j_{-\rho}(\boldsymbol{n}+\boldsymbol{\Delta}_\rho)} \geqslant 0$$

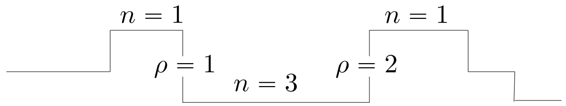
System entropy $$S = \sum_{\boldsymbol{n}} P_t(\boldsymbol{n})\big(S(\boldsymbol{n}) - \underbrace{k_b \log P_t(\boldsymbol{n})}_{\text{Shannon}}\big)$$

Free energy $$\Phi = \langle E\rangle - TS \qquad \Phi - \Phi^{eq} = k_b T D(p|p^{eq}) \geqslant 0$$

$$\left(D(p_i|p_i') \equiv \sum_i p_i \ln\frac{p_i}{p_i'} \geq 0 \right)$$ Kullback-Leibler divergence

Detailed balance dynamics, $W_\rho(\boldsymbol{n}) = 0$, minimizes free energy

Entropy production along a stochastic trajectory

$\Gamma_{\rightarrow}$: 

$$\sigma = k_B \ln \frac{\mathcal{P}[\Gamma_{\rightarrow}]}{\mathcal{P}[\Gamma_{\leftarrow}]}$$

Fluctuation theorem $$\frac{P(\sigma)}{P(-\sigma)} = e^{\sigma/k_B}$$

Overview: Rao, Esposito, *Entropy* **20**, **635** (2018)

$$\Sigma = \langle \sigma \rangle = D(\mathcal{P}_{\rightarrow}|\mathcal{P}_{\leftarrow}) \geq 0$$

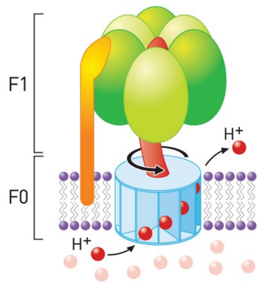
statistical measure
of time-reversal breaking

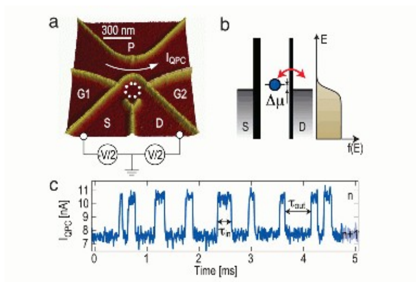
$$\left(D(p_i|p_i') \equiv \sum_i p_i \ln \frac{p_i}{p_i'} \geq 0 \right)$$
Kullback-Leibler divergence

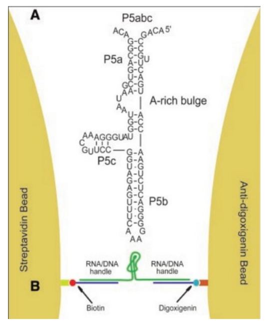
$$\frac{\langle O \rangle^2}{Var(O)} \leqslant \frac{\Sigma}{2k_B}$$

Thermodynamic uncertainty relation

Verified in many setups







Coarse graining underestimates entropy production $D(\mathcal{P}_{\rightarrow}|\mathcal{P}_{\leftarrow}) \geq D(\bar{\mathcal{P}}_{\rightarrow}|\bar{\mathcal{P}}_{\leftarrow})$

Macroscopic limit

Macroscopic limit at equilibrium

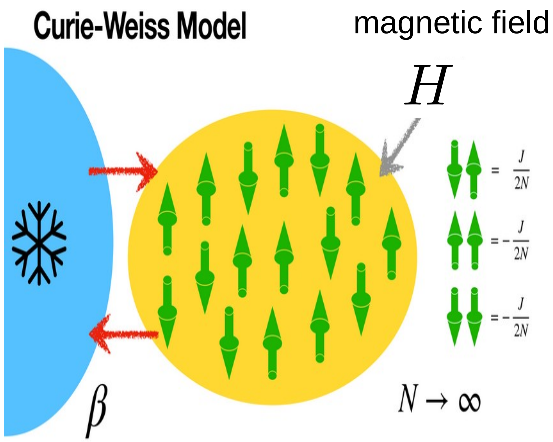
Free energy of state x

$$P_{\mathrm{eq}}(x) = \frac{e^{-\Phi(x)/k_b T}}{Z} \asymp e^{-\Omega(\phi(x)-\phi_{\min})/k_b T}$$

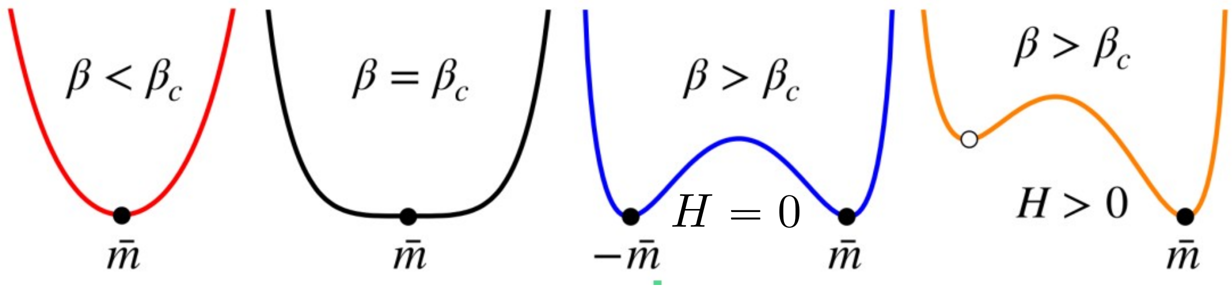
Ω: Scale parameter

Macro limit

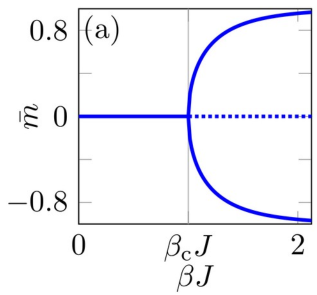
Phase transitions: changes in minima



Magnetization



Bifurcations



$H = 0$

Macroscopic dynamics

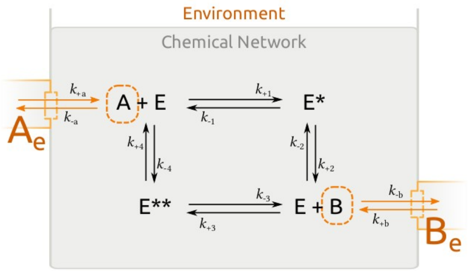
$$\partial_t P(\boldsymbol{n},t) = \sum_\rho [\lambda_\rho(\boldsymbol{n}-\boldsymbol{\Delta}_\rho)P(\boldsymbol{n}-\boldsymbol{\Delta}_\rho,t) - \lambda_\rho(\boldsymbol{n})P(\boldsymbol{n},t)]$$

Scale parameter Ω

$\Omega \to \infty$

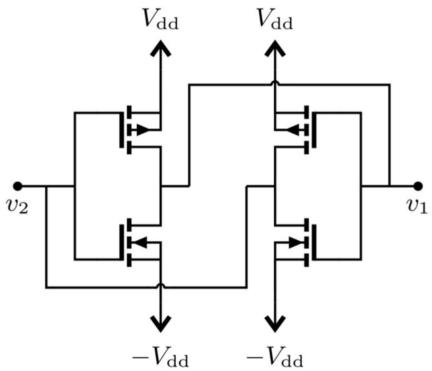
- Density $\boldsymbol{x} = \boldsymbol{n}/\Omega$ remains finite
- Transition rates scale linearly with Ω: $\omega_\rho(\boldsymbol{x}) = \lim_{\Omega\to\infty} \frac{\lambda_\rho(\Omega\boldsymbol{x})}{\Omega}$
- Free energies are extensive: $\phi(\boldsymbol{x}) = \lim_{\Omega\to\infty} \frac{\Phi(\Omega\boldsymbol{x})}{\Omega}$

Chemical Reaction Networks



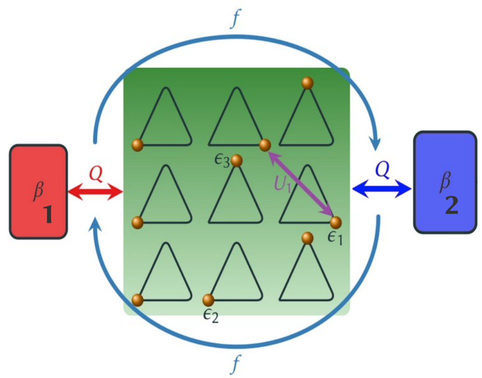
Rao, Esposito,
J. Chem. Phys. **149**, 245101 (2018)

Electronic Circuits

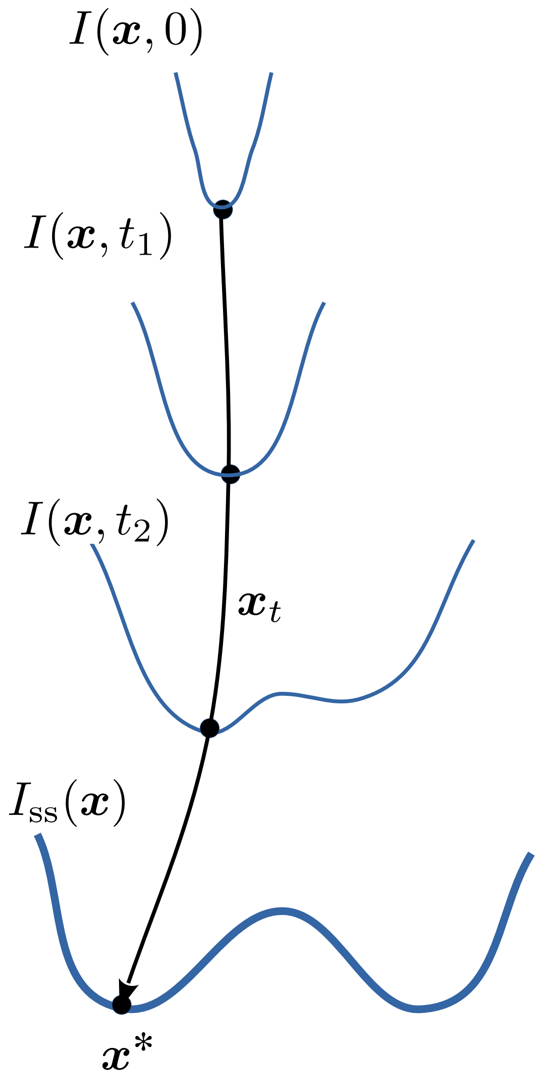


Freitas, Delvenne, Esposito,
Phys. Rev. X **11**, 031064 (2021)

Potts models



Herpich, Cossetto, Falasco, Esposito,
New J. Phys. **22**, 063005 (2020)



Macroscopic dynamics

Macroscopic Fluctuations $P(\boldsymbol{x},t) \asymp e^{-\Omega I(\boldsymbol{x},t)}$

Macroscopic Fluctuations

$$\partial_t I(\boldsymbol{x},t) = \sum_\rho \omega_\rho(\boldsymbol{x}) \left[1 - e^{\boldsymbol{\Delta}_\rho \cdot \partial_{\boldsymbol{x}} I(\boldsymbol{x},t)}\right]$$

Kubo 1973

Steady state

$$0 = \sum_\rho \omega_\rho(\boldsymbol{x}) \left[1 - e^{\boldsymbol{\Delta}_\rho \cdot \partial_{\boldsymbol{x}} I_{ss}(\boldsymbol{x})}\right] \qquad P_{ss}(\boldsymbol{x}) \asymp e^{-\Omega I_{ss}(\boldsymbol{x},t)}$$

Deterministic dynamics (minimum of $I(\boldsymbol{x},t)$)

$$d_t \boldsymbol{x}_t = \boldsymbol{u}(\boldsymbol{x}_t) = \sum_\rho \omega_\rho(\boldsymbol{x}_t) \boldsymbol{\Delta}_\rho$$

Fixed points $\boldsymbol{u}(\boldsymbol{x}^*) = 0$

$I_{ss}(\boldsymbol{x}_t)$ is a Lyapunov fct of the deterministic dynamics $-d_t I_{ss}(\boldsymbol{x}_t) \geqslant 0$

Falasco, Esposito, arXiv:2307.12406

Macroscopic nonequilibrium thermodynamics

$$\Omega \to \infty$$

Shannon entropy: $S_{\text{sh}} = -k_b \sum_{\boldsymbol{x}} P_t(\boldsymbol{x}) \log(P_t(\boldsymbol{x})) = k_b \Omega \sum_{\boldsymbol{x}} P_t(\boldsymbol{x}) I(\boldsymbol{x}, t) \simeq k_b \Omega I(\boldsymbol{x}_t, t) = 0$

2nd law $\dot{\Sigma}/\Omega = d_t S/\Omega - \langle \dot{Q} \rangle/(T\Omega) \simeq$

$$\dot{\sigma}(\boldsymbol{x}_t) = d_t s(\boldsymbol{x}_t) - \dot{q}(\boldsymbol{x}_t)/T = (\dot{w}(\boldsymbol{x}_t) - d_t \phi(\boldsymbol{x}_t))/T$$
$$= k_b \sum_{\rho>0} (\omega_\rho(\boldsymbol{x}_t) - \omega_{-\rho}(\boldsymbol{x}_t)) \ln \frac{\omega_\rho(\boldsymbol{x}_t)}{\omega_{-\rho}(\boldsymbol{x}_t)} \geqslant 0$$

1st law $d_t \langle E \rangle/\Omega = \langle \dot{W} \rangle/\Omega + \langle \dot{Q} \rangle/\Omega \simeq$

$$d_t e(\boldsymbol{x}_t) = \dot{w}(\boldsymbol{x}_t) + \dot{q}(\boldsymbol{x}_t)$$

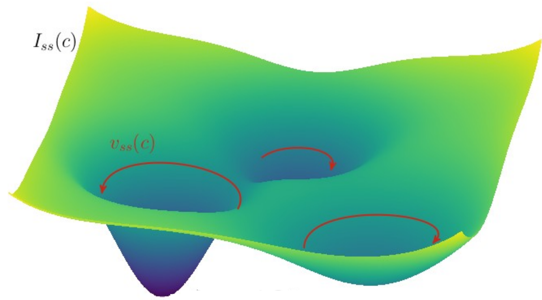
$\dot{w}(\boldsymbol{x}_t) = 0 \longrightarrow d_t \phi(\boldsymbol{x}_t) \leqslant 0$

Detailed balanced dynamics minimize the thermodynamic potential

Freitas, Esposito, Nat Com **13**, 5084 (2022)

Drift-field decomposition

$$d_t \boldsymbol{x}_t = \boldsymbol{u}(\boldsymbol{x}_t)$$



Deterministic drift vector field $\quad \boldsymbol{u}(\boldsymbol{x}) = \sum_\rho \omega_\rho(\boldsymbol{x}) \boldsymbol{\Delta}_\rho = \boldsymbol{v}_{\mathrm{ss}}(\boldsymbol{x}) - \boldsymbol{F}(\boldsymbol{x})$

Macro limit of the probability velocity $\quad \boldsymbol{v}_{\mathrm{ss}}(\boldsymbol{x}) = \sum_\rho \Delta_\rho \omega_\rho(\boldsymbol{x}) \dfrac{\mathrm{e}^{\Delta_\rho \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x})} - 1}{\Delta_\rho \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x})}$

Gradient-like vector field $\quad \boldsymbol{F}(\boldsymbol{x}) = \mathcal{M}(\boldsymbol{x}) \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x})$

"Mobility" matrix $= \sum_\rho \Delta_\rho \Delta_\rho \omega_\rho(\boldsymbol{x}) \dfrac{\mathrm{e}^{\Delta_\rho \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x})} - \Delta_\rho \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x}) - 1}{(\Delta_\rho \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x}))^2}$

Orthogonal decomposition: $\boldsymbol{v}_{\mathrm{ss}}(\boldsymbol{x}) \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x}) = 0 \qquad d_t I_{\mathrm{ss}}(\boldsymbol{x}_t) = -\boldsymbol{F}(\boldsymbol{x}_t) \cdot \partial_{\boldsymbol{x}} I_{\mathrm{ss}}(\boldsymbol{x}_t) \leqslant 0$

downhill motion in $I_{\mathrm{ss}}(\boldsymbol{x}_t)$ towards attractors with circulation on its level sets with $\boldsymbol{v}_{\mathrm{ss}}(\boldsymbol{x}_t)$

if $W_\rho = 0$ ⇒ $\boldsymbol{v}_{\mathrm{ss}}(\boldsymbol{x}) = 0$, $d_t \phi(\boldsymbol{x}) \leqslant 0$ ⇒

$$d_t \boldsymbol{x}_t = -D^{(0)}(\boldsymbol{x}_t) \cdot \partial_{\boldsymbol{x}_t} \phi(\boldsymbol{x}_t) + \mathcal{O}((\partial_{\boldsymbol{x}_t} \phi)^2)$$

Diffusion coefficient $D(x) = \dfrac{1}{2} \sum_\rho \Delta_\rho \Delta_\rho \omega_\rho(x)$

Gradient descend in free energy towards equilibrium fixed point
Not complex behavior: just fixed points!

Falasco, Esposito, arXiv:2307.12406

Gaussian approximation

$$\partial_t I(\boldsymbol{x},t) = \sum_\rho \omega_\rho(\boldsymbol{x}) \left[1 - e^{\boldsymbol{\Delta}_\rho \cdot \partial_{\boldsymbol{x}} I(\boldsymbol{x},t)}\right] \approx -\boldsymbol{u}(\boldsymbol{x}) \cdot \partial_{\boldsymbol{x}} I(\boldsymbol{x},t) - D(\boldsymbol{x}) \cdot \partial_{\boldsymbol{x}} I(\boldsymbol{x},t) \partial_{\boldsymbol{x}} I(\boldsymbol{x},t)$$

$$\sum_\rho \omega_\rho(\boldsymbol{x}) \boldsymbol{\Delta}_\rho \qquad \frac{1}{2}\sum_\rho \Delta_\rho \Delta_\rho \omega_\rho(\boldsymbol{x})$$

if $\partial_{\boldsymbol{x}} I_{\rm ss}(\boldsymbol{x})$ small (close to fixed points)

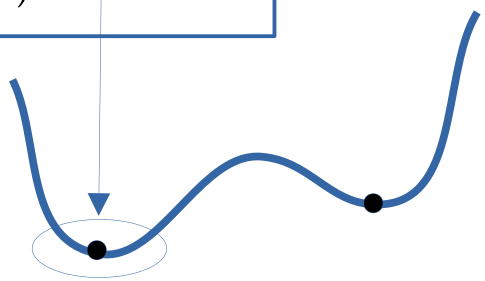
or **if** Δ_ρ small (diffusive limit)

$$d_t \boldsymbol{x}_t = \boldsymbol{u}(\boldsymbol{x}_t) + \frac{1}{\sqrt{\Omega}} \boldsymbol{\eta}(t)$$

Gaussian noise

$$\lim_{\Omega \to \infty} \frac{< \boldsymbol{\eta}(t) \boldsymbol{\eta}(t') >}{\Omega} = 2\boldsymbol{D}(\boldsymbol{x}_t) \delta(t - t')$$

In general thermo inconsistent



$\boldsymbol{x}^*$

Close to equilibrium:
Onsager-Machlup

Linear noise $\rho_t = x_t - \boldsymbol{x}_t$

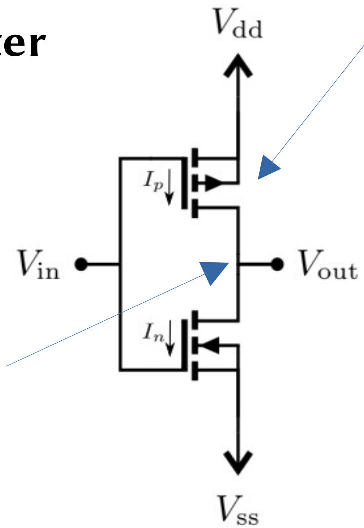
$$d_t \rho_t = \rho(t) \partial_x \boldsymbol{u}(x^{\rm eq}) + \frac{1}{\sqrt{\Omega}} \eta(t)$$

$$\partial_{\boldsymbol{x}} \boldsymbol{u}(\boldsymbol{x}^{\rm eq}) = -D(\boldsymbol{x}^{\rm eq}) \cdot \partial_{\boldsymbol{x}} \partial_{\boldsymbol{x}} \phi(\boldsymbol{x}_{\rm eq})$$

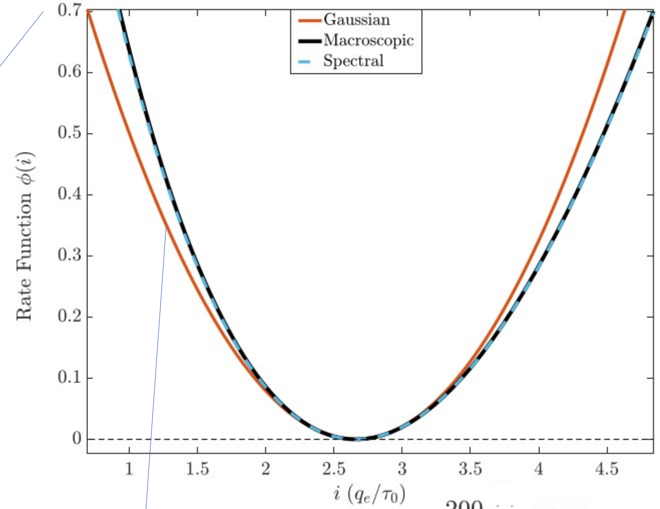
Thermo consistent
(ST for overdamped Langevin)

Falasco, Esposito, arXiv:2307.12406

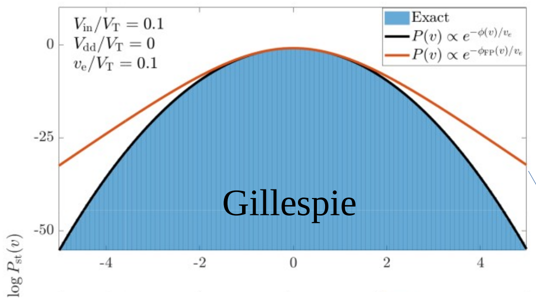
CMOS inverter



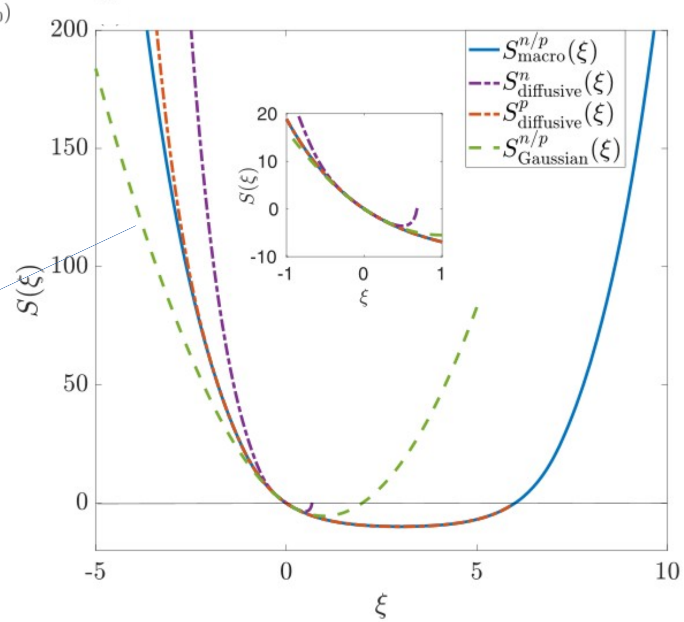
Stationary current rate function through pMOS



Stationary rate function of
voltage on the free conductor



Cumulant GF



Langevin does not work well
and breaks Fluctuation Theorem

Gopal, Esposito, Freitas, PRB **106**, 155303 (2022)

NESS fluctuations – macroscopic dissipation

Adiabatic non-adiabatic decomposition of entropy production: $\dot{\Sigma} = \dot{\Sigma}_{\rm a} + \dot{\Sigma}_{\rm na} \geqslant 0$

$\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \geqslant 0 \quad \geqslant 0$

$$\dot{\Sigma}_{\rm na} = -k_b\, d_t D \geq 0 \qquad D = \sum_{\boldsymbol{x}} P_t(\boldsymbol{x}) \log(P_t(\boldsymbol{x})/P_{\rm ss}(\boldsymbol{x})) \simeq \Omega \sum_{\boldsymbol{x}} P_t(\boldsymbol{x}) I_{\rm ss}(\boldsymbol{x}) \simeq \Omega I_{\rm ss}(\boldsymbol{x}_t)$$

NESS: $P_{\rm ss}(x) \asymp e^{-\Omega I_{\rm ss}(x)}$

Emergent 2nd law

$$\dot{\Sigma}_{\rm na}/\Omega \simeq \boxed{-k_b\, d_t I_{\rm ss}(\boldsymbol{x}_t) \geqslant 0}$$

Lyapunov fct of the det. dynamics

$$\dot{\Sigma}_{\rm a}/\Omega \simeq \boxed{\dot{\sigma}(\boldsymbol{x}_t) + k_b\, d_t I_{\rm ss}(\boldsymbol{x}_t) \geq 0}$$

Macroscopic entropy production — **Steady state fluctuations**

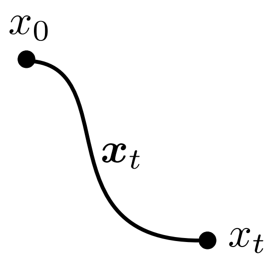
Freitas, Esposito, Nat Com **13**, 5084 (2022)

"Close" to equilibrium:
W_ρ small

Linear response theory for rate functions instead of probabilities !!!

$$\dot{\sigma}^{(0)}(\boldsymbol{x}_t)/k_b = \beta\big(\dot{w}^{(0)}(\boldsymbol{x}_t) - d_t\phi(\boldsymbol{x}_t)\big) \simeq -d_t I_{\rm ss}(\boldsymbol{x}_t)$$

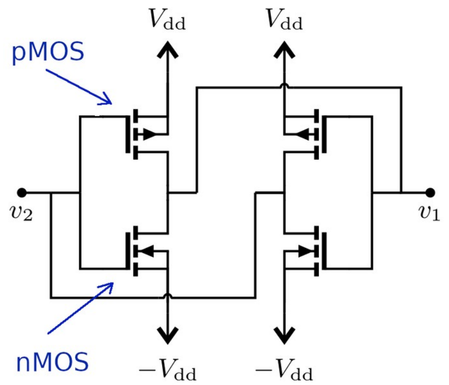
solution of the detailed balanced dynamics
$W_\rho = 0$

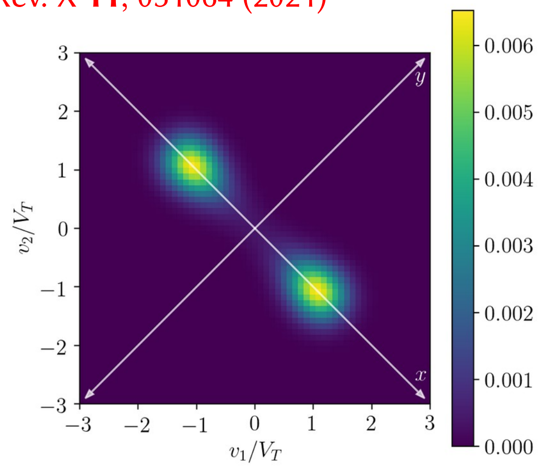


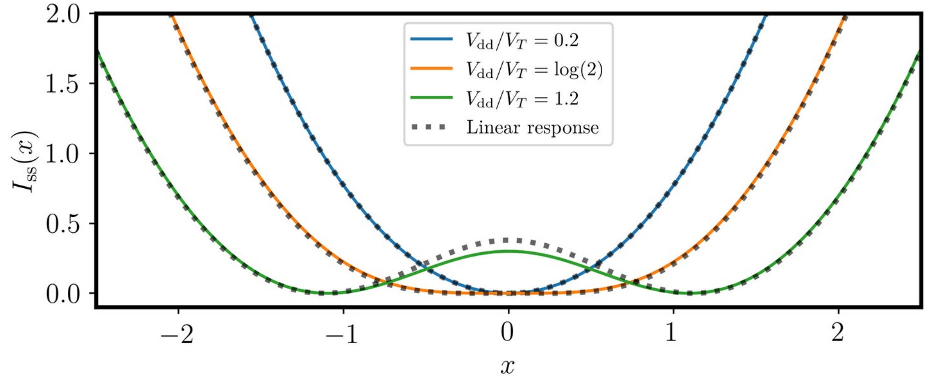
Freitas, Falasco, Esposito, *New J. Phys.* **23**, 093003 (2021)

Example of a CMOS bit

Freitas, Delvenne, Esposito, Phys. Rev. X **11**, 031064 (2021)







$v_e = q_e/C \qquad V_T = k_b T/q_e$

- **Bistability as a nonequilibrium phase transition**
- **Macro can be small !** $\Omega = V_T/v_e = 10$

Meso (stochastic) dynamics

$$d_t P(v_1, v_2, t) = PA|_{v_1 - v_e, v_2} + PB|_{v_1 + v_e, v_2} + PA^*|_{v_1, v_2 - v_e} + PB^*|_{v_1, v_2 + v_e} - P(A + B + A^* + B^*)|_{v_1, v_2},$$

$$\lambda_+^p(v_1, v_2) = (I_0/q_e)\, e^{(V_{\rm dd} - v_2 - V_{\rm th})/(nV_T)},$$

$$\lambda_-^p(v_1, v_2) = \lambda_+^p(v_1, v_2)\, e^{-(V_{\rm dd} - v_1)/V_T}\ e^{-(v_e/2)/V_T}$$

$$A(v_1, v_2) = \lambda_+^p(v_1, v_2) + \lambda_-^n(v_1, v_2),$$

$$B(v_1, v_2) = \lambda_-^p(v_1, v_2) + \lambda_+^n(v_1, v_2),$$

$$v_e = q_e/C$$

$$\Phi(v_1, v_2) = (C/2)(v_1^2 + v_2^2) + CV_{\rm dd}^2$$

Macro (deterministic) dynamics

$$C\frac{dv_1}{dt} = I_p(v_1, v_2) - I_n(v_1, v_2),$$

$$C\frac{dv_2}{dt} = I_p(v_2, v_1) - I_n(v_2, v_1).$$

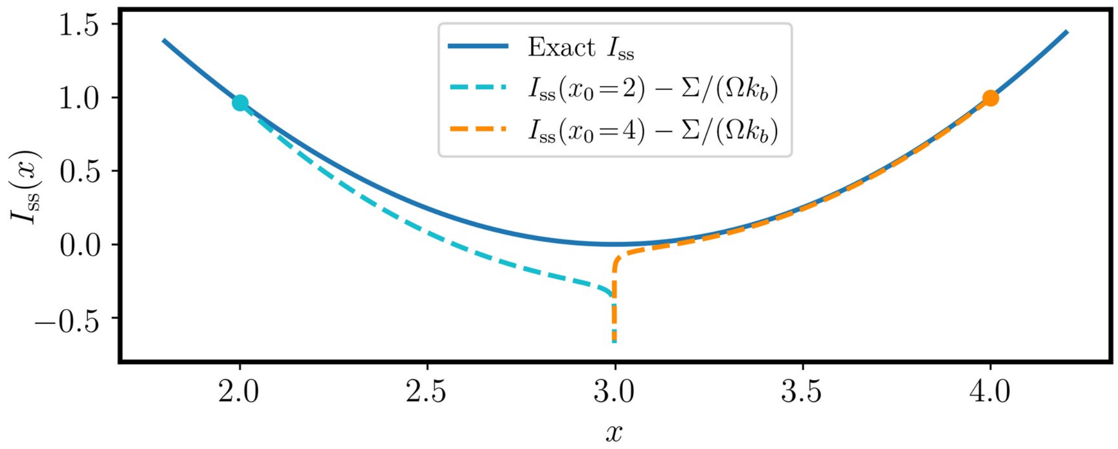
$$I_p(v, v_g) = I_0 e^{-V_{\rm th}/V_T}\ e^{(V_{\rm dd} - v_g)/(nV_T)}\ (1 - e^{-(V_{\rm dd} - v)/V_T})$$

$$I_n(v, v_g) = I_p(-v, -v_g)$$

- **Dissipation along the macro (deterministic) dynamics can be used to bound the steady state rate function**

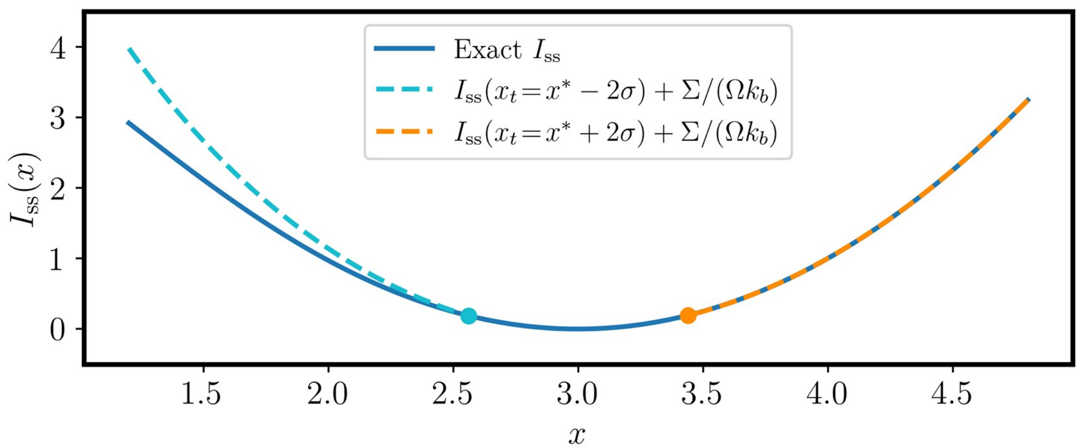
$$I_{\rm ss}(x_0) - \sigma(\boldsymbol{x}_t)/k_b \leq I_{\rm ss}(x_t)$$

$$\sigma(\boldsymbol{x}_t) = q(\boldsymbol{x}_t)/T$$



Freitas, Esposito,
Nat Com **13**, 5084 (2022)

$$I_{\rm ss}(x_t) + \sigma(\boldsymbol{x}_t)/k_b \geq I_{\rm ss}(x_0)$$

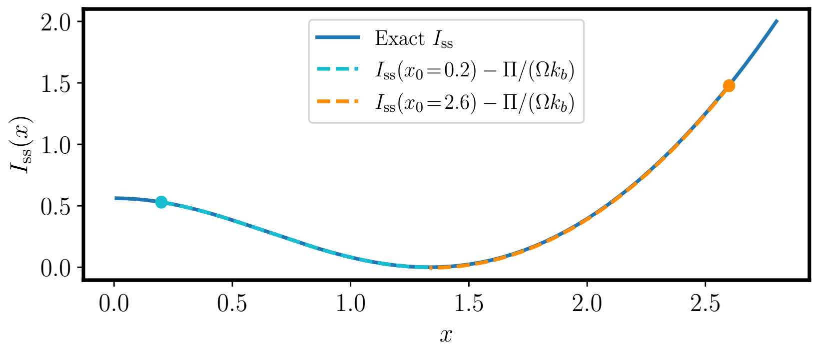


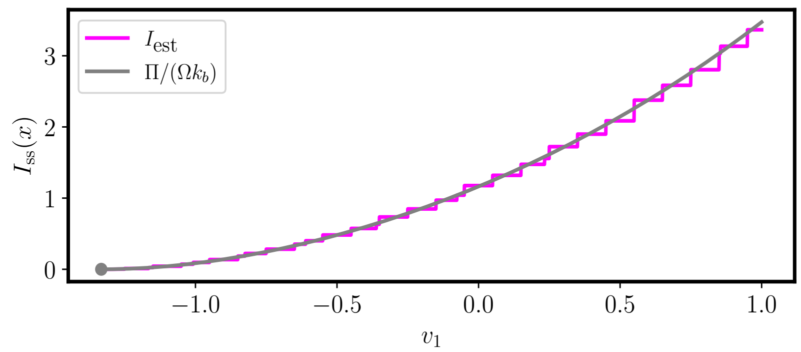
Tightening the bound: A method to compute steady state rate functions

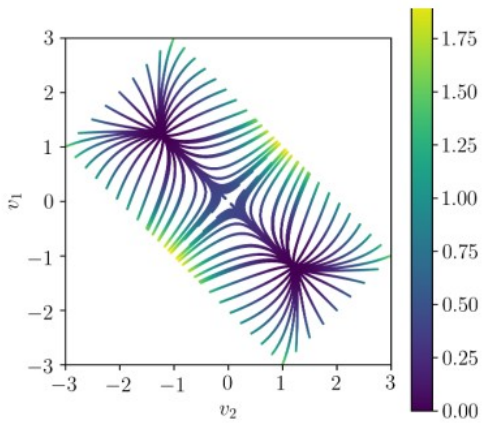
Physical dissipation: $\dot{\Sigma} \geq \dot{\Pi} = \frac{k_b}{2} \sum_{\rho, \boldsymbol{n}} (\tilde{j}_\rho(\boldsymbol{n}) - \tilde{j}_{-\rho}(\boldsymbol{n} + \tilde{\boldsymbol{\Delta}}_\rho)) \log \frac{\tilde{j}_\rho(\boldsymbol{n})}{\tilde{j}_{-\rho}(\boldsymbol{n} + \tilde{\boldsymbol{\Delta}}_\rho)}$

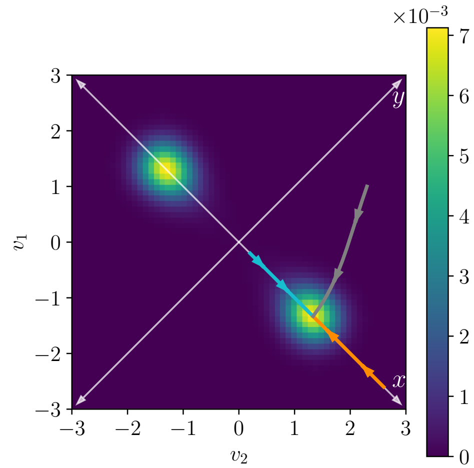
Coarse grained dissipation obtained by lumping transitions between same pairs of states

$$\pi(\boldsymbol{x}_t)/k_b \geq I(x_0) - I(x_t) \geq 0$$







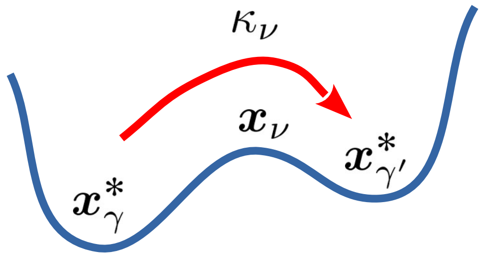


Full reconstruction

Freitas, Esposito, Nat Com **13**, 5084 (2022)

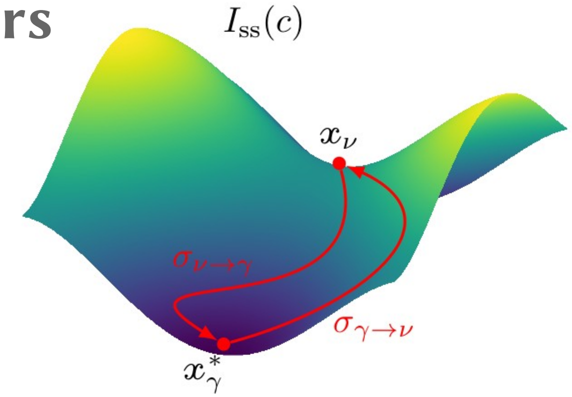
$k_b = 1$

Transition rates between attractors



$$\kappa_\nu \asymp e^{-V[I_{\rm ss}^{(\gamma)}(\boldsymbol{x}_\nu) - I_{\rm ss}^{(\gamma)}(\boldsymbol{x}^*_\gamma)]}$$

$\boldsymbol{u}(\boldsymbol{x}^*) = 0$ Fixed points of the det. dynamics



- W_ρ small ➡ Local detailed balance Falasco, Esposito, PRE **103**, 042114 (2021)

$$\lim_{V\to\infty} \frac{1}{V} \ln \frac{\kappa_\nu}{\kappa_{-\nu}} = \beta(\phi(\boldsymbol{x}^{\rm eq}_\gamma) - \phi(\boldsymbol{x}^{\rm eq}_{\gamma'})) + \sigma_\nu^{(0)}$$

$$\sigma_\nu^{(0)} := -\sigma_{\rm nc}^{(0)}(\boldsymbol{x}_\nu, \boldsymbol{x}^{\rm eq}_\gamma) + \sigma_{\rm nc}^{(0)}(\boldsymbol{x}_\nu, \boldsymbol{x}^{\rm eq}_{\gamma'})$$

$$\sigma_{\rm nc}^{\nu\to\gamma}(\boldsymbol{x}, \boldsymbol{x}') := \beta \int_{\boldsymbol{x}}^{\boldsymbol{x}'} dt \sum_\rho W_\rho\, \omega_\rho(\boldsymbol{x}(t))$$

relaxation — instanton

- General bound

$$-\sigma_{\nu\to\gamma} \leqslant \lim_{V\to\infty} \frac{1}{V} \ln \kappa_\nu \leqslant \sigma_{\gamma\to\nu}$$

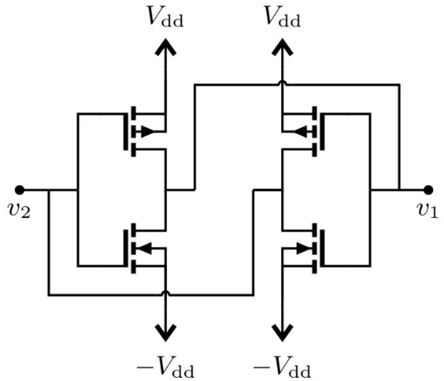
Falasco, Esposito, arXiv:2307.12406

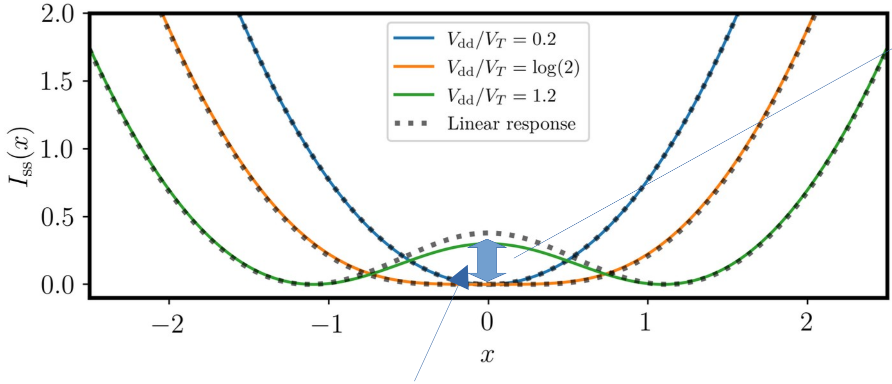
W_ρ small ➡ $-\sigma_{\nu\to\gamma} = \lim_{V\to\infty} \frac{1}{V} \ln \kappa_\nu = \sigma_{\gamma\to\nu} < 0$

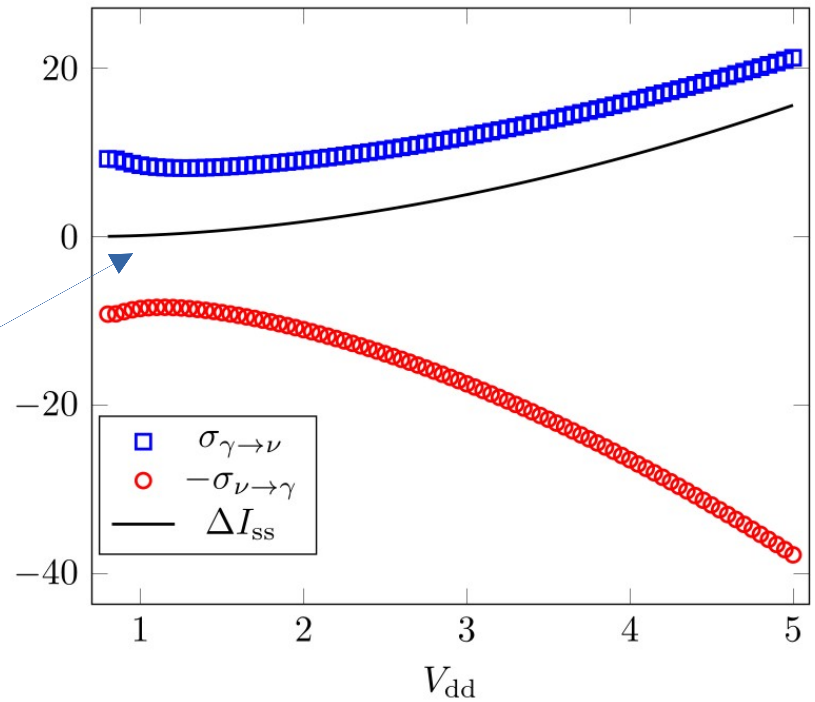
Attractor with largest lifetime has the largest relaxation entropy production !
(smallest κ_ν) (largest $\sigma_{\nu\to\gamma}$)

Remark: **If** most $\sigma_{\nu\to\gamma}$ occurs close to $\boldsymbol{x}^*_\gamma$ "maximum entropy production principle"

Example of a CMOS bit







$$\kappa \asymp e^{-[I_{ss}(0)-I_{ss}(v^*)]/v_e}$$

$$-\lim_{v_e \to 0} v_e \ln \kappa \propto \langle \dot{\sigma}_{\pm 1} \rangle^2$$

Error rate ~ (Dissipation)^2

Nonequilibrium Field Theories

- In general x=(r,c)

  c Internal degrees of freedom, e.g. chemistry

  r real space (diffusive scaling)

Falasco, Esposito, arXiv:2307.12406

- If x=r (diffusive limit)

$$\partial_t c(r,t) = -\nabla \cdot \left(j[c] + \frac{1}{\sqrt{\Omega}} \xi(r,t) \right) \qquad \langle \xi(r,t)\xi(r',t') \rangle = 2\chi(c(r,t))\delta(r-r')\delta(t-t')$$

$$j[c] := \chi \cdot \left(-\nabla \frac{\delta \phi}{\delta c} + f \right)$$

Mobility

$$\chi_\alpha(c)\nabla \frac{\delta \phi}{\delta c_\alpha} = D_\alpha(c)\nabla c \qquad D_\alpha = \chi_\alpha \partial^2_{c_\alpha} \phi$$

$$\phi[c] = \frac{1}{T} u[c] - s_{\mathrm{int}}[c]$$

Time-dependent DFT
Dean *JPA* **29**, L613 (1996)

$$u[c] = \frac{1}{2} \int dr \int dr' c(r) U(r-r') c(r')$$

$$s_{\mathrm{int}}[c] = -\int dr c(r)(\ln c(r) - 1)$$

$$\chi(c) \propto c$$

Simple exclusion
Bertini et al. *RMP* **87**, 593 (2015)

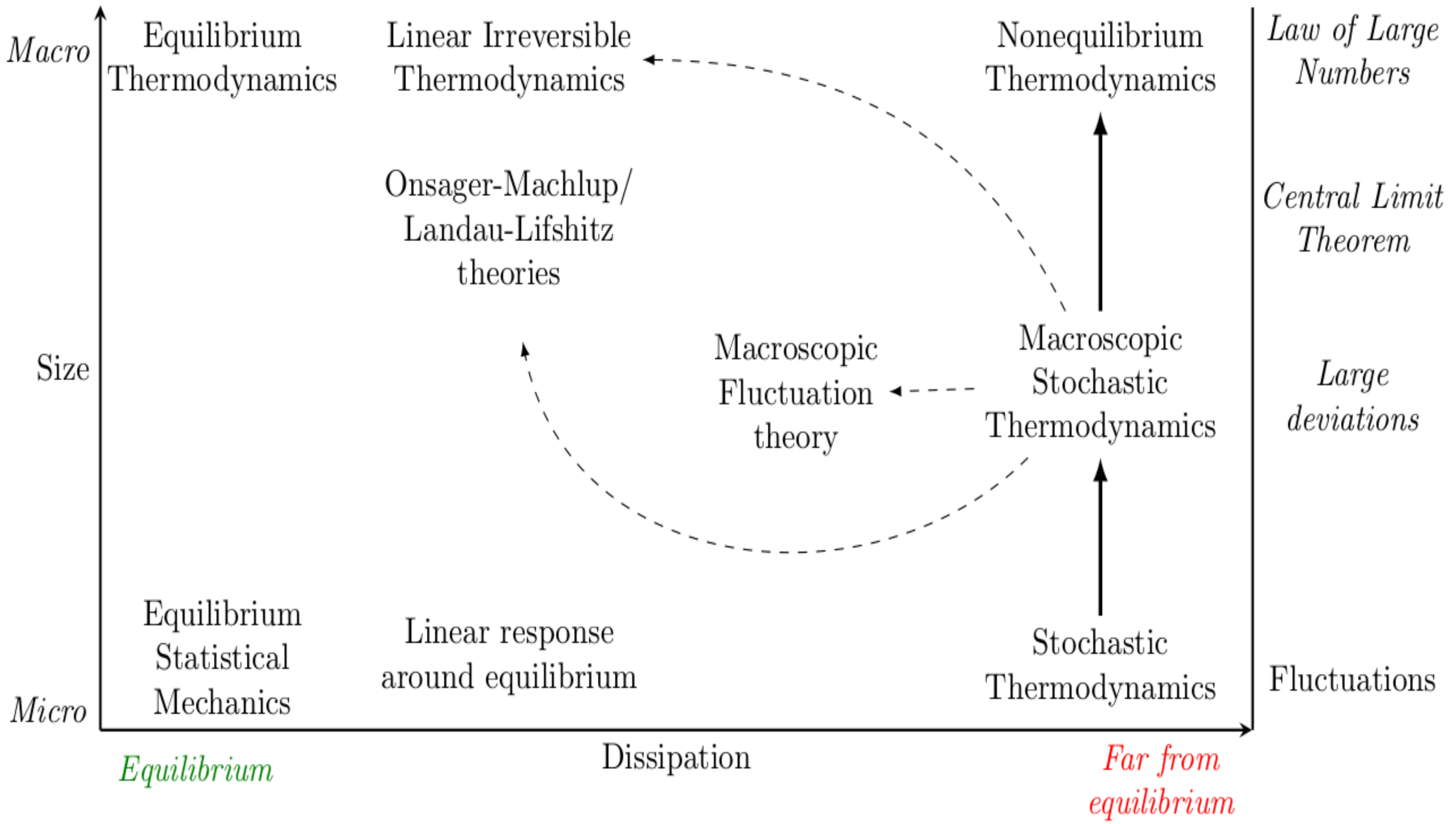
$$u[c] = 0$$

$$\chi(c) \propto c(1-c)$$

$$s_{\mathrm{int}}[c] = -\int dr [c(r) \ln c(r) + (1-c(r)) \ln(1-c(r))]$$

Conclusions

- Recovering classical “irreversible thermo” results from stochastic thermodynamics



Falasco, Esposito, *Macroscopic Stochastic Thermodynamics*, arXiv:2307.12406