UNIVERSITÉ DU LUXEMBOURG

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Dissipation in Open Quantum Systems

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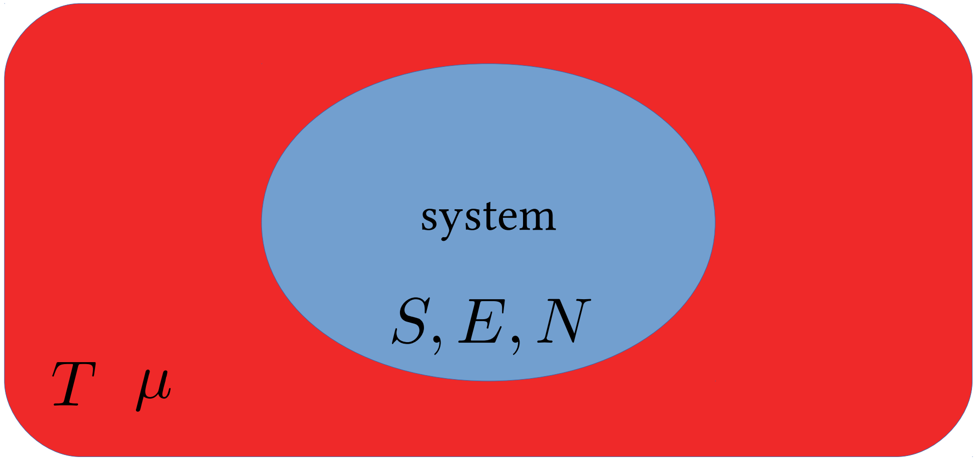
Outline

- Phenomenological Nonequilibrium Thermodynamics
- Hamiltonian formulation
- Born-Markov-Secular Quantum Master Equation (QME)
- Landau-Zener QME
- Repeated Interactions (Hamiltonian + QME formulation)

Phenomenological Nonequilibrium Thermodynamics



Zeroth law: System dynamics with an equilibrium

1st law:

$$d_t E = \dot{W} + \dot{Q}$$

2nd law:

$$\dot{\Sigma} = d_t S - \frac{\dot{Q}}{T} \geq 0$$

Slow transformation

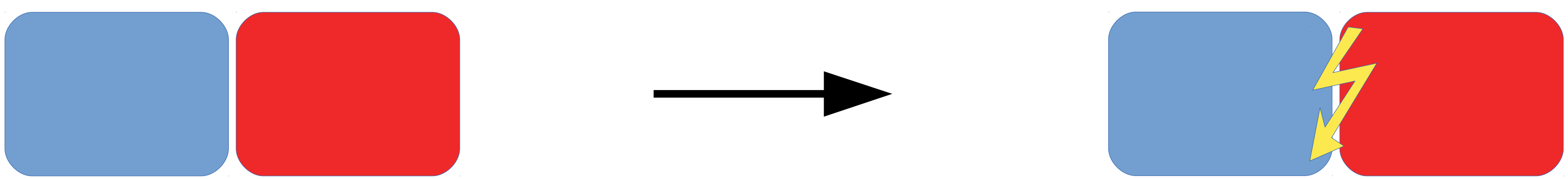
$$d_t S \approx \frac{\dot{Q}}{T}$$

Hamiltonian formulation

System X – System Y

$$H_{\text{tot}}(t) = H_X(t) + H_Y(t) + H_{XY}(t)$$

$$\rho_{XY}(0) = \rho_X(0)\rho_Y(0) \qquad \qquad \rho_{XY}(\tau) = U_\tau \rho_X(0)\rho_Y(0)U_\tau^\dagger$$



$$d_t E_{XY}(t) = \text{tr}_{XY}\left\{\rho_{XY}(t) d_t H_{\text{tot}}(t)\right\} \equiv \dot{W}(t)$$

$$I_{X:Y}(t) \equiv S_X(t) + S_Y(t) - S_{XY}(t) \qquad S_{XY}(t) \equiv -\text{tr}_{XY}\{\rho_{XY}(t)\ln\rho_{XY}(t)\}$$

$$= \Delta S_X(\tau) + \Delta S_Y(\tau) = D[\rho_{XY}(t)||\rho_X(t)\rho_Y(t)] \geq 0$$

System X – Reservoir R

$$\rho_{XR}(0) = \rho_X(0)\rho_\beta^R \qquad \rho_\beta^R \equiv \frac{e^{-\beta H_R}}{Z_R}$$

$$E_X(t) \equiv \mathrm{tr}_{XR}\{[H_X(t) + H_{XR}(t)]\rho_{XR}(t)\}$$

$$d_t E_X(t) = \dot{W}(t) + \dot{Q}(t) \qquad \begin{cases} \dot{W}(t) = d_t E_{XY}(t) \\ \dot{Q}(t) \equiv -\mathrm{tr}_R\{H_R d_t \rho_R(t)\} \end{cases}$$

$$\begin{aligned} \Sigma(\tau) \equiv \Delta S_X(\tau) - \beta Q(\tau) &= D[\rho_{XR}(\tau)||\rho_X(\tau)\rho_\beta^R] \\ &= D[\rho_R(\tau)||\rho_\beta^R] + I_{X:R}(\tau) \geq 0 \end{aligned}$$

[Esposito, Lindenberg, & Van den Broeck, NJP **12**, 013013 (2010)]

Ideal reservoir

Another identity: $TD[\rho_R(\tau)||\rho_\beta^R] = -Q(\tau) - T\Delta S_R(\tau) \geq 0$

$$\rho_R(\tau) = \rho_\beta^R + \epsilon\sigma_R \qquad D[\rho_R(\tau)||\rho_\beta^R] = \mathcal{O}(\epsilon^2)$$

$$\Delta S_R(\tau) = -\beta Q(\tau)$$

$$\Sigma(\tau) = I_{X:R}(\tau)$$

Summary:
- 1st, 2nd law, strong coupling
- no 0th law, $\Sigma \geq 0$ but not $\dot{\Sigma}$

Born-Markov-Secular QME

$$H_{XR} = \sum_k A_k \otimes B_k$$

Effective dynamics

$$d_t \rho_X(t) = -i[H_X(t), \rho_X(t)] + \mathcal{L}_\beta(t)\rho_X(t) \equiv \mathcal{L}_X(t)\rho_X(t),$$

$$\mathcal{L}_\beta(t)\rho(t) = \sum_\omega \sum_{k,\ell} \gamma_{k\ell}(\omega) \left(A_\ell(\omega)\rho(t)A_k^\dagger(\omega) - \frac{1}{2}\{A_k^\dagger(\omega)A_\ell(\omega), \rho(t)\} \right)$$

$$A_k(\omega) \equiv \sum_{\epsilon-\epsilon'=\omega} \Pi_\epsilon A_k \Pi_{\epsilon'} \qquad \gamma_{k\ell}(\omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \mathrm{tr}_R\{B_k(t)B_\ell(0)\rho_\beta^R\}$$

Local detailed balance: $\gamma_{k\ell}(-\omega) = e^{-\beta\omega}\gamma_{\ell k}(\omega)$

$$\mathcal{L}_\beta(t)\rho_\beta^X(t) = 0, \quad \rho_\beta^X(t) = \frac{e^{-\beta H_X(t)}}{Z_X(t)}$$

Thermodynamics

Energy: $E_X(t) = -\mathrm{tr}_X\{H_X(t)\rho_X(t)\}$

Entropy: $S_X(t) = -\mathrm{tr}_X\{\rho_X(t)\ln\rho_X(t)\}$

1st law $$d_t E_X(t) = \dot{W}(t) + \dot{Q}(t)$$

$$\dot{W}(t) = \mathrm{tr}_X\{\rho_X(t) d_t H_X(t)\}$$

$$\dot{Q}(t) = \mathrm{tr}_X\{H_X(t) d_t \rho_X(t)\} = \mathrm{tr}_X\{H_X(t)\mathcal{L}_X(t)\rho_X(t)\}$$

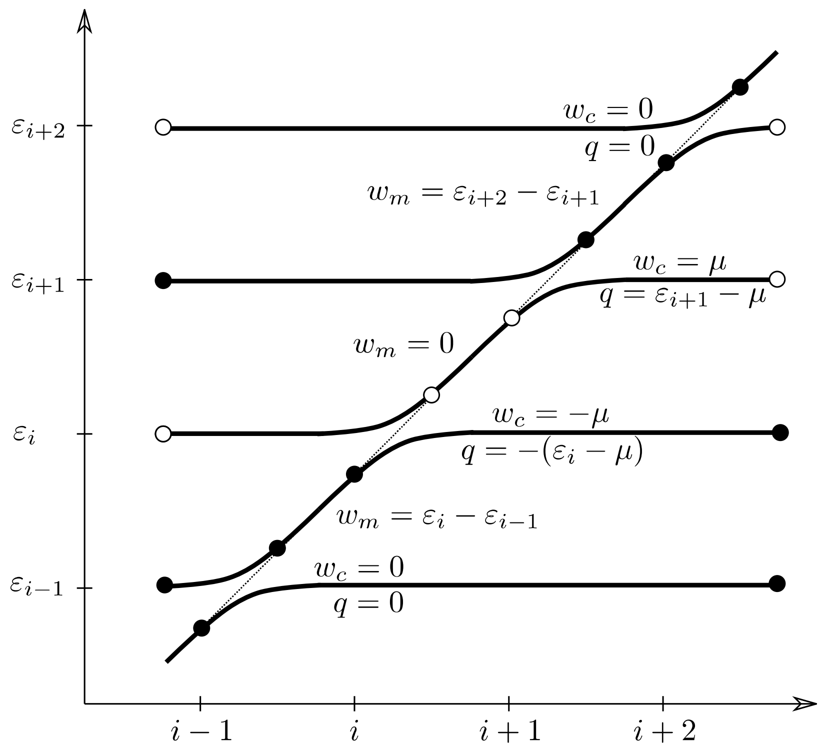
2nd law $$\dot{\Sigma}(t) = d_t S_X(t) - \beta\dot{Q}(t)$$

$$= -\mathrm{tr}\{[\mathcal{L}_X(t)\rho_X(t)][\ln\rho_X(t) - \ln\rho_\beta^X(t)]\} \geq 0$$

Summary:
- 0th, 1st, 2nd law, $\dot{\Sigma} \geq 0$, slow trsf. $\dot{\Sigma} \approx 0$
- but weak coupling

A Landau-Zener approach

$$H(t) = \epsilon_t c^\dagger c + \sum_{i=1}^{L} \varepsilon_i c_i^\dagger c_i + \gamma \sum_{i=1}^{L} (c^\dagger c_i + c_i^\dagger c)$$



Prob. diabatic transition:

$$R_i = \exp\{-\pi \delta_i^2 / (2\hbar \dot{\epsilon}_i)\}$$

$$t_i^{\mathrm{lz}} = \sqrt{\hbar/\dot{\epsilon}_i}\, \max[1, \sqrt{\delta_i^2/(\hbar\dot{\epsilon}_i)}]$$

Validity: $\Delta t_{i+} > t_i^{\mathrm{lz}}$ $\quad \Delta\varepsilon_{i+} > \delta_i$ ⇒ $\Delta\varepsilon_{i+} > \sqrt{\hbar\dot{\epsilon}_i}, \delta_i$

[Barra & Esposito, PRE **93**, 062118 (2016)]

Effective dynamics

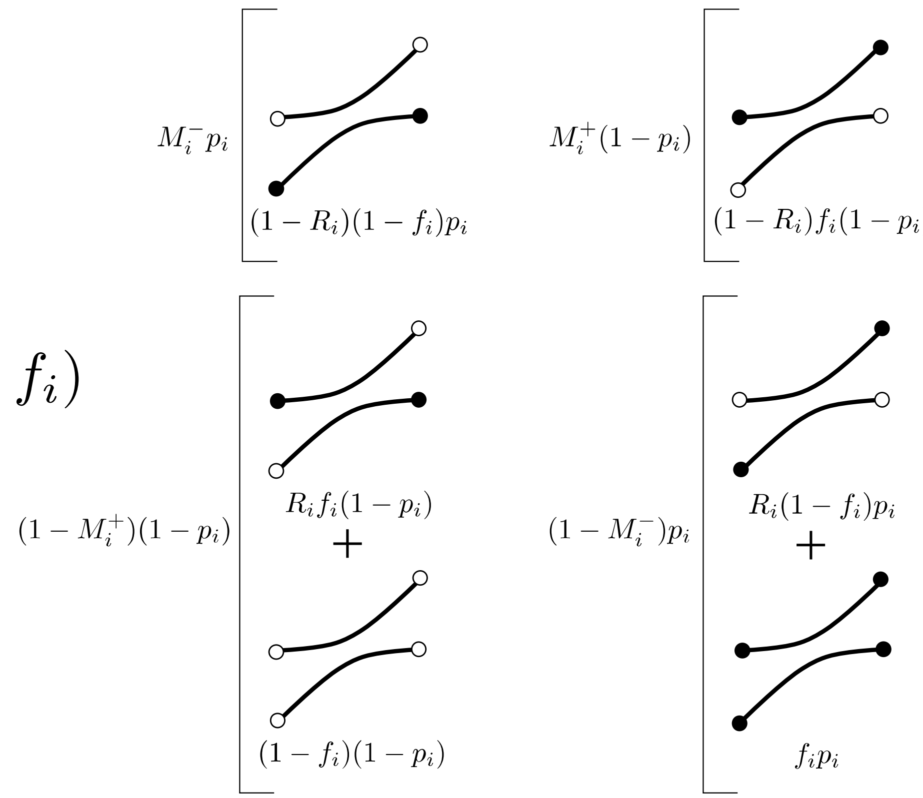
Master equation

$$p_{i+1} = (1 - M_i^-)p_i + M_i^+(1 - p_i)$$

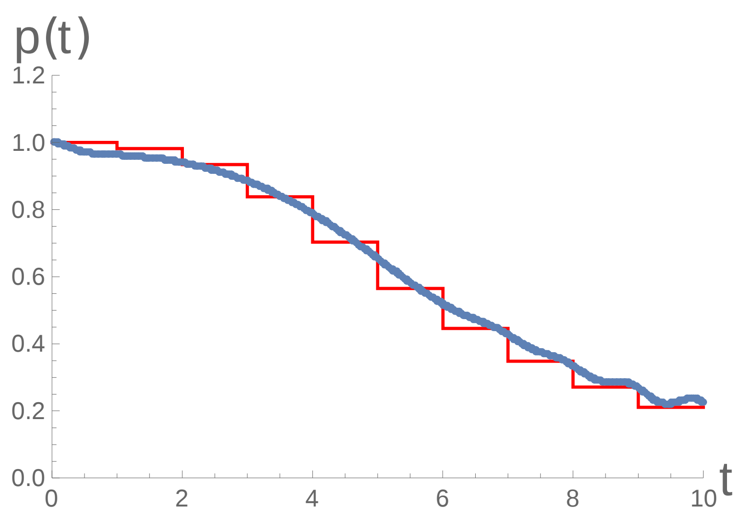
$$M_i^+ = (1 - R_i)f_i \qquad M_i^- = (1 - R_i)(1 - f_i)$$

Local detailed balance

$$M_i^+/M_i^- = e^{-\beta(\varepsilon_i - \mu)}$$

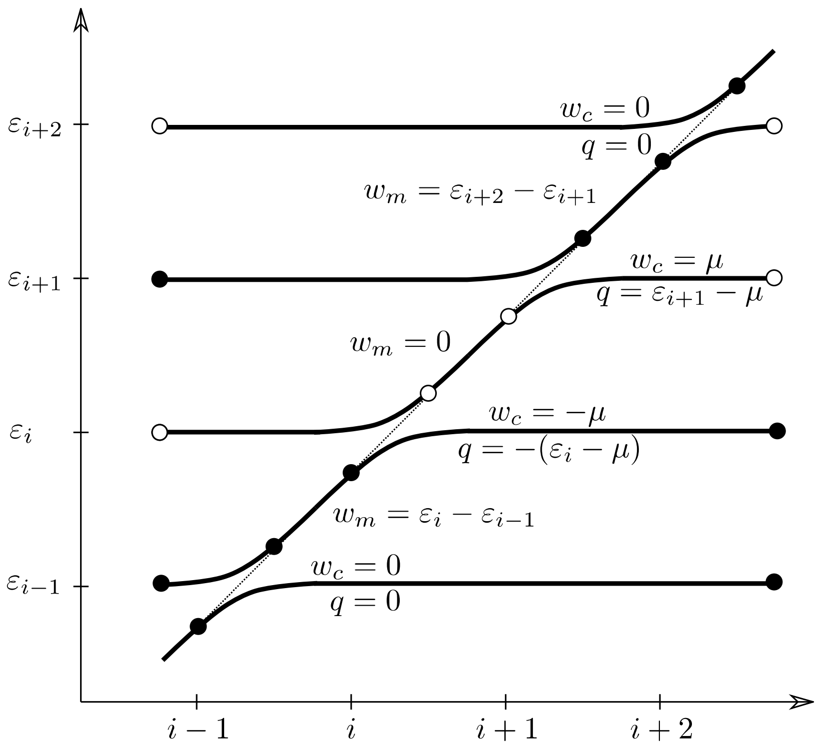


Exact vs stochastic dynamics



[Barra & Esposito, PRE **93**, 062118 (2016)]

Thermodynamics



1st law $\Delta E_{i+} = E_{i+1} - E_i = W_{i+} + Q_{i+}$

$$N_i = p_i \qquad E_i = \varepsilon_i p_i \qquad Q_{i+} = (\varepsilon_i - \mu)(p_{i+1} - p_i)$$

$$W_{i+} = W_{i+}^{\mathrm{m}} + W_{i+}^{\mathrm{c}} \quad \begin{cases} W_{i+}^{\mathrm{m}} = (\varepsilon_{i+1} - \varepsilon_i) p_{i+1} \\ W_{i+}^{\mathrm{c}} = \mu (p_{i+1} - p_i) \end{cases}$$

2nd law $\Delta S_{i+} = S_{i+1} - S_i = \Sigma_{i+} + Q_{i+}/T$

$$S_i = -k_B p_i \ln p_i - k_B (1 - p_i) \ln(1 - p_i)$$

$$\Sigma_{i+} = k_B M_i^+ (1 - p_i) \ln \frac{M_i^+ (1 - p_i)}{M_i^- p_i} + k_B M_i^- p_i \ln \frac{M_i^- p_i}{M_i^+ (1 - p_i)} - k_B D(p_{i+1} | p_i) \geq 0$$

[Barra & Esposito, PRE **93**, 062118 (2016)]

between crossing

$$\underbrace{W_{i+}^{\rm m} - \Delta\Omega_{i+}^{\rm eq}}$$

$$\Sigma_{i+} = \frac{W_{i+}^{\rm diss}}{T} - k_B D(p_{i+1}|f_{i+1}) + k_B D(p_i|f_i) \geq 0$$

at crossing

QM adiabatic regime (slow driving)

$$p_i = f_{i-1} \quad p_{i+1} = f_i$$

At the crossing: $\Sigma_{i+} = k_B D(f_{i-1}|f_i)$

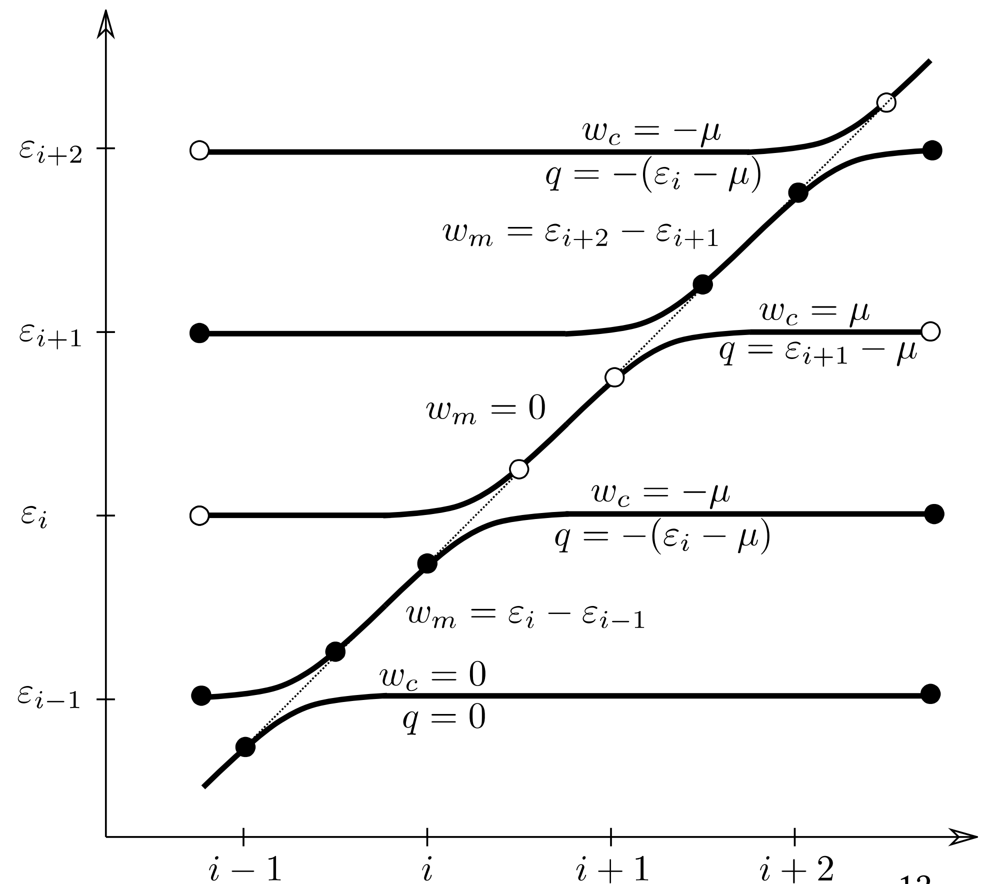
From $i \to i+1$: $W_{i+}^{\rm diss} = k_B T D(f_i|f_{i+1})$

Reversibility only occurs if:

$\Delta\varepsilon, \delta, \dot{\epsilon} \to 0$

$\Delta\varepsilon > \delta \gg \sqrt{\hbar\dot{\epsilon}}$

$\Sigma_{i+}\ ,\ W_{i+}^{\rm diss} \sim \Delta\varepsilon^2$



[Barra & Esposito, PRE **93**, 062118 (2016)]

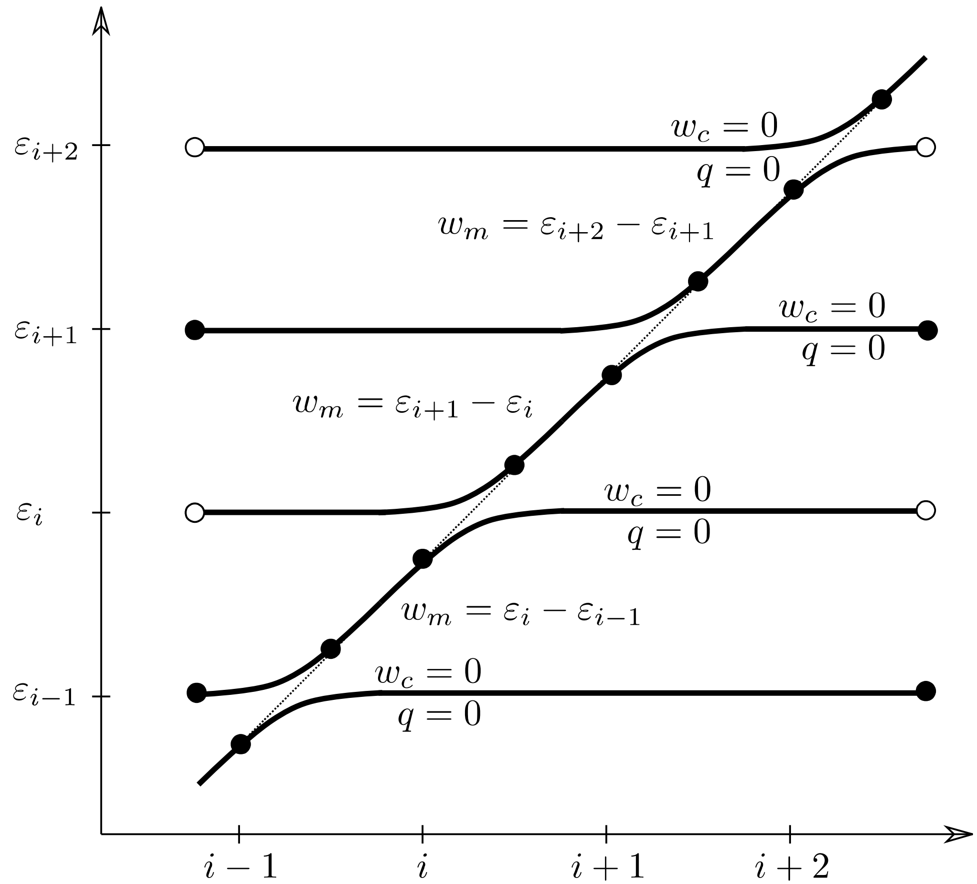
$$\Sigma_{i+} = \frac{W^{\text{diss}}_{i+}}{T} - k_B D(p_{i+1}|f_{i+1}) + k_B D(p_i|f_i) \geq 0$$

<u>QM diabatic regime</u> (fast driving)

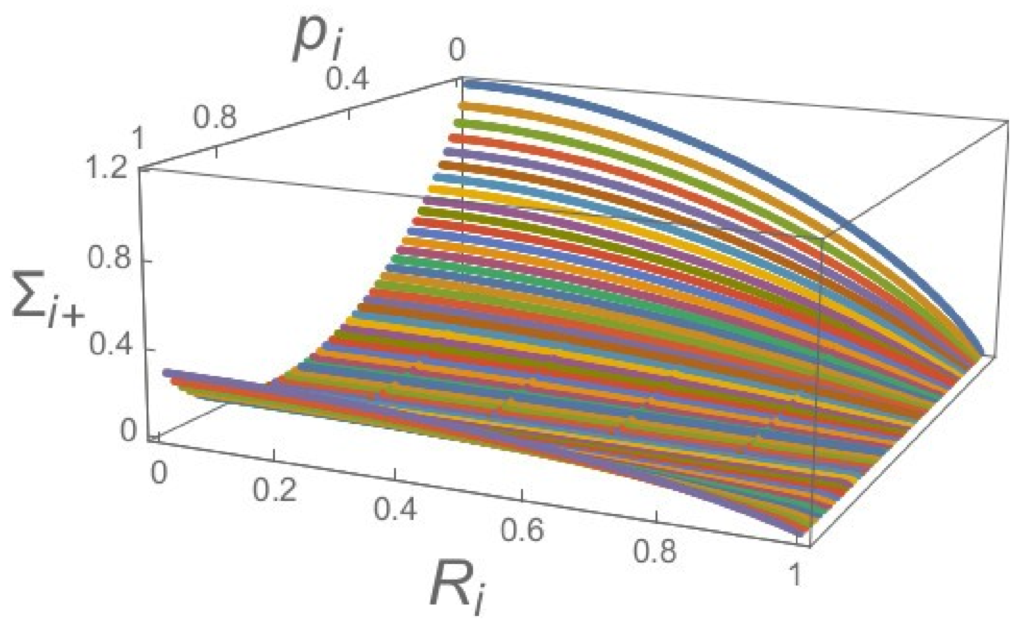
$$p_i = p_1$$

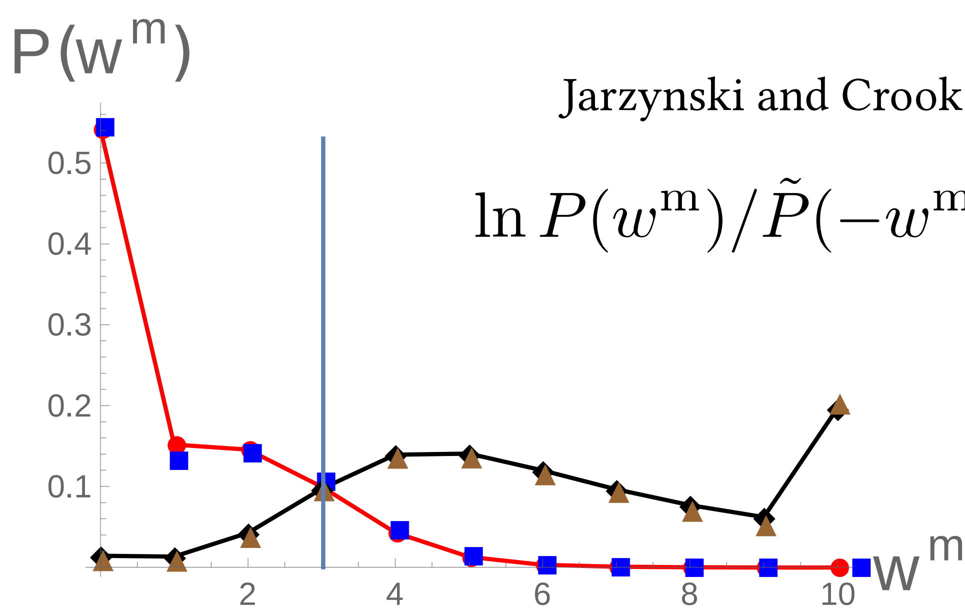
$$\Sigma = \Delta S = Q = 0$$

$$W^{\text{diss}} = k_B T \sum_i \big(D(p_1|f_{i+1}) - D(p_1|f_i) \big)$$



[Barra & Esposito, PRE **93**, 062118 (2016)]





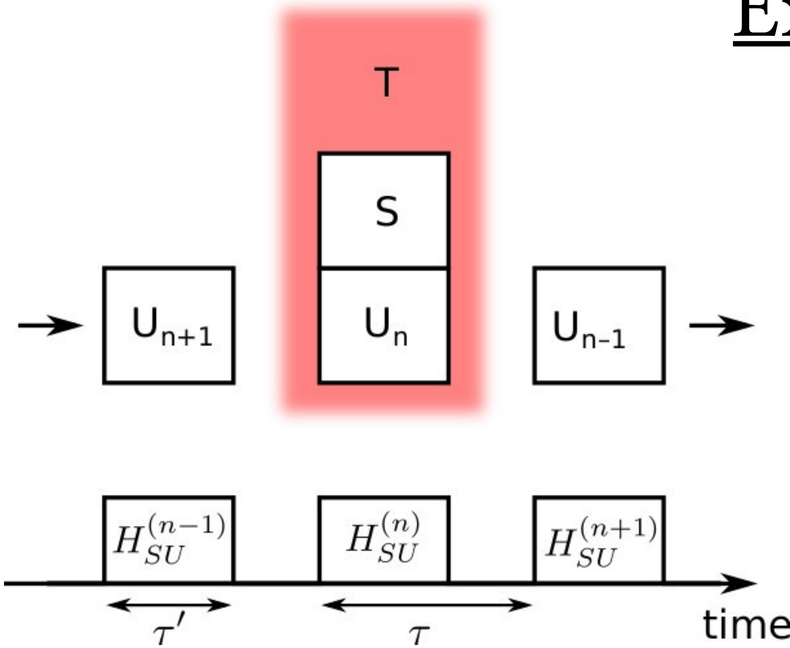
Jarzynski and Crooks fluctuation relation

$$\ln P(w^{\rm m})/\tilde{P}(-w^{\rm m}) = \beta(w^{\rm m} - \Delta\Omega^{\rm eq})$$

[Barra & Esposito, PRE **93**, 062118 (2016)]

Repeated interaction

Exact identities



$$\Delta E_X = \Delta E_U + \Delta E_S = W + Q$$

$$\Sigma = \underbrace{\Delta S_S + \Delta S_U - I_{S:U}(\tau)}_{\Delta S_X} - \beta Q \geq 0$$

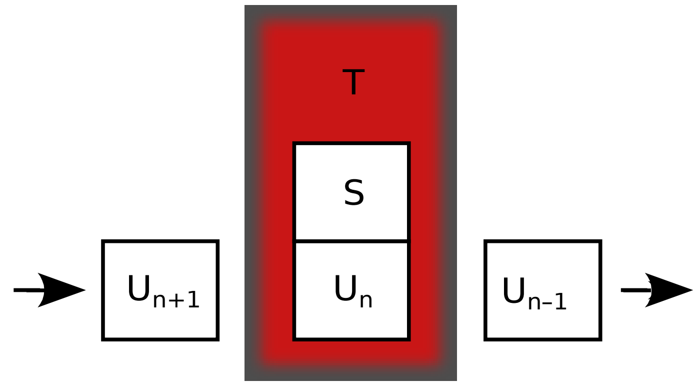
$$\Delta E_{SU} \equiv \lim_{\epsilon \searrow 0} \int_{-\epsilon}^{\tau-\epsilon} dt \frac{dE_X(t)}{dt} = \Delta E_S + \Delta E_U$$

$$W \equiv \lim_{\epsilon \searrow 0} \int_{-\epsilon}^{\tau-\epsilon} dt \dot{W}(t) = W_X + W_{\text{sw}}$$

$$Q \equiv \lim_{\epsilon \searrow 0} \int_{-\epsilon}^{\tau-\epsilon} dt \dot{Q}(t)$$

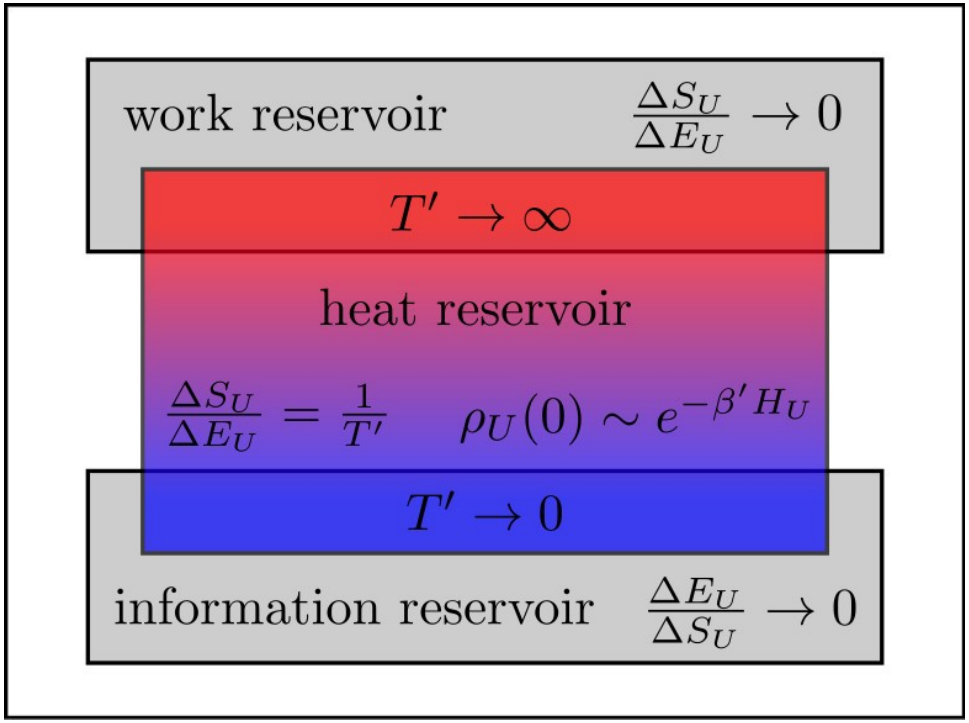
$$\begin{cases} W_X = \int_0^{\tau} dt \text{tr}_X \{\rho_X(t) d_t H_S(t)\} \\ \qquad + \lim_{\epsilon \searrow 0} \int_{\epsilon}^{\tau'-\epsilon} dt' \text{tr}_X \{\rho_X(t) d_t V_{SU}(t)\} \\ W_{\text{sw}} = \text{tr}_X \{V_{SU}(0)\rho_X(0) - V_{SU}(\tau')\rho_X(\tau')\} \end{cases}$$

[Strasberg, Schaller, Brandes & Esposito, PRX **7**, 021003 (2017)]



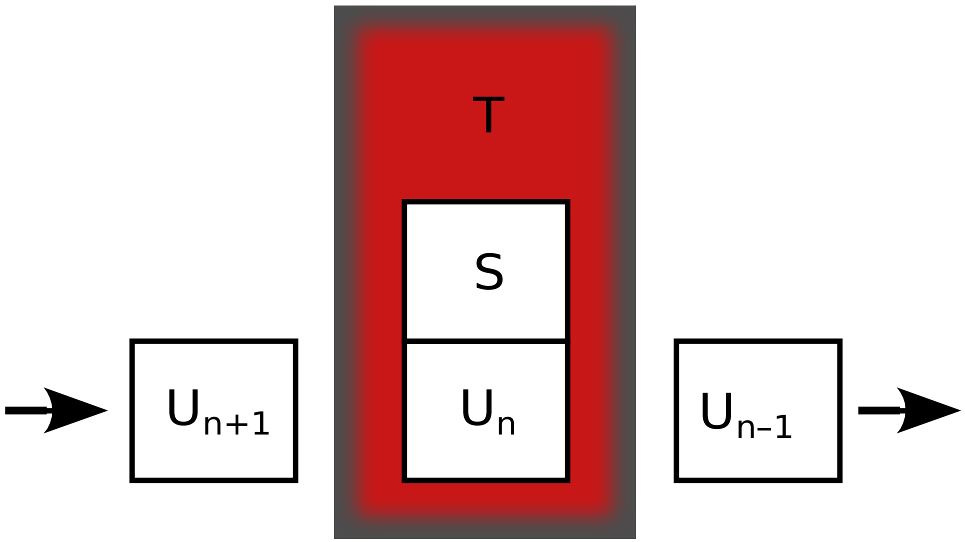
1st law $$\Delta E_S = W + Q - \Delta E_U$$

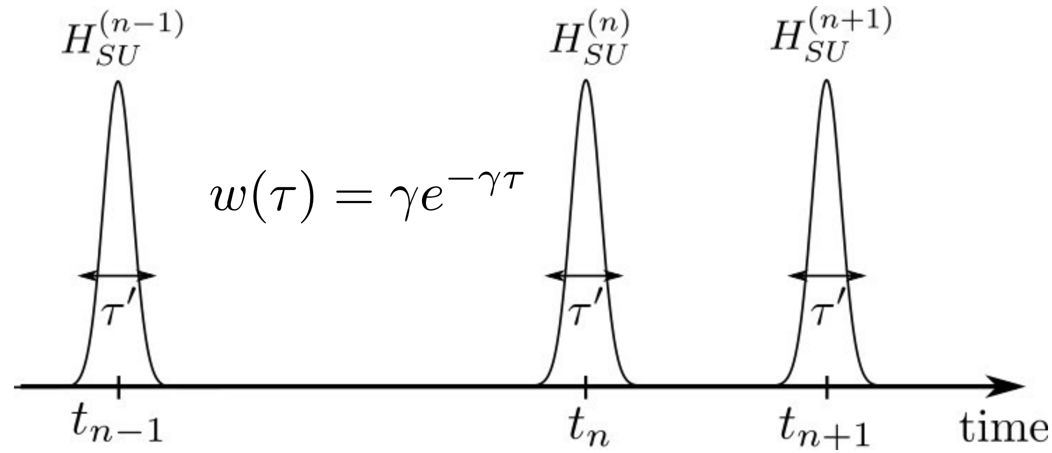
2nd law $$\Sigma_S \equiv \Delta S_S + \Delta S_U - \beta Q \geq I_{S:U}(\tau) \geq 0$$



[Strasberg, Schaller, Brandes & Esposito, PRX **7**, 021003 (2017)]

Repeated interaction QME





$$H_{SU}(t) = \sum_n \delta(t - t_n) V_{SU}$$

Effective dynamics

Effect of a kick: $U = e^{-iV_{SU}}$

$$\mathcal{J}_S \rho_S(t) \equiv \mathrm{tr}_U\{U \rho_S(t) \otimes \rho_U U^\dagger\}$$

$$\mathcal{J}_U \rho_U \equiv \mathrm{tr}_S\{U \rho_S(t) \otimes \rho_U U^\dagger\}$$

$$d_t \rho_S(t) = -i[H_S(t), \rho_S(t)] + \mathcal{L}_\beta \rho_S(t) + \mathcal{L}_{\mathrm{new}} \rho_S(t)$$

$$\mathcal{L}_{\mathrm{new}} \rho_S(t) \equiv \gamma(\mathcal{J}_S - 1)\rho_S(t)$$

[Strasberg, Schaller, Brandes & Esposito, PRX **7**, 021003 (2017)]

Thermodynamics

1st law
$$d_t E_S(t) = \dot{W}_S(t) + \dot{W}_{SU}(t) + \dot{Q}(t) - d_t E_U(t)$$

$$\dot{W}_S = \mathrm{tr}_S\{\rho_S(t) d_t H_S(t)\}$$

$$\dot{W}_{SU} = \gamma \mathrm{tr}_{SU}\{[H_S(t) + H_U][U\rho_S(t)\rho_U U^\dagger - \rho_S(t)\rho_U]\}$$
$$= \gamma \mathrm{tr}_S\{H_S(t)(\mathcal{J}_S - 1)\rho_S(t)\} + \gamma \mathrm{tr}_U\{H_U(\mathcal{J}_U - 1)\rho_U\}$$

$$\dot{Q}(t) = \mathrm{tr}_S\{H_S(t)\mathcal{L}_\beta \rho_S(t)\}$$

$$d_t E_U(t) = \dot{W}_{SU}(t) - \gamma \mathrm{tr}_S\{H_S(t)\mathcal{L}_{\mathrm{new}}\rho_S(t)\}$$

2nd law
$$\dot{\Sigma}_S(t) = d_t S_S(t) + d_t S_U(t) - \beta\dot{Q} \geq 0$$

$$\neq -\mathrm{tr}\{[\mathcal{L}_0\rho_S(t)][\ln\rho_S(t) - \ln\rho_\beta^S(t)]\} - \mathrm{tr}\{[\mathcal{L}_{\mathrm{new}}\rho_S(t)][\ln\rho_S(t) - \ln\bar{\rho}_{\mathrm{new}}]\}$$

thermodynamics cannot always be deduced from dynamics alone

[Strasberg, Schaller, Brandes & Esposito, PRX **7**, 021003 (2017)]

Units entropy changes

Approach 1: $$\rho_U(t) = \mathcal{J}_U \rho_U$$

$$d_t S_U(t) = \gamma(-\mathrm{tr}_U\{(\mathcal{J}_U \rho_U)\ln(\mathcal{J}_U \rho_U)\} + \mathrm{tr}_U\{\rho_U \ln \rho_U\})$$

Approach 2: Fraction of units which interacted $d_t n_t = \gamma N$

$$\bar{\rho}_U(t) = \frac{n_t}{N}\mathcal{J}_U \rho_U + \frac{N - n_t}{N}\rho_U$$

$$d_t \bar{S}_U(t) = -d_t \mathrm{tr}_U\{\bar{\rho}_U(t) \ln \bar{\rho}_U(t)\} = -\gamma \mathrm{tr}_U\{[(\mathcal{J}_U - 1)\rho_U] \ln \rho_U\}$$

Different by $d_t \bar{S}_U(t) - d_t S_U(t) = \gamma D(\mathcal{J}_U \rho_U \| \rho_U)$ "mixing" contribution

Thermal units $\rho_U = \rho^U_{\beta'}$

$$d_t S_U(t) = \beta' d_t E_U(t) - \gamma D(\mathcal{J}_U \rho^U_{\beta'} \| \rho^U_{\beta'})$$

$$d_t \bar{S}_U(t) = \beta' d_t \bar{E}_U(t)$$ ideal reservoir

[Strasberg, Schaller, Brandes & Esposito, PRX 7, 021003 (2017)]

There is more...

Quantum master equation including degenerate states:

[Bulnes-Cuetara, Esposito & Schaller, Entropy **18**, 447 (2016)]

Fast periodic driving using master equation and Floquet theory:

[Bulnes-Cuetara, Engel & Esposito, NJP **18**, 447 (2016)]

Strong coupling using polaron transformation and quantum master equation:

[Krause, Brandes, Esposito & Schaller, JCP **142**, 134106 (2015)]
[Schaller, Krause, Brandes & Esposito, NJP **15**, 033032 (2013)]

Strong coupling using Nonequilibrium Green's functions:

[Esposito, Ochoa & Galperin, PRL **114**, 080602 (2015)]
[Esposito, Ochoa & Galperin, PRB **92**, 235440 (2015)]

Strong coupling (classical) using time scale separation:

[Strasberg & Esposito, arxiv:1703.05098]
[Esposito, Phys. Rev. E **85**, 041125 (2012)]

Thank you