Entropy production in open systems: the predominant role of intra-environment correlations

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Stochastic Thermodynamics of Complex Systems

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Outline

- Main question: what is the microscopic nature of entropy production in open (quantum) systems?
- Second law of thermodynamics for open quantum systems out of equilibrium
- Contributions to the entropy production: system-environment mutual information and the relative entropy of the environment
- Demonstration of predominance of the relative entropy
- Physical meaning of the relative entropy: intra-environment correlations
- Post-thermalization: information spreading after thermalization

Second law of thermodynamics for open systems

- Second law of thermodynamics → thermodynamics irreversibility
- For transition between equilibrium states

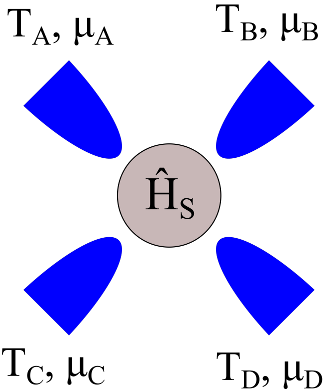
$$\Delta\mathcal{S} - Q/T \geq 0$$

- For open systems out of equilibrium [M. Esposito *et al.*, New J. Phys. **12**, 013013 (2010)]

$$\sigma = \Delta S_S - \sum_\alpha \beta_\alpha Q_\alpha \geq 0$$

where

  - σ – entropy production
  - $S_S = -\text{Tr}(\rho_S \ln \rho_S)$ – von Neumann entropy of the system
  - Q_α – heat delivered from the reservoir α



Derivation – assumptions

- Global Hamiltonian

$$\hat{H} = \hat{H}_S + \hat{H}_E + \hat{H}_I$$

where $\hat{H}_E = \sum_\alpha \hat{H}_\alpha$ (multiple baths)

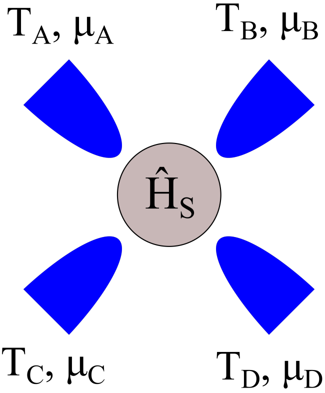
- Initially uncorrelated state

$$\rho_{SE}(0) = \rho_S(0) \otimes \rho_E^{\text{eq}}$$

- Initially thermal state of the environment

$$\rho_E^{\text{eq}} = \prod_\alpha Z_\alpha^{-1} e^{-\beta_\alpha \left(\hat{H}_\alpha - \mu_\alpha \hat{N}_\alpha\right)}$$

where $Z_\alpha = \text{Tr}\{\exp[-\beta_\alpha(\hat{H}_\alpha - \mu_\alpha \hat{N}_\alpha)]\}$



Derivation – assumptions

- Global unitary dynamics: $\Delta S_{SE} = 0$
- Generation of system-environment correlations

$$\Delta S_S + \Delta S_E = I_{SE} \geq 0$$

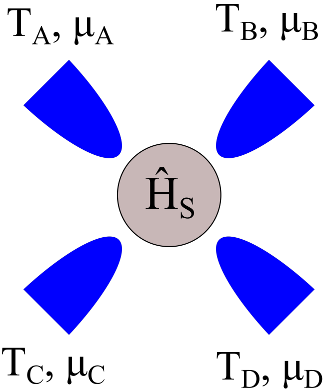
where $I_{SE} = S_S + S_E - S_{SE}$ – mutual information

- Von Neumann entropy change

$$\Delta S_E = -\sum_\alpha \beta_\alpha Q_\alpha - D(\rho_E || \rho_E^{\text{eq}})$$

where

- $Q_\alpha \equiv -\text{Tr}\left[(\rho_\alpha - \rho_\alpha^{\text{eq}})(\hat{H}_\alpha - \mu_\alpha \hat{N}_\alpha)\right]$ – heat delivered to system from bath α
- $D(\rho_E || \rho_E^{\text{eq}}) = \text{Tr}[\rho_E(\ln \rho_E - \ln \rho_E^{\text{eq}})] \geq 0$ – relative entropy



Contributions to the entropy production

- Finally

$$\sigma \equiv \Delta S_S - \sum_\alpha \beta_\alpha Q_\alpha = I_{SE} + D(\rho_E || \rho_E^{\text{eq}}) \geq 0$$

- Question: which contribution [I_{SE} or $D(\rho_E || \rho_E^{\text{eq}})$] is predominant
- Common argument:

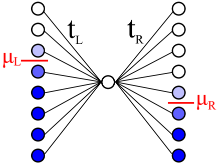
$$\Delta S_E = -\sum_\alpha \beta_\alpha Q_\alpha - D(\rho_E || \rho_E^{\text{eq}}) = -\sum_\alpha \beta_\alpha Q_\alpha + \mathcal{O}(\Delta \rho_E^2)$$

- $D(\rho_E || \rho_E^{\text{eq}})$ of the order of $\mathcal{O}(\Delta \rho_E^2)$, therefore negligible
- Implication: entropy production is related to correlation between the system and the environment

$$\sigma \approx I_{SE}$$

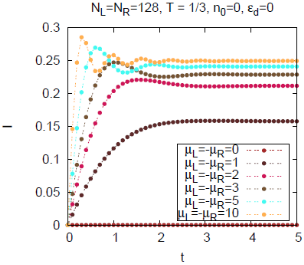
Saturation of mutual information (literature)

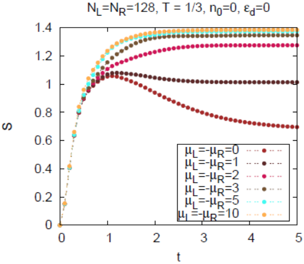
- Single resonant level [A. Sharma, E. Rabani, Phys. Rev. B **91**, 085121 (2015)]



$$\hat{H} = \epsilon_d c_d^\dagger c_d + \sum_{\alpha k} \epsilon_{\alpha k} c_{\alpha k}^\dagger c_{\alpha k} + \sum_{\alpha k} \left(t_{\alpha k} c_d^\dagger c_{\alpha k} + \text{h.c.} \right)$$

- Full description of system and environment (correlation matrix method)
- Mutual information I_{SE} saturates at the steady state
- Our conclusion: steady-state entropy production cannot result from the mutual information I_{SE}, but rather from the relative entropy (contrary to common opinion)



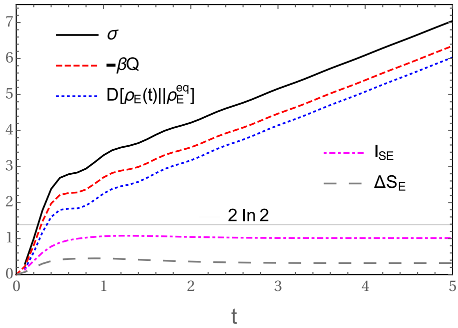


Single resonant level – thermodynamics (our results)

- Araki-Lieb inequality [H. Araki, E. H. Lieb, Commun. Math. Phys. **18**, 160 (1970)]

  $$I_{SE} \leq 2\min\{S_S, S_E\} \leq 2\ln\dim(\hat{H}_S)$$

  where $\dim(\hat{H}_S)$ – dimension of the Hilbert space of the system
- Mutual information I_{SE} saturates due to Araki-Lieb inequality
- Entropy production at long times results from the relative entropy $D(\rho_E||\rho_E^{eq})$



$\mu_L = -\mu_R = 1,\ \beta_L = \beta_R = \beta = 3,$
$\epsilon_{\alpha k} = (k-1)\Delta\epsilon - W/2,$
$\Delta\epsilon = W/(K-1),\ W = 20,\ K = 256$

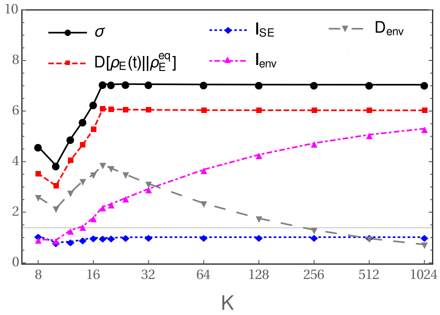
Contributions to the relative entropy

- Environment – noninteracting levels

$$\hat{H}_E = \sum_{\alpha k} \epsilon_{\alpha k} c^{\dagger}_{\alpha k} c_{\alpha k}$$

- Contributions to relative entropy

$$D(\rho_E || \rho_E^{\text{eq}}) = D_{\text{env}} + I_{\text{env}}$$



where

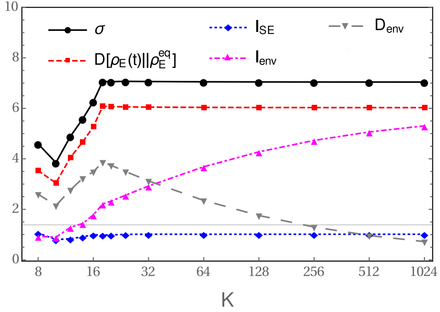
- $D_{\text{env}} = \sum_{\alpha k} D(\rho_{\alpha k} || \rho_{\alpha k}^{\text{eq}})$ – sum of relative entropies of the levels (deviations from equilibrium)

$\mu_L = -\mu_R = 1,\ \beta_L = \beta_R = \beta = 3,$
$\epsilon_{\alpha k} = (k-1)\Delta\epsilon - W/2,$
$\Delta\epsilon = W/(K-1),\ W = 20,\ t = 5$

- $I_{\text{env}} = \sum_{\alpha k} S_{\alpha k} - S_E$ with $S_{\alpha k} = -\text{Tr}(\rho_{\alpha k} \ln \rho_{\alpha k})$ – mutual information between the environmental degrees of freedom

Nature of the relative entropy

- D_{env} decreases with the number of sites K – level populations close to equilibrium ($n_i = \langle c_i^\dagger c_i \rangle \approx n_i^{eq}$)
- Mutual information I_{env} – results from the generation of two-point correlations ($\langle c_i^\dagger c_j \rangle \neq 0$)
- Preliminary results – I_{env} mainly related to the quantum coherence between the energy eigenstates of the bath



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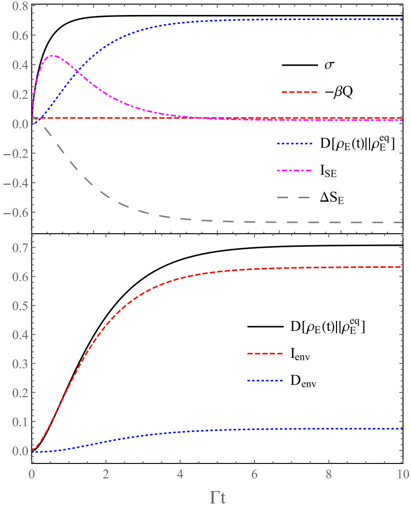
Entropy production during thermalization: Post-thermalization

- Whenever $\sigma \gg 2 \ln \dim(\hat{H}_S)$ the relative entropy production is the predominant contribution to σ
- Question: what happens when $\sigma \lessapprox 2 \ln \dim(\hat{H}_S)$?
- Preliminary results – "post-thermalization" – conversion of I_{SE} into the relative entropy (information spreading)
- Non-trivial dynamics of the environment at time-scales higher than the relaxation time!



Conclusions

- Entropy production at long times results from the displacement of the environment from equilibrium (relative entropy) rather than the mutual information between the system and the environment (contrary to common opinion)
- For large baths this results mainly from the correlation between the environmental degrees of freedom
- The environment may undergo nontrivial dynamics (associated with information spreading) even at time scales longer than the relaxation time
- Technical remark: the order of magnitude analysis should be applied with care

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Thank you for your attention!