Nature of Entropy Production in Open Systems

The Predominant Role of Intra-Environment Correlations

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Outline

- Main focus: connection between the information theory and 2nd law of thermodynamics
- Second law of thermodynamics for open quantum systems out of equilibrium
- Information-theoretic contributions to the entropy production: system-environment mutual information and the relative entropy of the environment
- Demonstration of predominance of the relative entropy (contrary to common view)
- Physical meaning of the relative entropy: intra-environment correlations

Second law of thermodynamics for open systems

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

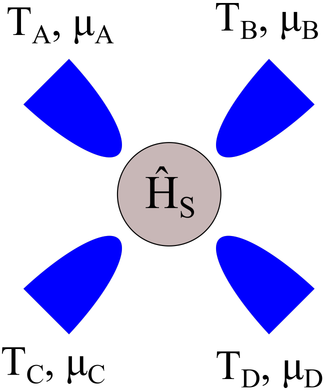
$$\Delta \mathcal{S} - Q/T \geq 0$$

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



Derivation of 2nd law – 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)

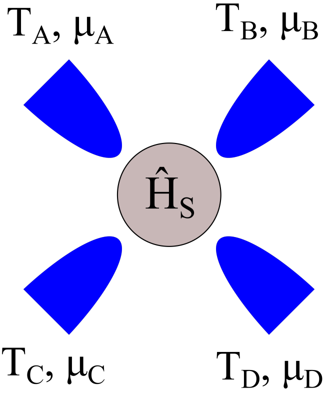
- Initially uncorrelated state

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

- 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 of 2nd law – assumptions

- Global unitary dynamics: $\Delta S_{SE} = 0$

$$\frac{d}{dt} = -\frac{i}{\hbar}[\hat{H}, \rho_{SE}]$$

- Generation of system-environment correlations

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

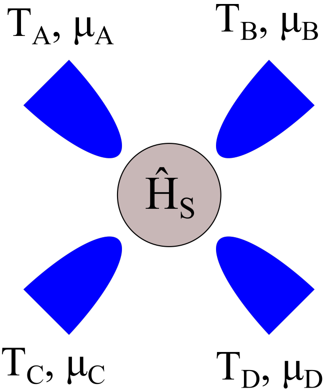
where $I_{SE} = S_S + S_E - S_{SE}$ – mutual information

- 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

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

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

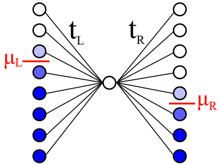
$$\Delta S_E = -\sum_\alpha \beta_\alpha Q_\alpha - D(\rho_E || \rho_E^{\mathrm{eq}}) = -\sum_\alpha \beta_\alpha Q_\alpha + \mathcal{O}(\Delta \rho_E^2)$$

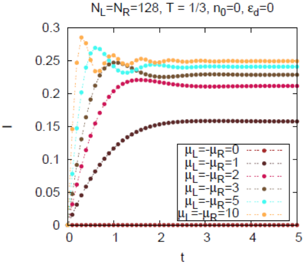
- $D(\rho_E || \rho_E^{\mathrm{eq}})$ of the order of $\mathcal{O}(\Delta \rho_E^2)$, therefore negligible for large baths
- ΔS_E related to heat (as in standard definition of entropy)
- Implication: entropy production is related to correlation between the system and the environment

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

Saturation of mutual information (literature)

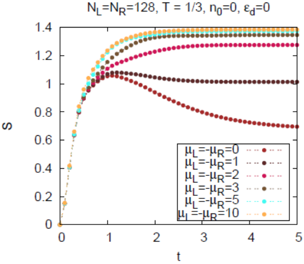
- Single resonant level [A. Sharma, E. Rabani, Phys. Rev. B **91**, 085121 (2015)]





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

- 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

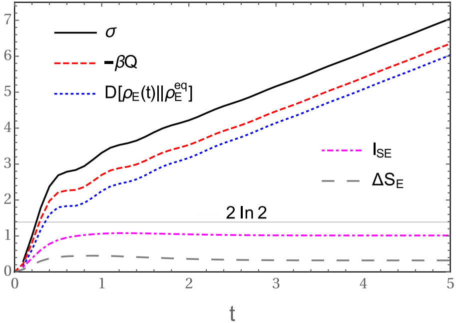


- Araki-Lieb inequality [H. Araki, E. H. Lieb, Commun. Math. Phys. **18**, 160 (1970)]

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

where $\dim(\hat{H}_S)$ – dimension of the Hilbert space of the system

- Mutual information I_{SE} saturates due to Araki-Lieb inequality
- ΔS_E also saturates – not directly related to heat
- 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

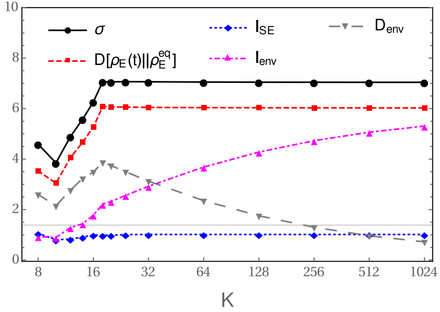
$$\hat{H}_E = \sum_{\alpha k} \epsilon_{\alpha k} c_{\alpha k}^{\dagger} c_{\alpha k}$$

- Contributions to relative entropy

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

where

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



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

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

Contributions to the relative entropy – interpretation

- $D_{\text{env}} = \sum_{\alpha k} D(\rho_{\alpha k} || \rho_{\alpha k}^{\text{eq}})$ – related to populations of the sites, which remain well thermalized in the thermodynamic limit

$$n_i = \langle c_i^\dagger c_i \rangle \approx \langle c_i^\dagger c_i \rangle_{\text{eq}}$$

  thus vanishes

- $I_{\text{env}} = \sum_{\alpha k} S_{\alpha k} - S_E$ – related to the generation of two point correlation functions

$$\langle c_i^\dagger c_j \rangle \neq 0$$

  which are not present in the equilibrium (thus $I_{\text{env}} > 0$)

- Entropy production is related to mutual information between the degrees of freedom in the environment rather than between the system and the environment

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 view)
- For large baths this results mainly from the correlation between the environmental degrees of freedom
- Methodology: the order of magnitude analysis should be applied with care

- More details: K. Ptaszyński and M. Esposito, *Entropy Production in Open Systems: The Predominant Role of Intra-Environment Correlations*, to appear in PRL (2019), arXiv:1905.03804

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