QUANTUM FEATURES OF IRREVERSIBILITY

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IRREVERSIBILITY AND ENTROPY PRODUCTION

UNDERSTAND AND QUANTIFY

- *Understanding* the emergence of irreversibility is a fundamental problem in physics.
- *Quantifying* it is crucial for several applications:
  - Engines, power plants, biological motors, electronic devices, &c.

- In thermodynamics, irreversibility is quantified by the **entropy production**.
- Thermodynamic processes obey the *Clausius inequality:*

$$\Delta S \geq \frac{\delta Q}{T}$$

- The difference is called the entropy production:

$$\Sigma := \Delta S - \frac{\delta Q}{T} \geq 0$$

- It is always non-negative and zero iff the process is reversible.

- Sometimes it is easier to work with *rates:*

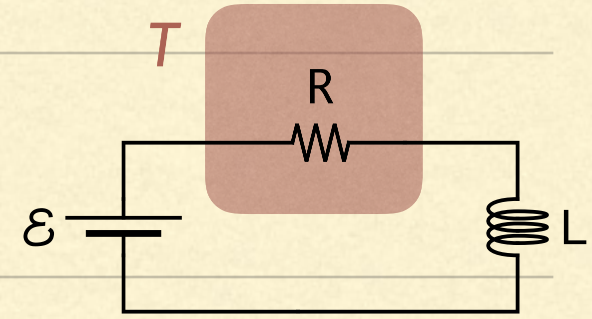
Rate of change of the entropy

$$\Pi = \frac{d\Sigma}{dt} \qquad \frac{dS}{dt} = \Pi - \Phi \qquad \Phi = -\frac{1}{T}\frac{dQ}{dt}$$

entropy production rate

entropy flux rate

EXAMPLE: ELECTRICAL CIRCUIT

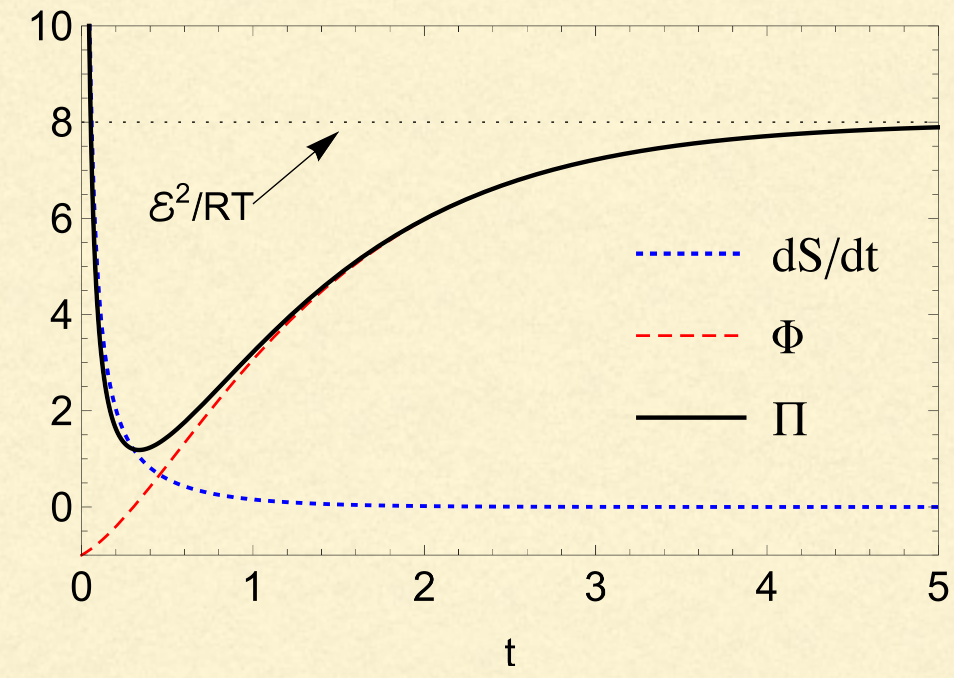


- The simplest example is an RL circuit connected to a bath and a battery.

$$\frac{dS}{dt} = \frac{R}{L}\frac{1}{e^{2Rt/L} - 1}$$

$$\Pi(t) = \frac{\mathcal{E}^2}{RT}(1 - e^{-Rt/L})^2 + \frac{R}{L}\frac{e^{-2Rt/L}}{e^{2Rt/L} - 1}$$

$$\Phi = \Pi - \frac{dS}{dt}$$



- In the long-time limit, this system will reach a *non-equilibrium steady state:*

$$\frac{dS}{dt} = 0 \qquad \text{but} \qquad \Pi_{ss} = \Phi_{ss} = \frac{\mathcal{E}^2}{RT}$$

GTL, T. Tomé and M. J. de Oliveira, *J. Phys. A*, **46**, 395001 (2013)

WHY ENTROPY PRODUCTION MATTERS

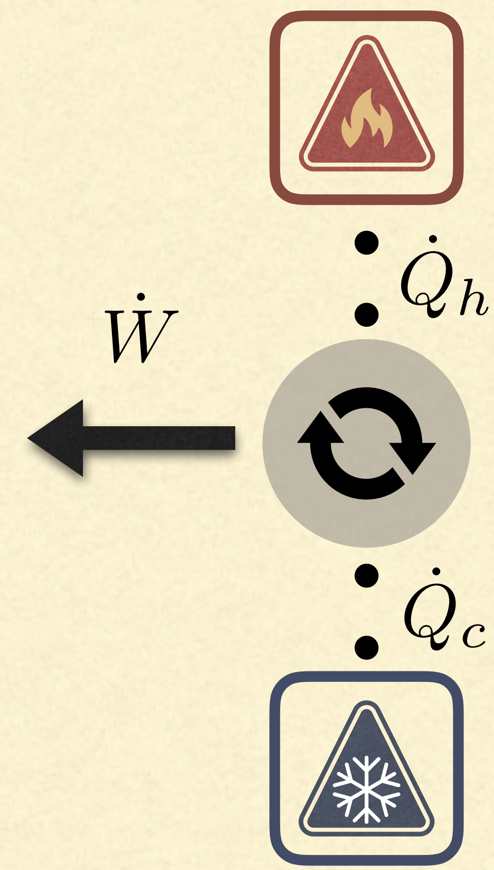
Thank you Wikipedia.

- The entropy production directly influences the efficiency of a heat engine.

- The 1st and 2nd laws *in the steady-state*, read:

$$\frac{dU}{dt} = \dot{Q}_h + \dot{Q}_c + \dot{W} = 0$$

$$\frac{dS}{dt} = \Pi + \frac{\dot{Q}_h}{T_h} + \frac{\dot{Q}_c}{T_c} = 0$$



- The efficiency in the steady-state reads:

$$\eta = -\frac{\dot{W}}{\dot{Q}_h} = 1 + \frac{\dot{Q}_c}{\dot{Q}_h} = 1 - \frac{T_c}{T_h} - \frac{T_c}{\dot{Q}_h}\Pi$$

- Entropy production is the reason why the efficiency is smaller than Carnot's.

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ARTICLE OPEN

The role of quantum coherence in non-equilibrium entropy production

Jader P. Santos[1], Lucas C. Céleri[2], Gabriel T. Landi[1] and Mauro Paternostro[3]

SCHNAKENBERG'S APPROACH

- Consider a discrete state system described by the classical master equation:

$$\frac{dp_n}{dt} = \sum_m \left\{ W(n|m)p_m - W(m|n)p_n \right\}$$

- We also assume detailed balance for simplicity (his result is actually more general):

$$\frac{W(n|m)}{W(m|n)} = \frac{p_n^{\text{eq}}}{p_m^{\text{eq}}} = e^{-\beta(E_n - E_m)}$$

- We now look at the evolution of the Shannon entropy:

$$S = -\sum_n p_n \ln p_n$$

Schnakenberg, Rev. Mod. Phys., **48**, 571 (1976)

- Schnakenberg showed that

$$\frac{dS}{dt} = \frac{1}{T}\frac{dQ}{dt} + \Pi$$

- where

$$\Pi = \frac{1}{2}\sum_{n,m}\Big\{W(n|m)p_m - W(m|n)p_n\Big\}\ln\frac{W(n|m)p_m}{W(m|n)p_n} \geq 0$$

- We can rewrite this formula in a neat way in terms of the *relative entropy (Kullback-Leibler divergence):*

$$\Pi = -\frac{d}{dt}S(\boldsymbol{p}(t)||\boldsymbol{p}^{\rm eq})$$

$$S(\boldsymbol{p}||\boldsymbol{q}) = \sum_n p_n \ln p_n/q_n$$

MASTER EQUATIONS AND THERMAL OPERATIONS

DAVIES MAPS

- The entropy production for Davies maps can be formulated in an analogous way:

$$\frac{d\rho}{dt} = \sum_i \gamma_i^- \left[A_i \rho A_i^\dagger - \frac{1}{2}\{A_i^\dagger A_i, \rho\} \right] + \gamma_i^+ \left[A_i^\dagger \rho A_i - \frac{1}{2}\{A_i A_i^\dagger, \rho\} \right]$$

(eigenoperator) $[H, A_i] = -\omega_i A_i$ $\qquad$ $\frac{\gamma_i^-}{\gamma_i^+} = e^{-\beta\omega_i}$ (detailed balance)

- The entropy production can be shown to be:

$$\Pi = -\frac{dS(\rho||\rho_{\mathrm{eq}})}{dt} \qquad S(\rho||\sigma) = \mathrm{tr}\left\{ \rho \ln \rho - \rho \ln \sigma \right\}$$

H. Spohn, *J. Math. Phys.*, **19**, 1227 (1978).
H.-P. Breuer, *Phys. Rev. A*, **68**, 032105 (2003)

- Davies maps select the energy basis as a preferred basis (*einselection*).

- This means the populations $p_n = \langle n|\rho|n\rangle$ will evolve according to

$$\frac{dp_n}{dt} = \sum_m \Big\{ W(n|m)p_m - W(m|n)p_n \Big\}$$

- We can now split

$$S(\rho||\rho_{\text{eq}}) = S(\boldsymbol{p}||\boldsymbol{p}_{\text{eq}}) + \mathcal{C}(\rho)$$

(relative entropy of coherence)

$$\mathcal{C}(\rho) = S(\boldsymbol{p}) - S(\rho)$$

- This yields:

$$\Pi = -\frac{dS(\boldsymbol{p}||\boldsymbol{p}_{\text{eq}})}{dt} - \frac{d\mathcal{C}}{dt}$$

- Coherence does *not* affect the entropy/heat flux.

- But decoherence is irreversible and thus affects the entropy production.

THERMAL OPERATIONS

- A thermal op. is a map of the form

$$\rho'_S = \mathcal{E}(\rho_S) = \mathrm{tr}_E\left\{U\left(\rho_S \otimes \frac{e^{-\beta H_E}}{Z_E}\right)U^\dagger\right\}$$

$$[U, H_S + H_E] = 0$$

- These maps are defined for any environment size and encompass Davies maps as a particular case.

- It also has a unique fixed point:

$$\mathcal{E}(e^{-\beta H_S}) = e^{-\beta H_S}$$

- Example:

$$U = e^{-iH_{SE}t} \qquad H_{SE} = \frac{\Omega}{2}(\sigma_z^S + \sigma_z^E) + g(\sigma_+^S\sigma_-^E + \sigma_-^S\sigma_+^E)$$

F. Brandão, M. Horodecki, J. Oppenheim, J. Renes & R. Spekkens, *Phys. Rev. Lett.*, **111**,250404 (2013).

- The entropy production for thermal operations is similarly defined as

$$\Sigma = S(\rho_S || \rho_S^{\text{eq}}) - S(\rho'_S || \rho_S^{\text{eq}})$$

- which can similarly be split as $\Sigma = \Sigma_d + \Xi$

$$\Sigma_d = S(\boldsymbol{p} || \boldsymbol{p}^{\text{eq}}) - S(\boldsymbol{p}' || \boldsymbol{p}^{\text{eq}})$$

$$\Xi = \mathcal{C}(\rho_S) - \mathcal{C}(\rho'_S)$$

- It is also possible to express the entropy production as

$$\Sigma = S(\rho'_E || \rho_E^{\text{eq}}) + \mathcal{I}(\rho'_{SE})$$

$$\mathcal{I}(\rho'_{SE}) = S(\rho'_S) + S(\rho'_E) - S(\rho'_{SE})$$ (SE mutual information)

M. Esposito, K. Lindenberg, C. Van Den Broeck, *New Journal of Physics*, **12,** 013013 (2010)

BASIS DEPENDENT QUANTUM DISCORD

- For thermal operations it follows that the total coherence is conserved,

$$\mathcal{C}(\rho_S) = \mathcal{C}(\rho'_{SE})$$

- We now define the *distributed coherence* (basis dependent discord):

$$\mathcal{C}_d(\rho'_{SE}) = \mathcal{C}(\rho'_{SE}) - \mathcal{C}(\rho'_S) - \mathcal{C}(\rho'_E)$$

$$= \mathcal{I}(\rho'_{SE}) - \mathcal{I}(\Delta(\rho'_{SE}))$$

- The coherence part of the entropy production will therefore also have two contributions,

$$\Xi = \mathcal{C}(\rho'_E) + \mathcal{C}_d(\rho'_{SE})$$

T. M. Kraft and M. Piani, arXiv 1801.03919

STOCHASTIC TRAJECTORIES

STOCHASTIC TRAJECTORIES

- We finally formulate the same problem using stochastic trajectories and the standard 2-point measurements.

(different bases)

$$\rho_S = \sum_\alpha p_\alpha |\psi_\alpha\rangle\langle\psi_\alpha| \qquad \rho_E = \sum_\mu q_\mu |\mu\rangle\langle\mu|$$

$$H_S = \sum_n E_n |n\rangle\langle n|$$

- Measure S+E in $|\psi_\alpha, \mu\rangle$
- Evolve with *U*.
- Measure only E (cool thing about thermal op.). Conditional final state of S:

$$|\Phi_{F|\alpha,\mu,\nu}\rangle = \frac{\langle\nu|U|\psi_\alpha,\mu\rangle}{\sqrt{P_F(\nu|\alpha,\mu)}} \qquad P_F(\nu|\alpha,\mu) = |\langle\nu|U|\psi_\alpha,\mu\rangle|^2$$

- The path probabilities are

$$\mathcal{P}_F[\alpha,\mu,\nu] = P_F(\nu|\alpha,\mu)p_\alpha q_\mu$$

- And the final state may be decomposed as an incoherent superposition of the quantum trajectories:

$$\rho_S' = \sum_{\alpha,\mu,\nu} \mathcal{P}[\alpha,\mu,\nu]|\Phi_{F|\alpha\mu\nu}\rangle\langle\Phi_{F|\alpha\mu\nu}|$$

- However, this is not an eigendecomposition. In general, we have

$$\rho_S' = \sum_\beta p_\beta'|\psi_\beta'\rangle\langle\psi_\beta'| \qquad p_\beta' = \sum_{\alpha,\mu,\nu} p_{\beta|\alpha\mu\nu}\mathcal{P}_F[\alpha,\mu,\nu] \qquad p_{\beta|\alpha\mu\nu} = |\langle\psi_\beta'|\Phi_{F|\alpha\mu\nu}\rangle|^2$$

- Notwithstanding, we can augment the trajectory as

$$\mathcal{P}_F[\alpha,\mu,\beta,\nu] = p_{\beta|\alpha\mu\nu}\;\mathcal{P}_F[\alpha,\mu,\nu] = |\langle\psi_\beta'|\Phi_{F|\alpha\mu\nu}\rangle|^2\;|\langle\nu|U|\psi_\alpha,\mu\rangle|^2 = |\langle\psi_\beta'\nu|U|\psi_\alpha\mu\rangle|^2$$

BACKWARD PROCESS

- Measure S+E in $|\psi'_\beta, \nu\rangle$
- Evolve with $U^\dagger$
- Measure E: the final state of the system conditioned on the trajectory will be

$$|\Phi_{B|\beta\mu\nu}\rangle = \frac{\langle\mu|U^\dagger|\psi'_\beta,\nu\rangle}{\sqrt{P_B(\mu|\alpha,\nu)}} \qquad P_B(\mu|\beta,\nu) = |\langle\mu|U^\dagger|\psi'_\beta,\nu\rangle|^2$$

- The probability for the backwards trajectory will then be

$$\mathcal{P}_B[\alpha,\mu,\beta,\nu] = p_{\alpha|\beta,\nu,\mu} P_B(\mu|\beta,\nu) p'_\beta q_\nu \qquad p_{\alpha|\beta,\nu,\mu} = |\langle\psi_\alpha|\Phi_{B|\beta\mu\nu}\rangle|^2$$

G. Manzano, J. M. Horowitz, J. M. R. Parrondo, *Phys Rev. X*, **8**, 031037 (2018).

STOCHASTIC ENTROPY PRODUCTION

- The stochastic entropy production is then defined as usual:

$$\sigma = \ln \frac{\mathcal{P}_F}{\mathcal{P}_B} = \ln \frac{p_\alpha q_\mu}{p'_\beta q_\nu}$$

- It is constructed so that

$$\langle e^{-\sigma} \rangle = 1 \qquad \langle \sigma \rangle = \Sigma = S(\rho_S || \rho_S^{\text{eq}}) - S(\rho'_S || \rho_S^{\text{eq}})$$

- But, in the spirt of the previous results, we now wish to separate it as

$$\sigma = \sigma_d + \xi$$

AUGMENTED TRAJECTORIES

- We introduce augmented trajectories

$$\tilde{\mathcal{P}}_F[\alpha, n, \mu, \beta, m, \mu] = p_{n|\alpha} p'_{m|\beta} \mathcal{P}_F[\alpha, \mu, \beta, \nu]$$

- where

$$p_{n|\alpha} = |\langle n|\psi_\alpha\rangle|^2 \qquad p'_{m|\beta} = |\langle m|\psi'_\beta\rangle|^2$$

- One may then define

$$\sigma_d = \ln \frac{p_n q_\mu}{p'_m q_\nu} \qquad \xi = \ln \frac{p_\alpha p'_m}{p'_\beta p_n}$$

P. A. M. Dirac, "On the analogy between classical and quantum mechanics". *Rev. Mod. Phys.* **17**, 195 (1945).

J. J. Park, S. W. K, V. Vedral, arXiv 1705.01750

- They give the correct averages:

$$\langle \sigma_d \rangle = \Sigma_d = S(\boldsymbol{p}||\boldsymbol{p}^{\mathrm{eq}}) - S(\boldsymbol{p}'||\boldsymbol{p}^{\mathrm{eq}})$$

$$\langle \xi \rangle = \Xi = \mathcal{C}(\rho_S) - \mathcal{C}(\rho_S')$$

- But they *do not* individually obey fluctuation theorems.

- The classical entropy production has to be corrected by the information gain:

$$\langle e^{-\sigma_d - \xi} \rangle = 1$$

- This is ultimately related to the incompatibility of quantum mechanical bases.

G. Francica, J. Goold and F. Plastina, 1707.06950

NON-LOCAL CONTRIBUTIONS TO ENTROPY PRODUCTION

In collaboration with Rafael Chaves, Lucas Céleri, and Paul Riechers.

- Each system interacts with a local bath.
- The systems do not interact with each other.
    - But they are prepared in a non-local state (only non-local contribution).
- The global map is then

$$\rho'_{SE} = U(\rho_S \otimes \rho_{E_1} \otimes \ldots \otimes \rho_{E_N})U^\dagger \qquad U = U_{S_1,E_1} \otimes \ldots \otimes U_{S_N,E_N}$$

- The unitaries may contain work.
    - We define heat as the change in energy of the environments.

$$Q_i = \langle H'_{E_i} \rangle - \langle H_{E_i} \rangle$$

D. Reeb and M.W.Wolf, *NJP*, **16**, 103011 (2014).

- We then define entropy production as:

$$\Sigma = \Delta \mathcal{S}_S + \sum_i \beta_i Q_i = \mathcal{I}_{\rho'_{SE}}(S:E) + \mathcal{S}(\rho'_E||\rho_E)$$

- We now introduce the total correlations

$$\mathcal{T}(\rho_S) = \mathcal{S}(\rho_S||\rho_{S_1} \otimes \ldots \otimes \rho_{S_N}) = \sum_i \mathcal{S}(\rho_{S_i}) - \mathcal{S}(\rho_S)$$

- The entropy production then becomes

$$\Sigma = \sum_i (\Delta \mathcal{S}_{S_i} + \beta_i Q_i) - \Delta \mathcal{T}$$

- Finally, we can also write this as

$$\Sigma = \sum_i \beta_i (W_i - \Delta F_i) - \Delta \mathcal{T} \qquad \Delta E_{S_i} = W_i - Q_i$$

QUANTUM CONTRIBUTIONS TO Σ

- We can split the total correlations into a classical term, related to the populations in the energy basis, plus the distributed coherence:

$$\mathcal{T}(\rho_S) = \mathcal{T}(\rho_S^{(d)}) + \mathcal{C}_d(\rho_S)$$

$$\mathcal{C}_d(\rho_S) = \mathcal{C}(\rho_S) - \sum_i \mathcal{C}(\rho_{S_i})$$

- The entropy production then becomes:

$$\Sigma = \sum_i (\Delta \mathcal{S}_{S_i} + \beta_i Q_i) - \Delta \mathcal{T}_c - \Delta \mathcal{C}_d$$

$$= \sum_i \beta_i (W_i - \Delta F_{S_i}) - \Delta \mathcal{T}_c - \Delta \mathcal{C}_d$$

- The positivity Σ then gives bounds on how distributed coherence affects the heat exchange (Landauer-style) and the amount of work that can be extracted.

Thank you!

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