Generalized Clausius inequality for nonequilibrium quantum processes

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Outline

1. Nonequilibrium entropy production
   - Microscopic expression
   - Geometric distance in Hilbert space
   - Generalized Clausius inequality
2. Nonequilibrium entropy production rate
   - Quantum speed limit
   - Maximal entropy production rate
   - Bremermann-Bekenstein bound

Introduction

Observation:

Thermodynamics describes equilibrium transformations

Challenge:

Generalization to arbitrary nonequilibrium processes

Motivation:

Far from equilibrium regime accessible in recent cold-atom experiments

Thermodynamics: a short reminder

Equilibrium (reversible) processes:

Entropy: $\Delta S_{rev} = Q/T$

Work: $W_{rev} = \Delta F$ ($F = U - TS$ = free energy)

Nonequilibrium (irreversible) processes:

Entropy: $\Delta S = Q/T + \Delta S_{irr}$

Work: $W = \Delta F + W_{irr}$

with $\Delta S_{irr} \geq 0$ and $W_{irr} \geq 0$ (Second law)

→ Thermodynamics does not allow computation of ΔS_{irr}, W_{irr}

Thermodynamics: a short reminder

Clausius inequality:

Clausius 1865

$$\Delta S_{irr} \geq 0$$

"Nonequilibrium entropy production always positive"

- lower bound "zero" is transformation independent
  → not useful for far from equilibrium processes
- sharper, transformation dependent lower bound necessary
  → use geometric distance from equilibrium

Macroscopic expression for ΔS_{irr}

Definition:

$$\Delta S_{irr} = \Delta S - Q/T$$

First law and free energy difference:

$$\Delta U = W + Q \qquad \text{and} \qquad \Delta F = \Delta U - T\Delta S$$

$$\longrightarrow \quad Q = \Delta F - W + T\Delta S$$

Nonequilibrium entropy production:

$$\Delta S_{irr} = \beta(W - \Delta F) = \beta W_{irr} \qquad \beta = 1/T$$

⟶ difference between total work and equilibrium work

Microscopic expression for ΔS_{irr}

Isolated, thermal quantum system with driven Hamiltonian H_τ

Work distribution:

Talkner, Lutz, Hänggi PRE (2007)(R)

$$\mathcal{P}(W) = \sum_{m,n} \delta\left(W - \left(E_m^\tau - E_n^0\right)\right) p_{m,n}^\tau p_n^0$$

→ thermal and quantum fluctuations

Nonequilibrium entropy production: $\Delta S_{irr} = \beta(\langle W \rangle - \Delta F)$

$$\Delta S_{\text{irr}} = S\left(\rho_\tau || \rho_\tau^{eq}\right) = \text{tr}\left\{\rho_\tau \ln\left(\rho_\tau\right) - \rho_\tau \ln\left(\rho_\tau^{eq}\right)\right\}$$

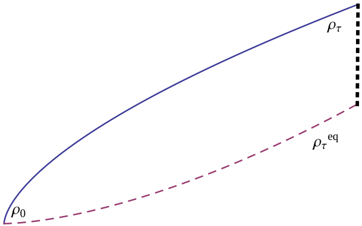
Fluctuation theorem:

Jarzynski PRL 1997

$$\langle \exp(-\beta W_{irr}) \rangle = 1$$

Quantum entropy production

$$\Delta S_{\text{irr}} = S\left(\rho_\tau || \rho_\tau^{eq}\right)$$



ρ_0 initial, thermal density operator

- ρ_τ nonequilibrium density operator
- ρ_τ^{eq} equilibrium density operator, $\rho_\tau^{eq} = \exp(-\beta H_\tau)/Z$

⟶ exact expression for ΔS_{irr}

but relative entropy not a true metric (asymmetric and no triangle inequality)

Distances: a reminder

Distance between two (unit) vectors:

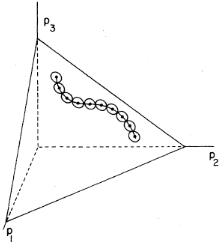
Angle: $\theta = \arccos \boldsymbol{a}.\boldsymbol{b} = \arccos \sum_i a_i b_i$

→ maximal distance $\theta = \pi/2$ (maximally distinguishable)

Distance between two pdfs (pure states in Hilbert space):

$$\ell = \arccos \int dx \sqrt{p_0(x) p_\tau(x)}$$

→ also number of distinguishable states between p_0 and p_τ



Wootters PRD 1981

'Angle' in Hilbert space

→ only Riemannian metric invariant under all unitary transformations

Distances: a reminder

Distance between two density operators (mixed states): Bures 1969

Bures length: $$\mathcal{L}(\rho_1, \rho_2) = \arccos\left(\sqrt{F(\rho_1, \rho_2)}\right)$$

→ generalization of Wootters' distance to mixed states

Braunstein and Caves PRL 1994

Fidelity: $$F\left(\rho_1, \rho_2\right) = \left[\mathrm{tr}\left\{\sqrt{\sqrt{\rho_1}\,\rho_2\,\sqrt{\rho_1}}\right\}\right]^2$$

→ For pure states = overlap $$F(\rho_1, \rho_2) = \mathrm{tr}\left\{\rho_1, \rho_2\right\}$$

$F = 1$ for identical states and $F = 0$ for orthogonal states

Lower bound for the relative entropy

Theorem:

Audenaert and Eisert, J. Math Phys. (2005)

For any unitarily invariant norm $d(\rho_1, \rho_2)$ and $e^{i,j} = |i\rangle\langle j|$

$$S(\rho_1||\rho_2) \geq 2\,\frac{d^2\left(\rho_1, \rho_2\right)}{d^2\left(e^{1,1}, e^{2,2}\right)}$$

For the Bures length $\mathcal{L}$, $F(e^{1,1}, e^{2,2}) = 0$

$$\Delta S_{\mathrm{irr}} \geq \frac{8}{\pi^2}\,\mathcal{L}^2\left(\rho_\tau, \rho_\tau^{\mathrm{eq}}\right)$$

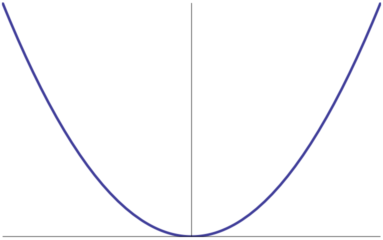
- → generalized Clausius inequality (beyond linear response)
- → valid for arbitrary nonequilibrium quantum processes
- → for classical, near equilibrium processes:

$$S\left(\rho^{\mathrm{eq}} + d\rho||\rho^{\mathrm{eq}}\right) \simeq 2\mathcal{L}^2\left(\rho^{\mathrm{eq}} + d\rho, \rho^{\mathrm{eq}}\right) \simeq d\ell^2\left(\rho^{\mathrm{eq}} + d\rho, \rho^{\mathrm{eq}}\right)/2$$

Salamon, Berry, PRL 51 (1983)

Time-dependent harmonic oscillator

Illustration:



Time-dependent frequency: $H = \frac{p^2}{2m} + \frac{m}{2}\,\omega^2(t)\,x^2$

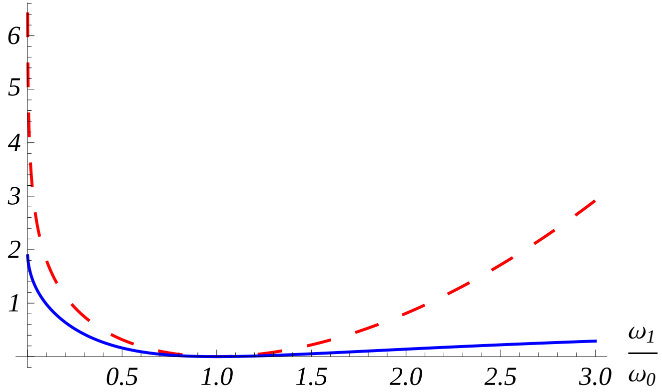
Initially thermalized, but otherwise isolated

⟶ describes modulated ion traps

Huber, Schmidt-Kaler, Deffner, Lutz, PRL (2008)

Generalized Clausius inequality

Harmonic oscillator:



Red: entropy production

Blue: squared Bures length

$$\omega_t^2 = \omega_0^2 + \left(\omega_1^2 - \omega_0^2\right)\, t/\tau$$

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Entropy production rate

Definition:

$$\sigma = \frac{\Delta S_{\text{irr}}}{\tau}$$

- fundamental quantity of nonequilibrium physics
- gives information about the speed of a process

In quantum nonequilibrium physics, there is a maximum entropy production rate

Quantum speed limit

Observation:

Hamiltonian (energy) is the generator of time evolution

⟶ energy sets limits on speed of quantum evolution

Uncertainty principle: $\tau \, \Delta E \geq \hbar$

⟶ minimal time to reach orthogonal state given by initial energy spread

Minimal time for nonorthogonal states: Giovannetti, Lloyd, Maccone PRA (2003)

$$\tau_{\text{min}} \simeq \max \left\{ \frac{2\hbar \, \mathcal{L}^2 \left(\rho_0, \rho_\tau\right)}{\pi \, E_0}, \frac{\hbar \, \mathcal{L} \left(\rho_0, \rho_\tau\right)}{\Delta E_0} \right\}$$

Slow process (time-independent Hamiltonian)

Maximum entropy production rate:

$$\sigma_{\text{max}} = \frac{\Delta S_{\text{irr}}}{\tau_{\text{min}}} \leq 2\beta\langle H_\tau\rangle \min\left\{\frac{\pi\, E_0}{\hbar\, \mathcal{L}^2\,(\rho_0, \rho_\tau)}, \frac{\Delta E_0}{\hbar\, \mathcal{L}\,(\rho_0, \rho_\tau)}\right\}$$

⟶ determined by initial energy and geometric distance to equilibrium

$$\Delta S_{\text{irr}} = \beta|\langle H_\tau\rangle - \langle H_0\rangle - \Delta F| \leq 2\beta\langle H_\tau\rangle$$

Bremermann-Bekenstein bound

Limit of far from equilibrium processes:

→ initial and maximum state orthogonal $\mathcal{L}(\rho_0, \rho_\tau) \simeq \pi/2$

Limit of high temperatures:

→ $E_0 \simeq 1/\beta$ and $\Delta E_0 \simeq E_0/\sqrt{N} \ll E_0$

$$\sigma \leq \frac{4}{\hbar\pi} \langle H_\tau \rangle$$

→ maximum communication rate (capacity) through noiseless channel with signals of finite duration Bremermann 1967, Bekenstein 1981

Fast process (time-dependent Hamiltonian)

Quantum speed limit time:

$$\tau_{\text{min}} = \max \left\{ \frac{\hbar \mathcal{L}(\rho_\tau, \rho_0)}{E_\tau}, \frac{\hbar \mathcal{L}(\rho_\tau, \rho_0)}{\Delta E_\tau} \right\}$$

with $E_\tau = (1/\tau)\int_0^\tau dt \langle H_t \rangle$ and $\Delta E_\tau = (1/\tau)\int_0^\tau dt\, (\langle H_t^2 \rangle - \langle H_t \rangle^2)^{1/2}$

⟶ time averaged quantities (and not initial values)

Minimum energy change for a give entropy variation:

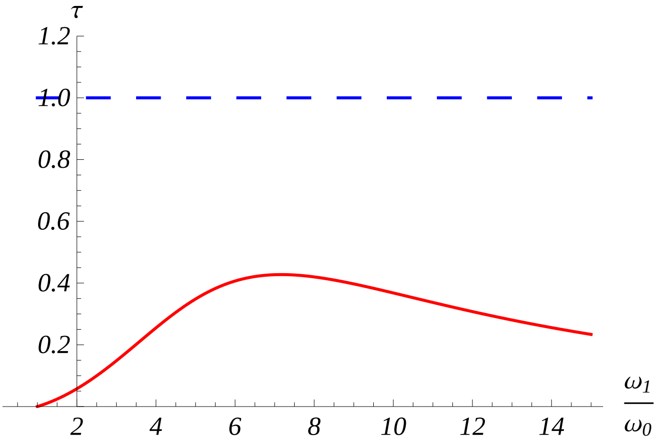
$$\frac{\langle H_\tau \rangle}{\Delta S_{\text{irr}}} \geq \frac{2\beta}{\tau} \min \left\{ \frac{E_\tau}{\hbar \mathcal{L}(\rho_\tau, \rho_0)}, \frac{\Delta E_\tau}{\hbar \mathcal{L}(\rho_\tau, \rho_0)} \right\}$$

Generalized Bremermann-Bekenstein bound, valid for

⟶ arbitrary distance between initial and final states
⟶ arbitrary initial temperature
⟶ arbitrary nonequilibium processes

Quantum speed limit time

Zero-temperature harmonic oscillator:



Red: quantum speed limit time

Blue: actual process duration

$$\omega_t^2 = \omega_0^2 + \left(\omega_1^2 - \omega_0^2\right)\, t/\tau$$

Summary

- generalization of the Clausius inequality for the entropy production to arbitrary nonequilibrium quantum processes

  → lower bound in terms of the geometric distance to equilibrium (Bures length)

- generalization of the Bremermann-Bekenstein bound for the entropy production rate to arbitrary quantum processes

  → upper bound in terms of the geometric distance to equilibrium and averaged energy