Entropy production and work in Generalised Gibbs Ensembles

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Quantum Thermodynamics and Quantum Information Theory
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Equilibration and Thermalisation in closed quantum systems

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And, if they equilibrate, do they reach thermalization? ("Proof" the appearance of Gibbs states).

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Quantum thermodynamics

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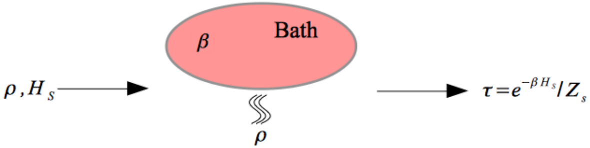
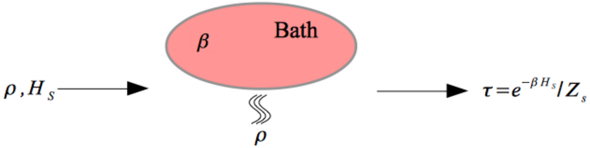
Examples:

- Heat engines.
- Resource theory of quantum thermodynamics. Gibbs states at ambient temperature are free resources, and the allowed operations are,

$$\rho \to \sigma = \mathrm{Tr}_B[U\rho \otimes \frac{e^{-\beta H}}{\mathcal{Z}} U^{\dagger}]$$

  with $[U, H_\rho + H] = 0$.





However, this picture is not quite true. Systems do not always thermalize, e.g.,

- strong coupling between system and bath,
- integrable systems,
- ...

An example: a chain of fermions

$$H = H_S + H_B + V$$

with

$$H_B = \sum_{i=1}^{N} a_i^\dagger a_i + g\left(a_i^\dagger a_{i+1} + a_{i+1}^\dagger a_i\right), \quad H_S = \epsilon c^\dagger c, \quad V = g\left(a_N^\dagger c + c^\dagger a_N\right).$$

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$$\rho_0 = \rho_s \otimes \frac{e^{-\beta H_B}}{\mathcal{Z}_B}$$

$$\rho(t) = U\rho_0 U^\dagger, \qquad U = e^{-iHt}$$

$$\text{population} = \mathrm{Tr}(c^\dagger c \rho(t))$$

$$\text{thermal state} = \frac{e^{-\beta H_S}}{\mathcal{Z}_S}$$

$$\text{Parameters}: N = 50,\ g = 0.3,\ \epsilon = 2$$

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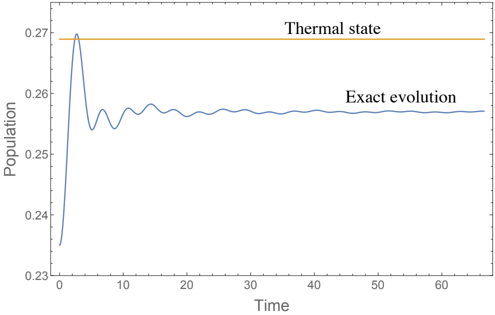

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Equilibration in closed quantum systems

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Equilibration in closed quantum systems

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Let a quantum system $\rho = |\psi_0\rangle\langle\psi_0|$ evolve under H, $\rho(t) = e^{-iHt}\rho e^{iHt}$.

Equilibration of subsystems [2]

For every ρ , the average distinguishability between $\rho_S(t) = \text{Tr}_B\rho(t)$ and time-averaged state $\omega_S = \text{Tr}_B\omega$ satisfies

$$\langle \mathcal{D}(\rho_S(t), \omega_S)\rangle_t \leq \frac{1}{2}\sqrt{\frac{d_S^2}{d^{\text{eff}}}}.$$

where $d^{\text{eff}} = \frac{1}{\sum_k |\langle E_k|\psi_0\rangle|^4}$ is the effective dimension.

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[2] P. Reimann, PRL. 101,190403 (2008), NJP 12, 055027 (2010); N. Linden, S. Popescu, A. Short and A. Winter, PRE 061103 (2009), NJP 12, 055021 (2010)

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Equilibration of subsystems

Equilibration of general observables [2]

For every ρ, and given a finite set of measurements $\mathcal{M}$, it is satisfied that

$$\langle \mathcal{D}(\rho_S(t), \omega_S)\rangle_t \leq \frac{\mathcal{N}(\mathcal{M})}{4\sqrt{d^{\mathrm{eff}}}}.$$

where $\mathcal{N}(\mathcal{M})$ is the total number of outcomes for all measurements in M.

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Equilibration of general observables

Closed finite quantum systems equilibrate *for all practical purposes*.

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$$\omega(\rho, H) := \lim_{T\to\infty} \frac{1}{T} \int_0^T \mathrm{e}^{-\mathrm{i}Ht}\, \rho\, \mathrm{e}^{\mathrm{i}Ht} \mathrm{d}t\,,$$

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A simple calculation yields,

$$\omega(\rho, H) = \sum_k P_k \rho P_k\,,$$

with $H = \sum_k E_k P_k$.

Thermalization

The equilibrium state $\omega(\rho, H)$ will in general not be a Gibbs state. In particular ω will depend on the initial state ρ.
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2. Subsystem state independence. If the subsystem is small compared to the bath, the equilibrium state of the subsystem should be independent of its initial state.

3. Gibbs form of the equilibrium state. Here we distinguish between,
   - weak thermal contact, $\rho_S = \frac{e^{-\beta H_S}}{\mathcal{Z}_S}$.
   - beyond weak interactions, $\rho_S = \mathrm{Tr}_B \frac{e^{-\beta H}}{\mathcal{Z}}$.

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Equilibration, thermalisation, and the maximum entropy principle

Let $H = \sum_k E_k P_k$ and $\rho(t) = e^{-iHt} \rho e^{iHt}$. Consider all conserved quantities A

$$\frac{d\,\mathrm{tr}(A\rho(t))}{dt} = 0, \qquad \text{with } [H, A] = 0.$$

If H is non-degenerate, then it suffices to take all P_k.

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- If one fixes all the conserved quantities $\mathrm{Tr} A\rho(t)\ \forall A$, then the time averaged state $\omega = \langle \rho \rangle_t$ is the state maximizing the Von Nemann entropy, $S = -\,\mathrm{tr}\, \rho \ln \rho$.

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- The Gibbs state $\omega_{\mathrm{Gibbs}}(\rho, H)$ maximises S when only *one* constant of motion, the energy $\mathrm{tr}(H\rho)$, is fixed. This maximization yields,

  $$\omega_{\mathrm{Gibbs}}(\rho, H) = \frac{e^{-\beta H}}{\mathcal{Z}}$$

  where β is found through $\mathrm{tr}(H\rho) = \mathrm{tr}(H\omega_{\mathrm{Gibbs}}(\rho, H)$.

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  where β is found through $\mathrm{tr}(H\rho) = \mathrm{tr}(H\omega_{\mathrm{Gibbs}}(\rho, H)$.
- Generalized Gibbs states[3] (GGE) lie in between. Given a set of conserved quantities $\{Q_i\}$, the GGE is the state maximising S, which gives,

  $$\omega_{\mathrm{GGE}}(\rho, H, \{Q_i\}) = \frac{e^{-\sum_i \beta_i Q_i}}{\mathcal{Z}}$$

  where β_i is found through $\mathrm{tr}(Q_i\rho) = \mathrm{tr}(Q_i\omega_{\mathrm{GGE}}(\rho, H, \{Q_i\}))$.

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Subjective and objective approach to choose Q_i

- *Subjective approach:*[4] the relevant conserved quantities are those that are experimentally accessible.
- *Objective approach:*[5] choose the ones that make the GGE as close as possible (e.g., in trace distance) to the time-averaged-state.

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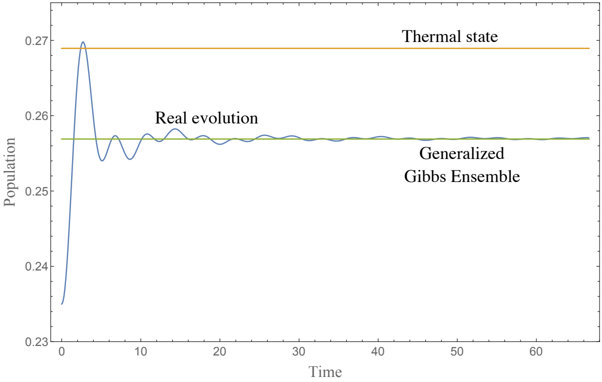
Choosing the constants of motion, an example.

Consider again a fermonic chain. Since the Hamiltonian is quadratic,

$$H = H_S + V + H_B = \sum_{ij} c_{ij} a_i^\dagger a_j = \sum_{k=1}^{N} \epsilon_k \eta_k^\dagger \eta_k = \sum_{k=1}^{N} h_k$$

Construct the GGE with N conserved quantities: $\mathrm{tr}(h_k \rho)$.



Thermodynamics with Generalised Gibbs Ensembles

0. Framework.

1. Entropy production.

2. Work extraction.

3. Optimal protocols and reversibility.

Framework: Quenches and equilibrations.

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Operations

Given some $\rho^{(i)}$, $H^{(i)}$ and

- Quenches: Fast change of the Hamiltonian $H^{(i)} \to H^{(i+1)}$. To it we associate a work cost,

$$W(\rho^{(i)}, \{H^{(i)}, H^{(i+1)}\}) := \mathrm{Tr}\left(\rho^{(i)}(H^{(i+1)} - H^{(i)})\right),$$

If we only change H_S: $W = \mathrm{Tr}\left(\rho_S^{(i)}(H_S^{(i+1)} - H_S^{(i)})\right)$.

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- Equilibration: After the quench, the state evolves as:

  $$\rho^{(i+1)}(t) = \mathrm{e}^{-\mathrm{i}tH^{(i+1)}}\rho^{(i)}\mathrm{e}^{\mathrm{i}tH^{(i+1)}}.$$

Effective description of the dynamics.

A (cyclic) work-extraction protocol is a sequence of N quenches:

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Under these quenches, the state of SB evolves as

$$\rho^{(0)} \to \rho^{(1)} \to \ldots. \to \rho^{(N-1)} \to \rho^{(N)}$$

$$\rho^{(i)} = \left(\bigotimes_i U_i \right) \rho \left(\bigotimes_i U_i^\dagger \right), \qquad U_k = e^{-itH^{(k)}}, \quad t \gg t_{\text{equilibration}}.$$

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We use an effective, time-independent description of the evolution:

$$\rho^{(0)} \to \omega^{(1)} \to \omega^{(2)} \to \ldots \to \omega^{(n)}$$

where ω is an equilibrium state (either Gibbs, GGE or time-average).
More precisely,

$$\omega^{(i+1)} = \omega_{\text{GGE}} \left(\omega^{(i)}, H, \{Q_i\} \right)$$

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Effective description with one constant of motion: the energy

Equilibrium states are Gibbs,

$$\omega^{(i)} = \frac{e^{-\beta^{(i)} H^{(i)}}}{\mathcal{Z}_i}$$

Notice that the temperature β changes through the protocol. It is find through the relation, $\mathrm{tr}(\omega^{(i)} H^{(i+1)}) = \mathrm{tr}(\omega^{(i+1)} H^{(i+1)})$.

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Recovering the classical thermodynamic limit

Temperature dependence: $\beta^{(i+1)} = \beta^{(i)} + \mathcal{O}\left(\frac{\text{Energy of the quench}}{\text{Total energy } S + B}\right)$.

Weak coupling limit: $e^{-\beta H} \approx e^{-\beta H_S^{(i)}} \otimes e^{-\beta H_B}$.

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Remark

The effective entropy defined here is different from the sum of local entropies,

$$S_{SB} = S(\rho_S) + S(\rho_B),$$

which is often used to compute entropy production. Note that S_{SB} can fluctuate when considering strongly interacting systems (it is only monotonically increasing under natural assumptions in the weak coupling limit).

Limit of very slow processes

$$\rho^{(0)} \to \omega^{(1)} \to \omega^{(2)} \to \dots \to \omega^{(N)}$$

In the limit of slow processes ($N \to \infty$), it is satisfied

$$S(\omega^{(N)}) = S(\omega^{(1)}) + \mathcal{O}\left(\frac{1}{N}\right).$$

In other words, no entropy is produced in infinitesimally slow processes. This introduces a notion of reversibility.

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Idea of the proof

By construction, the equilibrium states before and after the quench satisfy,

$$\mathrm{tr}(Q_{j+1}\omega^{(i)}) = \mathrm{tr}(Q_{j+1}\omega^{(i+1)}) \quad \forall j$$

where Q_j are all the conserved quantities. On the other hand, consider the (generalized) free energy functional $G_{\beta_{i+1}}(\sigma) = S(\sigma) - \sum_j \beta_{j+1} \mathrm{Tr}(Q_{j+1}\sigma)$. Since $\omega^{(i+1)}$ is a maximum $G_{\beta_{i+1}}(\sigma)$, one has $S(\omega^{(i+1)} + \delta\omega) - S(\omega^{(i+1)}) = \mathcal{O}(\delta\omega^2)$.

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Remark.

Besides $N \to \infty$, some further conditions on the Hamiltonian path need to be imposed to ensure entropy conservation.

Work extraction protocols.

Are optimal protocols for work extraction reversible?

Work extraction for Gibbs states

The total work cost reads,

$$\begin{aligned} W &= \mathrm{Tr}\left(\rho_S^{(0)}(H_S^{(0)} - H_S^{(1)})\right) + \sum_{i=1}^{n} \mathrm{Tr}\left(\rho_S^{(i)}(H_S^{(i)} - H_S^{(i+1)})\right) \\ &= \mathrm{Tr}\left(\rho_{SB}^{(0)}(H^{(0)} - H_{SB}^{(1)})\right) + \sum_{i} \mathrm{Tr}\left(\omega^{(i)}(H^{(i)} - H^{(i+1)})\right) \\ &= \mathrm{Tr}\left(H^{(0)}\left(\rho_{SB}^{(0)} - \omega^{(n)}\right)\right) \end{aligned}$$

where the ω's are equilibrium states for S+B, and we used that $\mathrm{Tr}\left(H^{(i+1)}\left(\omega^{(i)} - \omega^{(i+1)}\right)\right) = 0$.

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Clearly, the optimal protocol is the one minimising $\mathrm{tr}\left(H^{(0)}\omega^{(n)}\right)$. Since entropy and energy are monotonically related for Gibbs states, the optimal protocol is always the one minimising the entropy production.

Note that this property holds for any protocol. That is, once the first quench is realised, work is always maximised in the slowest path (minimal work principle).

Work extraction with GGE

For GGE equilibrium states, the one-to-one correspondence between energy and entropy is lost. This opens the door towards breaking the minimal work principle.

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For GGE equilibrium states, the one-to-one correspondence between energy and entropy is lost. This opens the door towards breaking the minimal work principle. A case study: quadratic fermionic Hamiltonians,

$$H = \sum_{ij} c_{ij} a_i^\dagger a_j$$

with $a_i^\dagger, a_j = \delta_{ij}$, and $\{a_i, a_j\} = \{a_i^\dagger, a_j^\dagger\} = 0$.

Work extraction from fermonic systems I

Optimal protocol

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Work extraction from fermonic systems I

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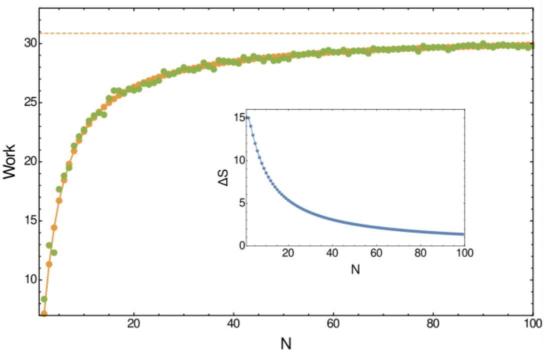
The optimal protocol can be found using the notion of passive states[6], and it is found to be *reversible*, in the sense that no entropy is produced in our effective description.

Work extraction from fermonic systems I

The optimal protocol is reversible.

Example: Chain of fermions



Comparison between unitary dynamics and effective description

Excellent agreement.

Our description does not capture fluctuations in time of the magnitude of interest.

Protocols constrained to actions on S

Now we consider a more realistic scenario where the Hamiltonian transformations are restricted to S,

$$H = H_S(t) + H_B + V.$$

Here the extracted work becomes a local quantity.

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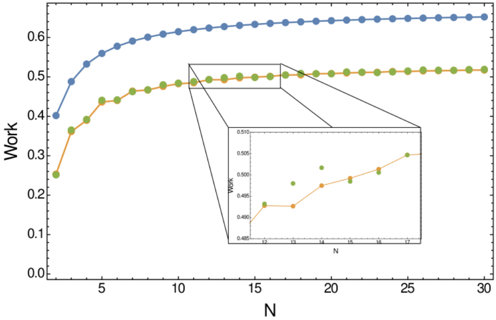
Case study: a chain of fermions.

Initial conditions: $\rho^{(0)} = \rho_S \otimes \frac{e^{-\beta H_B}}{\mathcal{Z}_{\mathcal{B}}}$.



The minimal work principle is not always satisfied for GGE.

Since equilibrium states here are not well described by Gibbs state by rather by GGE states, it is natural to generalise the initial state to

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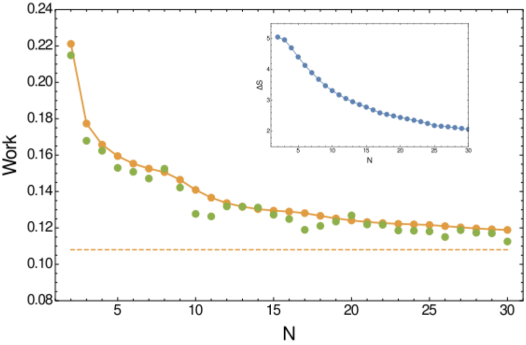
Given this new freedom, there are choices of ω_{GGE}, such as,

$$\mathrm{Tr}(\omega^{(B)}_{\mathrm{GGE}} \eta^{(B)\dagger}_k \eta^{(B)}_k) = \begin{cases} 1 & k \geq K \\ 0 & k < K \end{cases}$$

for which the minimal work principle does not hold.



Conclusions

- Coarse-grained description of the evolution of equilibrium states.
- Entropy production and reversibility in quantum closed systems.
- Implications for the relation between reversibility and maximal work extraction.

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Thank you very much for your attention.