Information Theory — Foundations and Applications

Quantum thermodynamics

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The dawn of irreversibility

> Newton's laws are fundamentally reversible. Why do we see irreversible process all around us?

> **Knowledge**
> The answer relies on our lack of knowledge.

But from where does this ignorance come from?

The thermodynamic limit

Physical quantities must be defined in terms of length and time measurements. What is a macroscopic measurement?

In the thermodynamic limit

The precision of our rulers and clocks are much bigger than the fundamental length and time scales at the atomic level. **Fluctuations** are suppressed and we only see the time and space averages of the complex underlying dynamics. Classical macroscopic measurements are naturally **coarse-grained**.

Thermodynamic quantities

From this procedure, thermodynamic quantities emerge and we have a framework to describe a complex system based on a few macroscopic variables.

The paradigm of thermodynamics

Classical thermodynamics
Thermodynamics relies on the **subjective** lack of knowledge arising from the impossibility to follow the complex underlying dynamics of a macroscopic system.

Quantum thermodynamics — Gauge perspective
In the same spirit, it is proposed that the relevant physical quantities should not take into account all the information contained in the quantum state of the system.

Quantum thermodynamics

There are several approaches to quantum thermodynamics

- Quantum statistical mechanics[1]
- Resource theory[2]
- Density functional theory[3]
- Axiomatic formulation[4]
- Information theory[5]

We are here interested in the **information** approach to thermodynamics.

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[1] M. Esposito, U. Harbola and S. Mukamel, Rev. Mod. Phys. **81**, 1665 (2009)
[2] M. Lostaglio, Rep. Prog. Phys. **82** 114001 (2019)
[3] M. Herrera, R. M. Serra and I. D'Amico, Sci Rep **7**, 4655 (2017)
[4] E. H. Lieb and J. Yngvason, Physics Reports **310**, 1 (1999)
[5] S. Deffner and S. Campbell, *Quantum thermodynamics* (Iop Concise Physics, 2019)

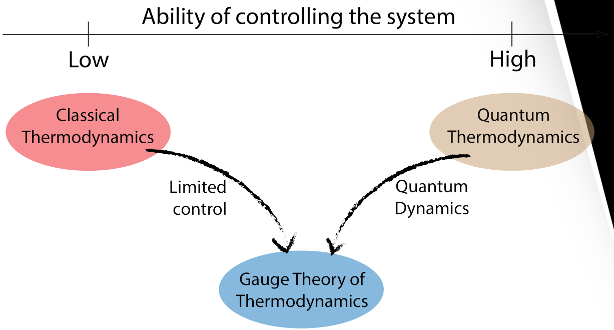
The scope of the theory

The general goal
How thermodynamic concepts like heat and work can be taken to the quantum realm, where fluctuations and randomness are fundamentally unavoidable?

Our approach
Keeping the same spirit of classical thermodynamics, and based on the *gauge invariance principle*, we propose a gauge group that washes out the irrelevant information contained in the quantum state of the system, thus introducing the coarse-grained procedure from what the thermodynamic quantities emerge.

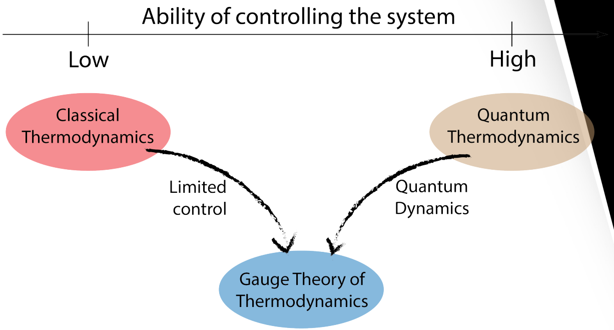
Why the gauge principle?

We have full control of the quantum system (we known the quantum state). Information theory enters the game in order to define thermodynamic quantities. However, the full quantum description is richer than the classical one. We also have information about bases.



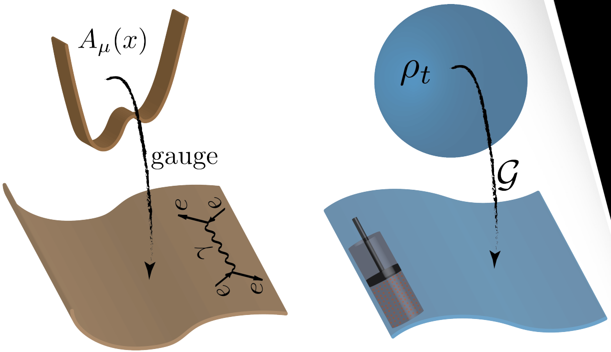
Why the gauge principle?

Most of this information is **redundant** from the point of view of thermodynamics, in the same sense that the positions and velocities of all particles in a system are not relevant for classical thermodynamics.



Why the gauge principle?[6]

Following the spirit of classical thermodynamics, we need to eliminate such redundancy. This is exactly the job of the **gauge invariance** principle: Physically meaningful quantities must be invariant under certain symmetry group.



[6] N. Cabibbo, L. Maiani and O. Benhar, *An introduction to gauge theories* (CRC Press, 2017)

Thermodynamic relevant quantities

We assume that all relevant quantities can be expressed as functionals of the density matrix ρ_t

$$F\left[\rho_t\right]$$

Some of particular interest here are the mean energy

$$U\left[\rho_t\right] = \mathrm{Tr}\rho_t H_t$$

and the work associated with a given process that takes place during the time interval $t \in [0, \tau]$[7]

$$W\left[\rho_t\right] = \int_0^\tau \mathrm{d}t \mathrm{Tr}\left[\rho_t \frac{\mathrm{d}H_t}{\mathrm{d}t}\right]$$

In this context, heat is defined as the difference between these last two equations.

[7] R. Alicki, J. Phys. A **12**, L103 (1979)

The allowed gauge transformations

- In our theory, the role of the potentials is played by carriers of quantum information, namely, the density matrices ρ_t.
- The gauge transformations must be represented by unitary matrices V_t acting as follows $\rho_t \mapsto V_t \rho_t V_t^\dagger$.

What kind of transformations are allowed?

Definition 1 (Emergent thermodynamic gauge)

Unitary transformations are admissible gauge transformations if they preserve the mean energy

$$U\left[V_t \rho_t V_t^\dagger\right] = U\left[\rho_t\right],$$

for all ρ_t, where $U\left[\rho_t\right] = \mathrm{Tr} \rho_t H_t$.

The construction of the thermodynamic gauge

Assuming that we are working with a d-dimensional system, the set of transformations V_t (that commutes with H_t) forms a subgroup of $\mathcal{U}(d)$, the set of $d \times d$ unitary matrices. Let H_t be a time dependent Hamiltonian and u_t the matrix that diagonalizes H_t. The thermodynamic group is the set

$$\mathcal{T}_H = \left\{ V_t \in \mathcal{U}(d) | \, [V_t, H] = 0, V_t = u_t \left(\bigoplus_{k=1}^{p} v_t^k \right) u_t^\dagger \right\}$$

wih $v_t^k \in \mathcal{U}(n_t^k) \subset \mathcal{U}(d)$ and $\Gamma = \{n_t^k\}_{k=1,\ldots,p}$ is the set of degeneracies at every instant t

From a topological point of view, this emergent gauge group is isomorphic to

$$\mathcal{G} = \mathcal{U}(n_1) \times \mathcal{U}(n_2) \times \ldots \times \mathcal{U}(n_p)$$

Gauge invariant thermodynamic quantities

Therefore, we have the Haar measure $\mathrm{d}\mathcal{G}$. Group averaging allows one to assign to each relevant quantity its gauge invariant version

If if F is not isomeric invariant

$$F_{\text{inv}}[\rho] = \int \mathrm{d}\mathcal{G} F\left[V_t \rho V_t^\dagger\right].$$

If F is invariant under unitaries, then

$$F\left[\mathrm{D}(\rho)\right] = F[\rho_{dd}^E]$$

in which $\mathrm{D}(\cdot) \equiv \int \mathrm{d}\mathcal{G} V_t (\cdot) V_t^\dagger$ and

$$\rho_{dd}^E \equiv \bigoplus_{k=1}^{p\leq d} \frac{\mathrm{Tr}\{\rho_{n_t^k}^E\}}{n_t^k} \mathbb{1}_{n_t^k}.$$

Gauge invariant work

The usual notion of work is not gauge invariant

$$W\left[\rho_t\right] \mapsto W\left[\rho_t\right] + \int_0^\tau \mathrm{d}t \mathrm{Tr}\left[H_t, \rho_t\right] V_t^\dagger \frac{\mathrm{d}V_t}{\mathrm{d}t}$$

We instead propose the following form for the **quantum work**

Definition 2 (Gauge invariant work)
Let $h_t = u_t^\dagger H_t u_t$ be the diagonal form of the Hamiltonian H_t, with u_t unitary. Then, the notion of work which is invariant with respect to the emergent thermodynamic gauge is given by

$$W_{\mathrm{inv}}[\rho_t] = \int_0^\tau \mathrm{d}t \mathrm{Tr}\left[\rho_t u_t \dot{h}_t u_t^\dagger\right]$$

Gauge invariant heat

From conservation of energy the invariant heat can be written as $Q_{\mathrm{inv}} = Q_u + Q_c$, where the usual heat reads

$$Q_u = \int_0^\tau \mathrm{d}t \mathrm{Tr}\left[\dot{\rho}_t H_t\right] \equiv \int_0^\tau \mathrm{d}t \mathrm{Tr}\left[\dot{\rho}_t u_t h_t u_t^\dagger\right],$$

while the **coherent heat** is defined as

$$Q_c = \int_0^\tau \mathrm{d}t \mathrm{Tr}\left[\rho_t \dot{u}_t h_t u_t^\dagger + \rho_t u_t h_t \dot{u}_t^\dagger\right].$$

Q_c contains **only** contributions from the coherences in the energy eigenbasis!

The Gauge entropy

We take von Neumann entropy of the quantum states as the measure of the total information contained in the considered state. By applying our theory to this quantity, we obtain the invariant notion of entropy

$$S_{\mathcal{G}}(\rho) = S(\rho_{dd}^{E})$$

with

$$\rho_{dd}^{E} \equiv \bigoplus_{k=1}^{p \leq d} \frac{\mathrm{Tr}\{\rho_{n_t^k}^{E}\}}{n_t^k} \mathbb{1}_{n_t^k}.$$

It is interesting to note that this quantity turns out to be exactly equal to the observational entropy and it is deeply related to the diagonal entropy[8]

[8] G. F. Ferrari, Ł. Rudnicki and L. C. Céleri, arxiv: 2409.07676

Properties of the entropy

By defining $V_t = u_t \mathcal{V}_t u_t^\dagger$ and the quantum channel as

$$\Lambda_{\mathcal{G}}\left[\rho\right] = \int \mathrm{d}\mathcal{G} \mathcal{V}_t \rho \mathcal{V}_t^\dagger$$

the gauge entropy can be written as

$$S_{\mathcal{G}}(\rho) = S_{\mathcal{G}}\left(\Lambda_{\mathcal{G}}\left[\rho_{\text{diag}}^E\right]\right)$$

Another interesting property is that

$$\Delta S_{\mathcal{G}} \geq 0$$

for all processes.

Gauge potential

We can rewrite both expressions by introducing the gauge potential $A_t = i\dot{u}_t u_t^\dagger$.

$$W_{\text{inv}}[\rho_t] = \int_0^\tau \mathrm{d}t \, \mathrm{Tr}\left[\rho_t D_t H_t\right] \quad \text{and} \quad Q_{\text{inv}}[\rho_t] = \int_0^\tau \mathrm{d}t \, \mathrm{Tr}\left[H_t D_t \rho_t\right],$$

with the covariant derivative defined as

$$D_t(\cdot) = \partial_t(\cdot) + i[A_t, (\cdot)]$$

The invariance of W_{inv} and Q_{inv} under V_t comes from the fact that the potential transforms as

$$A_t \mapsto A_t' = V_t^\dagger A_t V_t - i V_t^\dagger \dot{V}_t$$

Take home messages

- Although (mean) energy is well defined, the classical notions of work and heat cannot be directly translated to the quantum world, thus leading us to several definitions that are, in general, nonequivalent, but operationally well defined[9].
- The theory proposed here leads to gauge invariant definitions of thermodynamic quantities. Heat and work are not solely related with the changes in the information entropy. Work is associated with the changes in the eigenvalues of the Hamiltonian, while heat is connected with the changes in the eigenbasis of the Hamiltonian, thus being deeply linked with energy delocalization.
- There is a well defined notion of entropy that increases for every quantum operation, staying constant only in the case of adiabatic transformations.

[9] P. Talkner and P. Hänggi, Phys. Rev. E **93**, 022131 (2016)

Thank you for your attention

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