Colóquio do Instituto de Física da Universidade de São Paulo

Quantum thermodynamics and irreversibility

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Summary

- * Quantum Thermodynamics?
 - * Motivation from Quantum Information Sciences.
- * Recent progress and general trends in the field.
- * Quantifying irreversibility at the quantum level.

We live in the age of quantum technologies

- Since its conception, quantum mechanics has already provided us with remarkable technologies:
 - * Lasers.
 - Semiconductors: solar panels, LEDs, computers, smartphones.
 - * Nuclear magnetic resonance, electron microscopy, etc.
- These are now called Quantum Technologies 1.0 (UK Defence Science and Technology Laboratory)

But quantum mechanics also predicts other properties, such as *coherence* and *entanglement*, which are not usually employed in these applications.

Coherence

 In QM we learn that a superposition of states is also a valid state:

 $|\psi\rangle = a|1\rangle + b|2\rangle$

- But when we construct the periodic table, we don't care about this: we just "put" the electrons in each state.
- * That's not very quantum:
 - * Its quantum because the energy levels are discrete.
 - * But other than that, its classical.



 $|2\rangle$

 $|1\rangle$

Decoherence

- * Coherences and entanglement are usually washed away very quickly by the contact of a system with its environment.
- * We start with a pure state:

$$|\psi\rangle = a|0\rangle + b|1\rangle \qquad \Longrightarrow \qquad \rho = |\psi\rangle\langle\psi| = \begin{pmatrix} |a|^2 & ab^*\\ a^*b & |b|^2 \end{pmatrix}$$

Then the contact with the environment will gradually degrade the coherences:

$$\rho(t) = \begin{pmatrix} |a|^2 & e^{-\gamma t} a b^* \\ e^{-\gamma t} a^* b & |b|^2 \end{pmatrix}$$

* If we wait long enough, we eventually get a classical state:

$$\rho(\infty) = \begin{pmatrix} |a|^2 & 0\\ 0 & |b|^2 \end{pmatrix}$$

Isolate, experiment, understand...

- And so began a long quest to isolate, experiment and understand with these more exotic *quantum resources*:
 - Coherence, entanglement, squeezing, asymmetry, purity, discord, &c.
- We now have are many platforms where we can have impressive control over individual quantum systems:
 - Quantum optics, trapped ions, superconducting qubits, NMR, NV centers in diamond, Bose-Einstein condensates, ultra-cold atoms in optical lattices, &c.



Quantum Technologies 2.0

- Together with these experimental advances, it also became clear that we could harness these quantum resources to produce new technologies:
 - * Secure communications with *quantum cryptography*.
 - * Exponentially faster algorithms with *quantum computers*.
 - * Higher sensitivity with *quantum metrology*.
- * Will any of these ever see the light of day?
 - * Based on the history of physics, we will *definitely* see some applications.
- * But even if no direct applications appear:
 - What we learned so far in this field is already helping in many other areas, such as e.g. *strongly correlated systems* (in this context correlation = entanglement).

Quantum Thermodynamics

- It is now straightforward to define what is the goal of "Quantum Thermodynamics":
 - * To understand the role of quantum resources in thermodynamic quantities such as heat and work.
- Topics of current interest include:
 - * The role of measurements in thermodynamic processes.
 - * Thermal transformations under the presence of quantum fluctuations.
 - How coherence, entanglement and squeezing affect the operation of heat engines.
 - * Irreversibility at the quantum level.

Review of the recent literature

Quantum measurement

PHYSICAL REVIEW E 75, 050102(R) (2007)

Fluctuation theorems: Work is not an observable

Peter Talkner, Eric Lutz, and Peter Hänggi

PRL 118, 070601 (2017) PHYSICAL REVIEW LETTERS 17 FEBRUARY 2017

in Coherent Quantum Systems

Martí Perarnau-Llobet,^{1,*} Elisa Bäumer,^{1,2,†} Karen V. Hovhannisyan,^{1,‡} Marcus Huber,^{3,4,§} and Antonio Acin^{1,5,¶}

The role of quantum measurement in stochastic thermodynamics

Cyril Elouard¹, David A. Herrera-Martí¹, Maxime Clusel² and Alexia Auffèves¹ *npj Quantum Information* (2017)3:9

Thermal operations

Published 27 Jun 2014 Work extraction and thermodynamics for individual quantum systems

Paul Skrzypczyk¹, Anthony J. Short² & Sandu Popescu²

NATURE COMMUNICATIONS | 5:4185 | DOI: 10.1038/ncomms5185 |

Published 26 Jun 2013 Fundamental limitations for quantum and nanoscale thermodynamics

Michał Horodecki^{1,*} & Jonathan Oppenheim^{2,3,*}

NATURE COMMUNICATIONS | 4:2059 | DOI: 10.1038/ncomms3059 |

The second laws of quantum thermodynamics

Fernando Brandão^{a,1}, Michał Horodecki^b, Nelly Ng^c, Jonathan Oppenheim^{c,d,2}, and Stephanie Wehner^{c,e}

PNAS | March 17, 2015 | vol. 112 | no. 11 | 3275–3279

The second laws of quantum thermodynamics

Fernando Brandão^{a,1}, Michał Horodecki^b, Nelly Ng^c, Jonathan Oppenheim^{c,d,2}, and Stephanie Wehner^{c,e} PNAS | March 17, 2015 | vol. 112 | no. 11 | 3275–3279

Rényi entropy
$$S_{\alpha} = -\frac{1}{1-\alpha}\log \mathrm{tr} \rho^{\alpha}$$

von Neumann entropy

$$S_1 = -\mathrm{tr}(\rho \ln \rho)$$

$$F_{\alpha}(\rho,\rho_{\beta}) \coloneqq kTD_{\alpha}(\rho \| \rho_{\beta}) - kT\log Z,$$

with the Rényi divergences $D_{\alpha}(\rho \| \rho_{\beta})$ defined as

$$D_{\alpha}(\rho \| \rho_{\beta}) = \frac{\operatorname{sgn}(\alpha)}{\alpha - 1} \log \sum_{i} p_{i}^{\alpha} q_{i}^{1 - \alpha},$$

A transition is allowed when:

$$F_{\alpha}(\rho,\rho_{\beta}) \ge F_{\alpha}(\rho',\rho_{\beta})$$

Generalizes the second law. For macroscopic systems all Rényi entropies converge to von Neumann.

More general heat engines



Viewpoint: Squeezed Environment Boosts Engine Performance

James Millen, Vienna Center for Quantum Science and Technology, University of Vienna, 1090

Vienna, Austria

September 13, 2017 • *Physics* 10, 99

Selected for a Viewpoint in *Physics* PHYSICAL REVIEW X 7, 031044 (2017)

Squeezed Thermal Reservoirs as a Resource for a Nanomechanical Engine beyond the Carnot Limit

Jan Klaers,^{*} Stefan Faelt, Atac Imamoglu, and Emre Togan Institute for Quantum Electronics, ETH Zürich, CH-8093 Zürich, Switzerland (Received 25 April 2017; revised manuscript received 25 July 2017; published 13 September 2017)



Coherence producing engine

Autonomous thermal machine for amplification and control of energetic coherence

Gonzalo Manzano,^{1,2} Ralph Silva,³ and Juan M.R. Parrondo¹



Measures of Irreversibility

Entropy production

* The energy of a system satisfies a continuity equation:

$$\frac{d\langle H\rangle}{dt} = -\Phi_E$$

* For the entropy that is not true:

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

П represents the entropy production rate due to the irreversible dynamics:

 $\Pi \ge 0$ and $\Pi = 0$ only in equilibrium

Dinâmica estocástica e irreversibilidade, T. Tomé e M. J. de Oliveira

Traditional formulation

* The traditional theory of entropy production, for both quantum and classical systems, is based on the following formulas:

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

Entropy production

$$\Pi = -\frac{d}{dt}S(\rho||\rho_{\rm eq})$$

$$S(\rho || \rho^{\rm eq}) = \operatorname{tr}(\rho \ln \rho - \rho \ln \rho^{\rm eq})$$

(Relative entropy)

Entropy flux

$$\Phi = \frac{\Phi_E}{T}$$
$$\left(dS = \frac{dE}{T}\right)$$

J. Schnakenberg, *Rev. Mod. Phys.* 48, 571 (1976).
H. Spohn, *J. Math. Phys.*, 19, 1227 (1978)
T. Tomé and M. J. de Oliveira, *Phys. Rev. Lett*, 108, 020601 (2012)

Entropy production and loss of coherence

* The environment selects a preferred basis for the system.

$$\rho = \begin{pmatrix} p_0 & q \\ q^* & p_1 \end{pmatrix}$$

- When the system interacts with an environment, two things happen simultaneously:
 - * The *populations* adjust to the levels imposed by the bath: $p_n = \langle n | \rho | n \rangle$
 - The system looses coherence.
- * We may write the relative entropy as

$$S(\rho||\rho_{\rm eq}) = S(p||p_{\rm eq}) + C(\rho)$$

$$S(p||p_{eq}) = \sum_{n} p_n \ln p_n / p_n^{eq}$$
$$C(\rho) = S(p) - S(\rho)$$

 $\Pi = \Pi_d + \Pi_{\rm coh}$

Entropy is produced due to the "classical" transitions between energy levels and also due to the loss of coherence

Problems with the standard formulation

$$\frac{dS}{dt} = \Pi - \Phi \qquad \qquad \Pi = -\frac{d}{dt}S(\rho||\rho_{eq}) \qquad \qquad \Phi = \frac{\Phi_E}{T}$$

- * Difficult to extend to systems connected to multiple reservoirs.
- * Cannot be extended to non-equilibrium reservoirs:
 - * Squeezed baths, dephasing baths, engineered baths, &c.
- * Breaks down at T = 0.

Spontaneous emission is at T = 0

- * Every system is nature is connected to a bath:
 - *Vacuum fluctuations act as a zero-temperature bath.*
 - Explains why atoms emit photons and relax to the ground-state.
- * The theory of open quantum systems accounts for this type of process quite naturally.
- * Everything is well behaved.
- * But Π and Φ diverge when $T \rightarrow 0$.



Dynamics of open quantum systems

Most used approaches

- * Keldysh Green's functions (discussed in Altland's book on Cond. Mat. Field Theory).
- Quantum Fokker-Planck-Kramers equation.
 - * M. J. de Oliveira, PRE, 94, 012128 (2016)
- Quantum Brownian motion:
 - * A. Caldeira and A. Leggett, *Physica A*, **121**, 587 (1983).
 - * L. Pucci, M. Esposito and L. Peliti, J. Stat. Mech. 13, P04005 (2013).



Lindblad dynamics

 Most widely used tool to describe experiments in Quantum Information setups.

$$\frac{d\rho}{dt} = -i[H,\rho] + D(\rho)$$

$$D(\rho) = \sum_{\alpha} L_{\alpha} \rho L_{\alpha}^{\dagger} - \frac{1}{2} \{ L_{\alpha}^{\dagger} L_{\alpha}, \rho \}$$

* Idea: the most general evolution of a closed system is a Unitary. The most general evolution of an open system is a *Kraus map*:

$$o \to \sum_k M_k \rho M_k^{\dagger}, \qquad \sum_k M_k^{\dagger} M_k = 1$$

* Lindblad's theorem: if such a map is also Markovian (forms a semigroup), then it can be expressed as a Lindblad master equation.

Open quantum harmonic oscillator

* We revisit this problem using the simplest model in quantum mechanics: the harmonic oscillator:

$$H = \omega(a^{\dagger}a + 1/2)$$

$$D(\rho) = \gamma(\bar{n}+1) \left[a\rho a^{\dagger} - \frac{1}{2} \{ a^{\dagger}a, \rho \} \right] + \gamma \bar{n} \left[a^{\dagger}\rho a - \frac{1}{2} \{ aa^{\dagger}, \rho \} \right]$$
$$\bar{n} = \frac{1}{e^{\beta\omega} - 1}$$

Classical dynamics describes emission and absorption of quanta. But also captures quantum features.



PHYSICAL REVIEW LETTERS

PRL 118, 220601 (2017)

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Wigner Entropy Production Rate

Jader P. Santos,¹ Gabriel T. Landi,² and Mauro Paternostro³ ¹Universidade Federal do ABC, 09210-580 Santo André, Brazil ²Instituto de Física da Universidade de São Paulo, 05314-970 São Paulo, Brazil ³Centre for Theoretical Atomic, Molecular and Optical Physics, School of Mathematics and Physics, Queen's University Belfast, Belfast BT7 1NN, United Kingdom (Received 6 March 2017; revised manuscript received 10 April 2017; published 1 June 2017)

Phase space

* Instead of using wavefunctions or density matrices, we work in *phase space* using the *Wigner function*:

$$W(\alpha, \alpha^*) = \frac{1}{\pi^2} \int d^2 \lambda e^{-\lambda \alpha^* + \lambda^* \alpha} \operatorname{tr} \left\{ \rho e^{\lambda a^\dagger - \lambda^* a} \right\}$$

* Phase space is now the complex plane, with:

$$x = \sqrt{2} \operatorname{Re}(\alpha), \qquad p = \sqrt{2} \operatorname{Im}(\alpha)$$

* Thermal equilibrium is a Gaussian

$$W_{\rm eq} = \frac{1}{\pi(\bar{n}+1/2)} \exp\left\{-\frac{|\alpha|^2}{\bar{n}+1/2}\right\}$$

 For T = 0 this gives the vacuum state, which still has a non-zero width: *quantum fluctuations*.



Rényi-2 and Wigner entropy

The second laws of quantum thermodynamics

Fernando Brandão^{a,1}, Michał Horodecki^b, Nelly Ng^c, Jonathan Oppenheim^{c,d,2}, and Stephanie Wehner^{c,e}

PNAS | March 17, 2015 | vol. 112 | no. 11 | 3275–3279

* The authors of this paper showed that for quantum systems all Rényi entropies have thermodynamic significance.

$$S_{\alpha} = \frac{1}{1 - \alpha} \ln \mathrm{tr} \rho^{\alpha}$$

* The simplest one to use is the Rényi-2 entropy:

$$S_2 = -\ln \mathrm{tr}\rho^2$$

* In *PRL* **109**, 190502 (2012) the authors showed that for Gaussian states, this actually coincides with the *Wigner entropy*

$$S = -\int d^2 \alpha W(\alpha, \alpha^*) \ln W(\alpha, \alpha^*)$$

Quantum Fokker-Planck equation

$$\frac{d\rho}{dt} = -i[H,\rho] + D(\rho)$$

 In terms of the Wigner function, the Lindblad equation becomes a quantum Fokker-Planck equation:

$$\partial_t W = -i\omega \left[\partial_{\alpha^*}(\alpha^* W) - \partial_{\alpha}(\alpha W) \right] + \mathcal{D}(W)$$

 $\mathcal{D}(W) = \partial_{\alpha} J(W) + \partial_{\alpha^*} J^*(W)$

$$J(W) = \frac{\gamma}{2} \left[\alpha W + (\bar{n} + 1/2) \partial_{\alpha^*} W \right]$$

This is a continuity equation and J(W) is the irreversible component of the probability current.

$$J(W_{\rm eq}) = 0$$

U. Seifert, Rep. Prog. Phys. 75, 126001 (2012)

Wigner entropy production and flux

 We use 3 different methods to show that the Wigner entropy production for a harmonic oscillator will be:

$$\Pi = \frac{4}{\gamma(\bar{n}+1/2)} \int d^2 \alpha \frac{|J(W)|^2}{W}$$

* The entropy flux rate then becomes

$$\Phi = \frac{\gamma}{\bar{n} + 1/2} \left[\langle a^{\dagger} a \rangle - \bar{n} \right] = \frac{\Phi_E}{\omega(\bar{n} + 1/2)}$$

* At high temperatures $\omega(\bar{n} + 1/2) \simeq T$ so we get

$$\Phi \simeq \frac{\Phi_E}{T}$$

* Now both Π and Φ remain finite at T = 0.

M. Brunelli, et. al. arXiv:1602.06958

Experiments





Generalizations

J. P. Santos, L. C. Céleri, GTL, M. Paternostro, arXiv:1707.08946

Spins and qubits

* We would like to have a similar framework for spin systems.

Spin coherent states: $|\Omega\rangle = e^{-\phi J_z} e^{-\theta J_y} |J, J\rangle$

Husimi-Q function: $Q(\Omega) = \langle \Omega | \rho | \Omega \rangle$

Wehrl entropy:
$$\Sigma = -\int d\Omega Q(\Omega) \ln Q(\Omega)$$

 The Quantum Fokker-Planck equation is now written in terms of orbital angular momentum operators.

$$-i[J_z,\rho] \quad \to \quad \mathcal{J}_z(\mathcal{Q}) = -i\frac{\partial}{\partial\phi}\mathcal{Q}$$

Dephasing and amplitude damping

* The dephasing bath induces no population changes, only decoherence:

$$D(\rho) = -\frac{\lambda}{2} [J_z, [J_z, \rho]]$$

* It leads to no entropy flux, only an entropy production:

$$\Pi = \frac{\lambda}{2} \int d\Omega \frac{|\mathcal{J}_z(\mathcal{Q})|^2}{\mathcal{Q}}$$

* We compare this with the amplitude damping:

$$D(\rho) = \gamma(\bar{n}+1) \left[J_{-}\rho J_{+} - \frac{1}{2} \{ J_{+}J_{-}, \rho \} \right] + \gamma \bar{n} \left[J_{+}\rho J_{-} - \frac{1}{2} \{ J_{-}J_{+}, \rho \} \right]$$

 We now see the separation of a contribution from population changes and a contribution from decoherence.

$$\Pi = \frac{\gamma}{2} \int \frac{d\Omega}{Q} \left\{ \frac{[2JQ\sin\theta + (\cos\theta - (2\bar{n}+1))\partial_{\theta}Q]^2}{(2\bar{n}+1) - \cos\theta} + |\mathcal{J}_z(Q)|^2 \left[(2\bar{n}+1)\cos\theta - 1 \right] \frac{\cos\theta}{\sin^2\theta} \right\}$$

Squeezed baths

Example of a non-equilibrium reservoir.

$$\mathcal{D}_{z}(\rho) = \gamma (N+1) \left[a\rho a^{\dagger} - \frac{1}{2} \{ a^{\dagger} a, \rho \} \right]$$
$$+ \gamma N \left[a^{\dagger} \rho a - \frac{1}{2} \{ aa^{\dagger}, \rho \} \right]$$
$$- \gamma M \left[a^{\dagger} \rho a^{\dagger} - \frac{1}{2} \{ a^{\dagger} a^{\dagger}, \rho \} \right]$$
$$- \gamma M^{*} \left[a\rho a - \frac{1}{2} \{ aa, \rho \} \right]$$

 $J_E = \frac{d\langle a^{\dagger}a \rangle}{dt} = \gamma (N - \langle a^{\dagger}a \rangle)$

 $J_S = \frac{d\langle aa \rangle}{dt} = \gamma(M - \langle aa \rangle)$

 $N + 1/2 = (\bar{n} + 1/2) \cosh 2r$ $M = -(\bar{n} + 1/2)e^{i\theta} \sinh(2r)$

Onsager theory for squeezing

- * Our formalism allows us to cast this problem within the same thermodynamic framework of Onsager's transport theory:
 - Joint transport of energy and squeezing.
 - * We can even define a Squeezing Peltier and Squeezing Seebeck effect.

 $J_E = \mathcal{T}_{1,1}\delta\bar{n} + \mathcal{T}_{1,2}\delta r$ $J_S = \mathcal{T}_{2,1}\delta\bar{n} + \mathcal{T}_{2,2}\delta r$

 Entropy production and flux can be written like in standard thermodynamics:

$$\Phi = \bar{f}_E J_E + \bar{f}_S J_S + \bar{f}_S^* J_S^*$$
$$\Pi = (\bar{f}_E - f_E) J_E + (\bar{f}_S - f_S) J_S + (\bar{f}_S^* - f_S^*) J_S^*$$

Conclusions

- * Quantum Information Sciences: *understand and exploit the role of quantum resources, such as coherence and entanglement.*
- * Quantum thermodynamics: *understand how these resources affect properties such as heat, work and entropy production.*
- * Theory of irreversibility for open quantum systems is incomplete.
- * We proposed an alternative for Gaussian states using the Wigner entropy.
 - This approach solves the T = 0 problem and is also useful to study engineered reservoirs.

Collaborators:

- Jader. P. Santos (post-doc)
- Mauro Paternostro (Queen's @ Belfast)
- Lucas Céleri (UFG)
- Dragi Karevski and Malte Henkel (Uni Lorraine @ Nancy)
- André Timpanaro and Fernando Semião (UFABC)
- Sascha Wald (SISSA @ Trieste)
- Cecilia Cormick (NUC @ Cordoba)
- Giovanna Morigi (Särbrucken)

Students:

- Wellington Ribeiro: dephasing in fermionic systems.
- William Malouf: entropy production and mutual information.
- Heitor Casagrande: DMRG simulations of open quantum systems.
- **Pedro Portugal:** backflow of information in Non-Markovian dynamics.
- Franklin Luis: transport of squeezing in opto-mechanical systems.
- **Bruno Goes:** irreversibility in dissipative quantum phase transitions.
- Mariana Cipolla: entropy production and entanglement in the spin-boson model.

Thank you.

Stochastic trajectories and fluctuation theorems

- * We can also arrive at the same result using a completely different method.
 - * We analyze the stochastic trajectories in the complex plane.
- * The quantum Fokker-Planck equation is equivalent to a Langevin equation in the complex plane:

$$\frac{dA}{dt} = -i\omega A - \frac{\gamma}{2}A + \sqrt{\gamma(\bar{n} + 1/2)}\xi(t)$$
$$\langle \xi(t)\xi(t')\rangle = 0, \qquad \langle \xi(t)\xi^*(t')\rangle = \delta(t - t')$$

 We can now define the entropy produced in a trajectory as a functional of the path probabilities for the forward and reversed trajectories:

$$\Sigma[\alpha(t)] = \ln \frac{\mathcal{P}[\alpha(t)]}{\mathcal{P}_R[\alpha^*(\tau - t)]}$$

This quantity satisfies a fluctuation theorem

$$\langle e^{-\Sigma} \rangle = 1$$

* We show that we can obtain exactly the same formula for the entropy production rate if we define it as

$$\Pi = \frac{\langle d\Sigma[A(t)] \rangle}{dt}$$

Example: RL circuit



Example: two inductively coupled RL circuits



$$\Pi_{\rm ss} = \frac{\mathcal{E}_1^2}{R_1 T_1} + \frac{\mathcal{E}_2^2}{R_2 T_2} + \frac{m^2 R_1 R_2}{(L_1 L_2 - m^2)(L_2 R_1 + L_1 R_2)} \frac{(T_1 - T_2)^2}{T_1 T_2}$$

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

Example: evolution of a coherent state

 Consider the evolution of a harmonic oscillator starting from a coherent state:

 $\rho(0) = |\mu\rangle\langle\mu|$

The evolution remains as a (pure) coherent state:

$$\rho(t) = |\mu_t\rangle \langle \mu_t|$$
$$\mu_t = \mu e^{-(i\omega + \gamma/2)t}$$



- * The entropy is zero throughout, but Π and Φ would both be infinite.
- * This is clearly an inconsistency of the theory.

Squeezed baths and gravitational waves



Observation of strong radiation pressure forces from squeezed light on a mechanical oscillator

Jeremy B. Clark, Florent Lecocq, Raymond W. Simmonds, José Aumentado and John D. Teufel*



 For the squeezed bath we find that the entropy production rate is given by

$$\Pi = \frac{4}{\gamma(\bar{n}+1/2)} \int \frac{d^2\alpha}{W} \left| J_z \cosh r + J_z^* e^{i(\theta - 2\omega_s t)} \sinh r \right|^2$$

$$J_z(W) = \frac{\gamma}{2} \left[\alpha W + (N+1/2)\partial_{\alpha^*} W + M_t \partial_{\alpha} W \right]$$

* The entropy flux rate is given by

$$\Phi = \frac{\gamma}{\bar{n} + 1/2} \left[\cosh(2r) \langle a^{\dagger} a \rangle - \bar{n} + \sinh^2(r) - \frac{\operatorname{Re}[M_t^* \langle aa \rangle]}{\bar{n} + 1/2} \right]$$