Seminário para a Universidade Federal de Minas Gerais

Quantum thermodynamics and irreversibility

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Summary

- * Quantum Thermodynamics?
 - * Motivation from Quantum Information Sciences.
- * Recent progress and general trends in the field.
- * Our contribution: 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.







Interaction with the environment

- * Consider a 2-level system in an arbitrary state.
- * For a pure state we have

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

More generally, we have

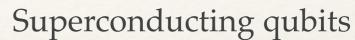
$$\rho = \begin{pmatrix} p_0 & q \\ q^* & p_1 \end{pmatrix}$$

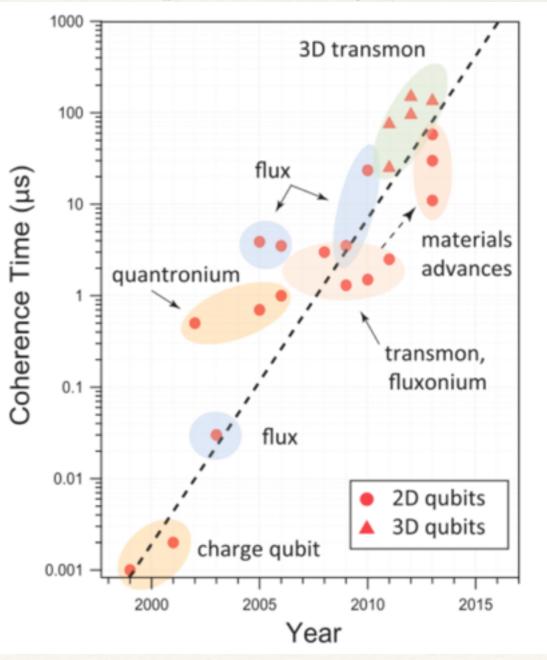
- * The interaction with the environment does two things:
 - 1. Changes the populations in a certain basis.
 - 2. Destroys coherences.

$$\begin{pmatrix} p_0 & q \\ q^* & p_1 \end{pmatrix} \to \begin{pmatrix} p_0' & 0 \\ 0 & p_1' \end{pmatrix}$$

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

week ending 17 FEBRUARY 2017



No-Go Theorem for the Characterization of Work Fluctuations in Coherent Quantum Systems

Martí Perarnau-Llobet, 1,* Elisa Bäumer, 1,2,† Karen V. Hovhannisyan, 1,‡ Marcus Huber, 3,4,8 and Antonio Acin 1,5,5

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}

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Rényi entropy

$$S_{\alpha} = -\frac{1}{1-\alpha} \log \operatorname{tr} \rho^{\alpha}$$

von Neumann entropy

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

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

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

<u>James Millen</u>, Vienna Center for Quantum Science and Technology, University of Vienna, 1090 Vienna, Austria

September 13, 2017 • Physics 10, 99

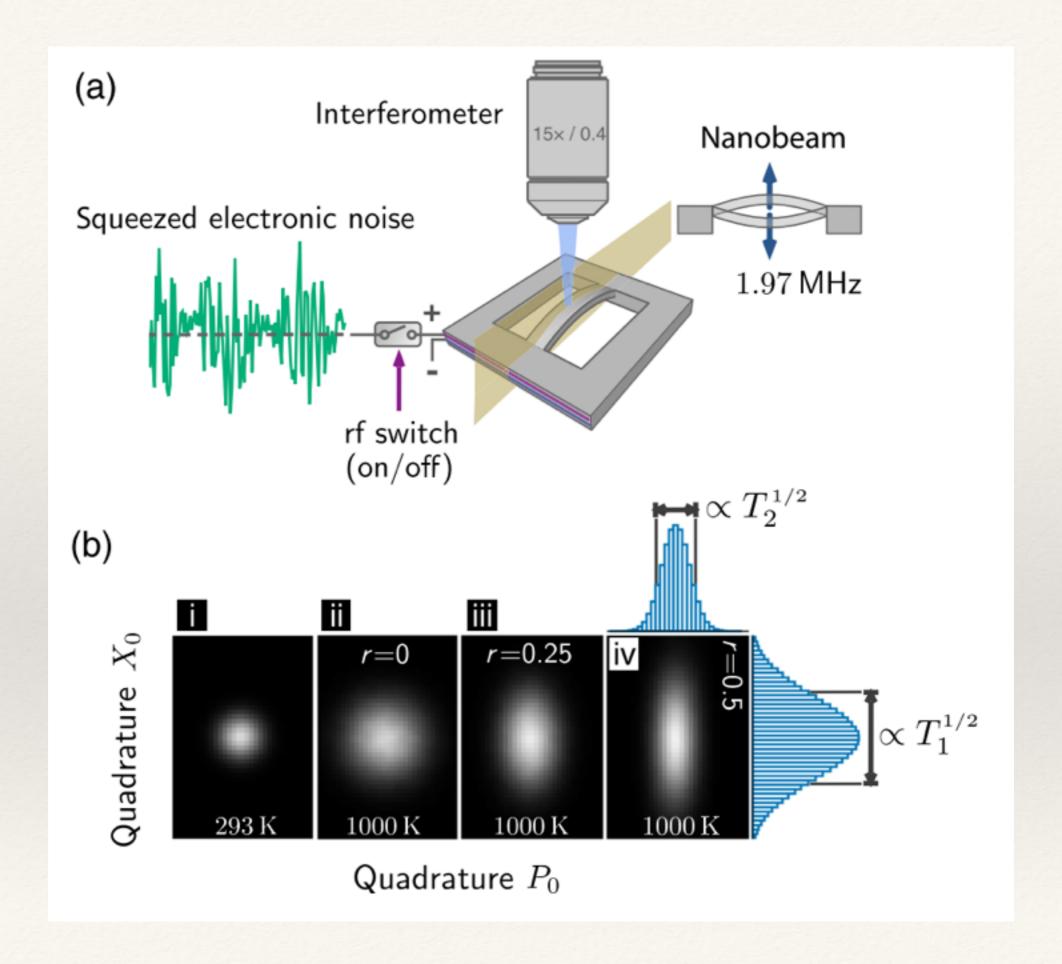
Selected for a Viewpoint in *Physics* PHYSICAL REVIEW X 7, 031044 (2017)

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

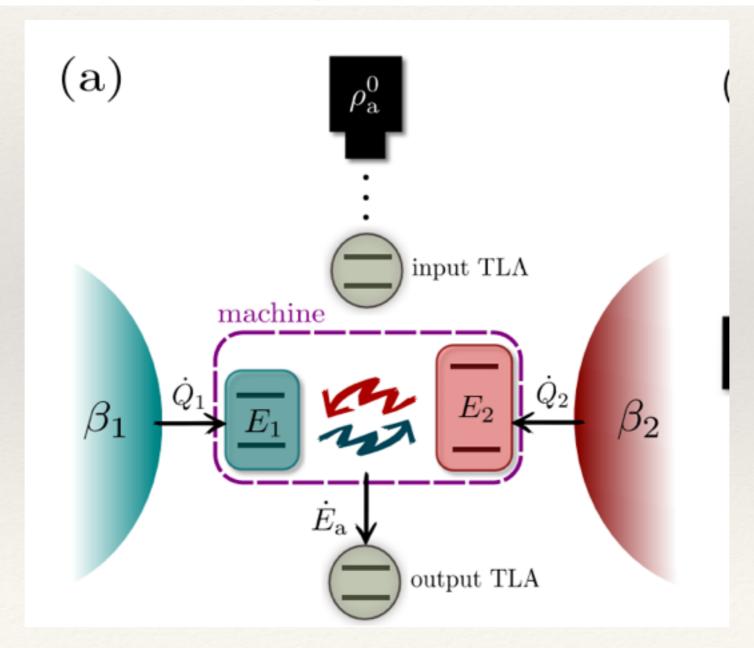
(Received 25 April 2017; revised manuscript received 25 July 2017; published 13 September 2017)



Coherence producing engine

Autonomous thermal machine for amplification and control of energetic coherence

Gonzalo Manzano, 1, 2 Ralph Silva, 3 and Juan M.R. Parrondo 1



Measures of Irreversibility

Entropy production

* The energy of a system satisfies a continuity equation:

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

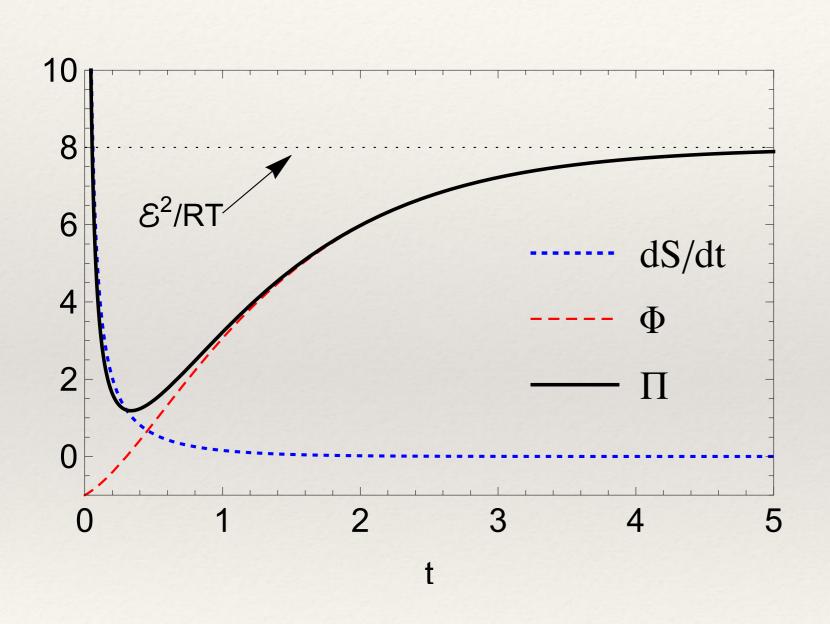
* For the entropy that is not true:

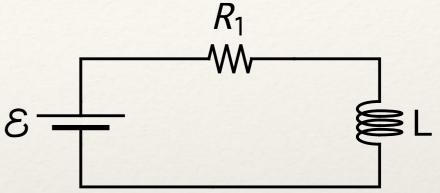
$$\frac{dS}{dt} = \Pi - \Phi$$

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

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

Example: RL circuit



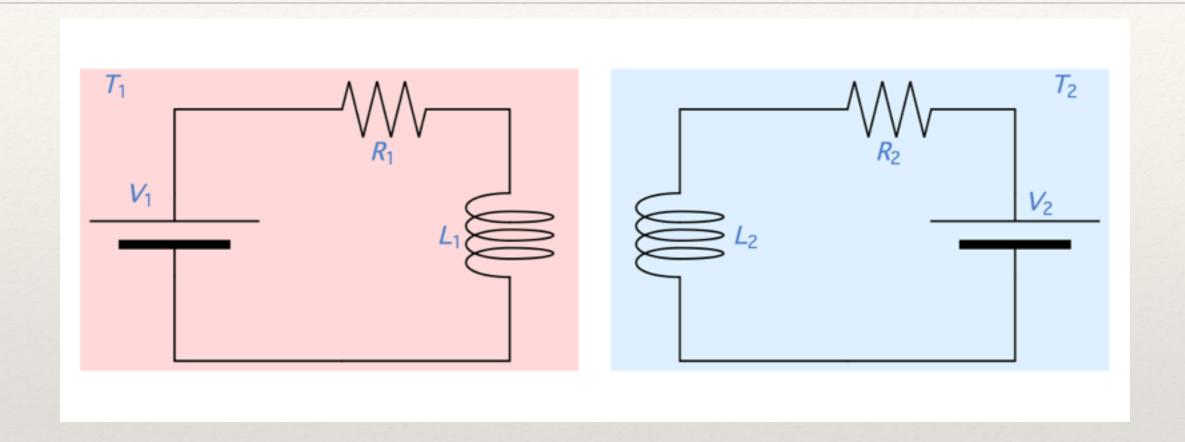


Steady-state

$$\frac{dS}{dt} = 0$$

$$\Pi_{\rm ss} = \Phi_{\rm ss} = \frac{\mathcal{E}^2}{RT}$$

Example: two inductively coupled RL circuits



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

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

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 flux

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

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

Entropy production

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

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

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

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

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

$$C(\rho) = S(p) - S(\rho)$$

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

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

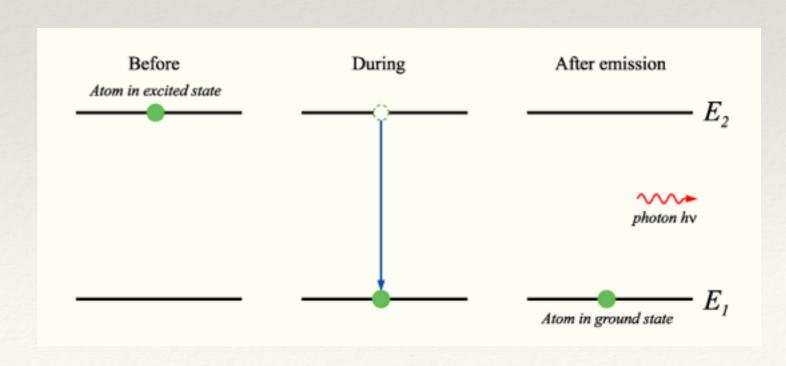
Problems with the standard formulation

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

- 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 $T \rightarrow 0$.



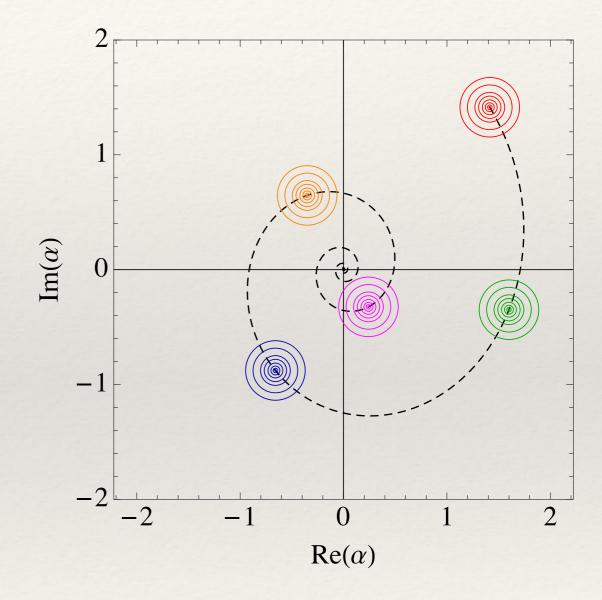
Example: evolution of a coherent state

* 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.

Dynamics of open quantum systems

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*:

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

* 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:

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

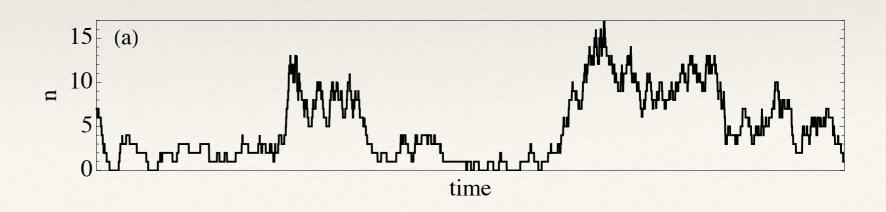
The dissipator describing the contact with a thermal bath is

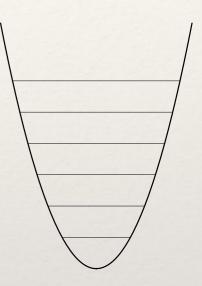
$$D(\rho) = \gamma(\bar{n}+1) \left[a\rho a^{\dagger} - \frac{1}{2} \{ a^{\dagger}a, \rho \} \right] + \gamma \bar{n} \left[a^{\dagger}\rho a - \frac{1}{2} \{ aa^{\dagger}, \rho \} \right]$$

$$\bar{n} = \frac{1}{e^{\beta\omega} - 1}$$

Classical dynamics describes emission and absorption of quanta.

But also captures quantum features.







Wigner Entropy Production Rate

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Phase space

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

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

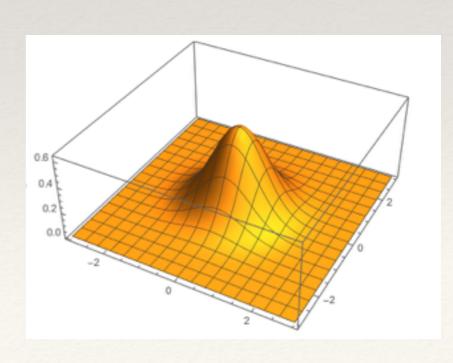
Phase space is now the complex plane, with:

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

* Thermal equilibrium is a Gaussian

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

* 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.

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

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

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

* 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. $J(W_{eq}) = 0$

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.

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

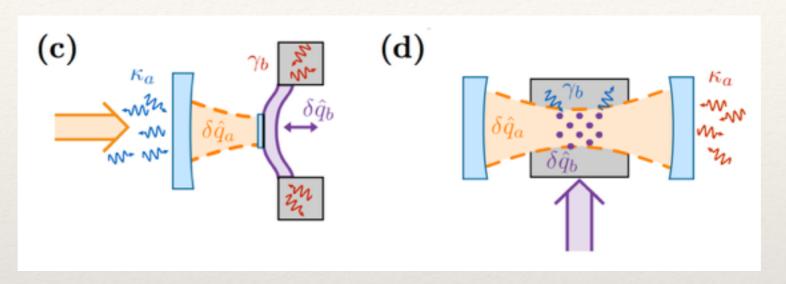
$$\langle e^{-\Sigma} \rangle = 1$$

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

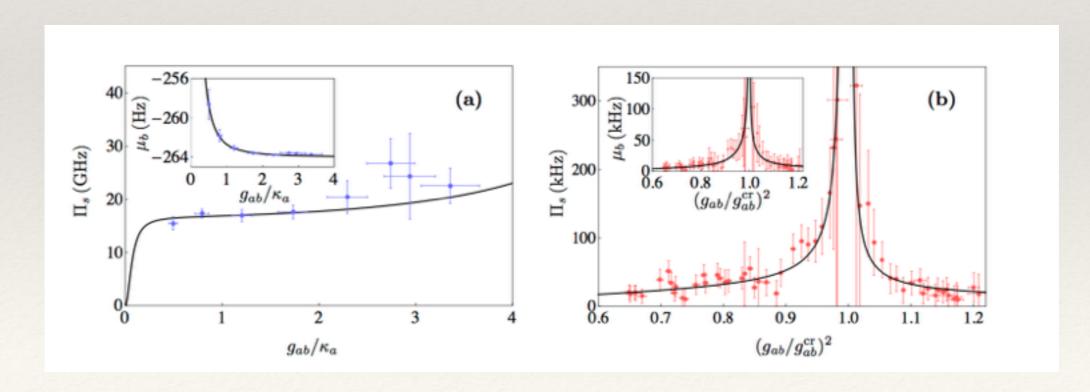
$$\Pi = \frac{\langle d\Sigma[A(t)] \rangle}{dt}$$

Experiments

Optomechanical system (Vienna)



BEC in a highfinesse cavity (ETH)



Generalizations

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:
$$\Sigma = -\int d\Omega \mathcal{Q}(\Omega) \ln \mathcal{Q}(\Omega)$$

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

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

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.

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

Squeezed baths

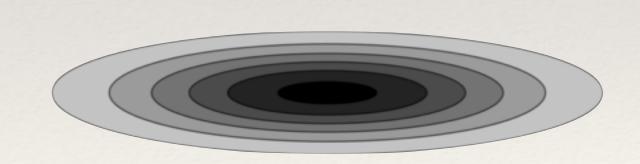
* Example of a non-equilibrium reservoir.

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

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

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

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



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

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

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

The entropy flux rate is given by

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

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: dynamics of dissipative quantum phase transitions.
- Mariana Cipolla: entropy production and entanglement in the spin-boson model.



Squeezed baths and gravitational waves

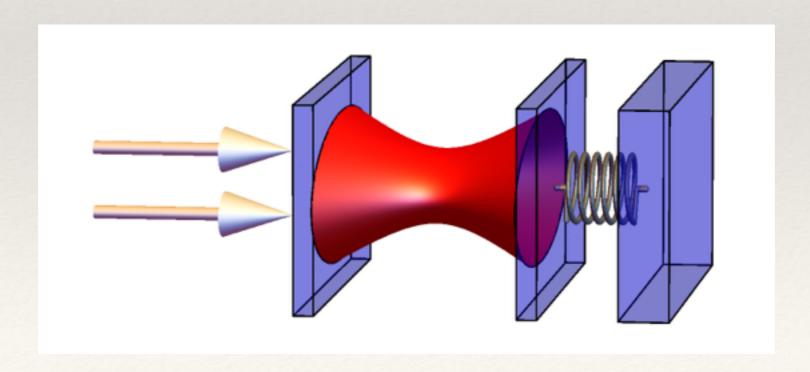


LETTERS

PUBLISHED ONLINE: 28 MARCH 2016 | DOI: 10.1038/NPHYS3701

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*



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).

ARTICLE

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Observation of non-Markovian micromechanical Brownian motion

S. Gröblacher^{1,2}, A. Trubarov², N. Prigge³, G.D. Cole², M. Aspelmeyer^{2,3} & J. Eisert³

