Seminário do grupo de física estatística - 25 de maio de 2017

Measures of irreversibility for open quantum systems

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In collaboration with Jader Pereira dos Santos (post-doc) and Mauro Paternostro from Queens University, Belfast.

Irreversibility

- * Irreversibility is one of the most fundamental concepts in thermodynamics.
- * *Quantifying the degree of irreversibility* of a general process is a task of great technological importance.
- * This idea was originally developed for macroscopic systems.
- However, it also finds broad applications in micro and mesoscopic systems. e.g.:
 - * Molecular motors.
 - * Nano-devices.
 - * Open quantum systems.

Micro and meso heat engines



LETTERS PUBLISHED ONLINE: 26 OCTOBER 2015 | DOI: 10.1038/NPHYS3518

Brownian Carnot engine

I. A. Martínez^{1,2*†}, É. Roldán^{1,3,4*†}, L. Dinis^{4,5}, D. Petrov¹, J. M. R. Parrondo^{4,5} and R. A. Rica^{1*}

THERMODYNAMICS

A single-atom heat engine

Johannes Roßnagel,¹* Samuel T. Dawkins,¹ Karl N. Tolazzi,² Obinna Abah,³ Eric Lutz,³ Ferdinand Schmidt-Kaler,¹ Kilian Singer^{1,4}*

SCIENCE 15 APRIL 2016 • VOL 352 ISSUE 6283

Fluctuations of heat and work

Verification of the Crooks fluctuation theorem and recovery of RNA folding free energies

D. Collin¹*, F. Ritort²*, C. Jarzynski³, S. B. Smith⁴, I. Tinoco Jr⁵ & C. Bustamante^{4,6}

nature Vol 437|8 September 2005|doi:10.1038/nature04061



Work extraction and thermodynamics for individual quantum systems

Paul Skrzypczyk¹, Anthony J. Short² & Sandu Popescu²

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

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

Open quantum systems

- Here we address the question of how to quantify the degree of irreversibility of a quantum system undergoing open dynamics.
- * The interesting aspect about quantum dynamics is the possibility of constructing *engineered/non-equilibrium reservoirs*:
 - * Zero temperature baths (vacuum fluctuations).
 - Decoherence baths.
 - * Squeezed thermal baths.

Observing the Progressive Decoherence of the "Meter" in a Quantum Measurement

M. Brune, E. Hagley, J. Dreyer, X. Maître, A. Maali, C. Wunderlich, J. M. Raimond, and S. Haroche Laboratoire Kastler Brossel,* Département de Physique de l'Ecole Normale Supérieure, 24 Rue Lhomond, F-75231 Paris Cedex 05, France (Received 10 September 1996)

Decoherence of quantum superpositions through coupling to engineered reservoirs

C. J. Myatt*, B. E. King*, Q. A. Turchette, C. A. Sackett, D. Kielpinski, W. M. Itano, C. Monroe & D. J. Wineland

National Institute of Standards and Technology, Div. 847.10, 325 Broadway, Boulder, Colorado 80303, USA

NATURE VOL 403 20 JANUARY 2000 www.nature.com

LETTER

doi:10.1038/nature12801

Dissipative production of a maximally entangled steady state of two quantum bits

Y. Lin¹*, J. P. Gaebler¹*, F. Reiter², T. R. Tan¹, R. Bowler¹, A. S. Sørensen², D. Leibfried¹ & D. J. Wineland¹

VOL 504 | NATURE | 415



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*



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Nanoscale Heat Engine Beyond the Carnot Limit

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(Received 12 September 2013; revised manuscript received 4 December 2013; published 22 January 2014)





Quantum computation and quantum-state engineering driven by dissipation

Frank Verstraete^{1*}, Michael M. Wolf² and J. Ignacio Cirac^{3*}

- * In general, the environment is a problem for quantum computing because it destroys coherences.
- * In this paper they show that the environment can actually be used to make the quantum computation itself.
 - * Any universal quantum gate implementable as a unitary dynamics can also be implemented by an engineered reservoir.
- * If we could engineer reservoirs we would be able to do quantum computing where noise is not a problem, but instead is the solution.

How to quantify irreversibility

How to quantify irreversibility?

* 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

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, M. J. de Oliveira, J. Phys. 46 (2013) 395001

П and the relative entropy

 There is a famous formula which has been used both in the classical and quantum cases:

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

* which is written in terms of the *Kullback-Leibler divergence* (*relative entropy*):

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

* When the density matrices are both diagonal we obtain instead:

$$S(p||p^{\text{eq}}) = \sum_{n} (p_n \ln p_n - p_n \ln p_n^{\text{eq}}) \qquad p_n = \langle n|\rho|n\rangle$$

Entropy production for quantum dynamical semigroups

Herbert Spohn^{a)}

Department of Physics, Princeton University, Princeton, New Jersey 08540 (Received 15 August 1977)

PHYSICAL REVIEW A 68, 032105 (2003)

Quantum jumps and entropy production

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Fachbereich Physik, Carl von Ossietzky Universität, D-26111 Oldenburg, Germany and Physikalisches Institut, Universität Freiburg, D-79104 Freiburg, Germany (Received 29 January 2003; published 26 September 2003)

PRL 107, 140404 (2011)

PHYSICAL REVIEW LETTERS

week ending 30 SEPTEMBER 2011

Nonequilibrium Entropy Production for Open Quantum Systems

Sebastian Deffner and Eric Lutz

Department of Physics, University of Augsburg, D-86135 Augsburg, Germany (Received 28 March 2011; revised manuscript received 29 July 2011; published 30 September 2011)

Example: master equation

$$\frac{dp_n}{dt} = \sum_m \left\{ W(n|m)p_m - W(m|n)p_n \right\}$$
$$\Pi = -\frac{d}{dt}S(p||p^{eq}) = -\sum_n \frac{dp_n}{dt}\ln p_n/p_n^{eq}$$
$$= \sum_{n,m} W(m|n)p_n \ln \left[\frac{W(m|n)p_n}{W(n|m)p_m}\right]$$

where I assumed detailed balance holds

$$W(n|m)p_m^{\rm eq} = W(m|n)p_n^{\rm eq}$$

J. Schnakenberg, Rev. Mod. Phys. 48, 571 (1976).

1.

The entropy flux then becomes

$$\Phi = \Pi - \frac{dS}{dt} = \sum_{n} \frac{dp_n}{dt} \ln p_n^{\text{eq}}$$

If

$$p_n^{\rm eq} = \frac{e^{-\beta E_n}}{Z}$$

$$\Phi = -\frac{1}{T} \sum_{n} E_n \frac{dp_n}{dt} = \frac{\Phi_E}{T}$$

This is the standard thermodynamic relation between dS and dE

Open quantum dynamics

- Here we will be interested in the dynamics of a quantum system in contact with a reservoir.
- We will assume that this dynamics can be modeled by a Lindblad master equation

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

* where D is called the Lindblad dissipator

* To be concrete, let us first consider the simplest example possible: a quantum harmonic oscillator

$$\begin{split} D(\rho) &= \gamma (\bar{n}+1) \bigg[a\rho a^{\dagger} - \frac{1}{2} \{ a^{\dagger} a, \rho \} \bigg] + \gamma \bar{n} \bigg[a^{\dagger} \rho a - \frac{1}{2} \{ aa^{\dagger}, \rho \} \bigg] \\ H &= \omega a^{\dagger} a \qquad \bar{n} = \frac{1}{e^{\beta \omega} - 1} \end{split}$$

* If we look at the diagonal elements of the density matrix

$$\langle n | \frac{d\rho}{dt} | n \rangle = \frac{dp_n}{dt} = \langle n | D(\rho) | n \rangle$$

 We then get the standard master equation for the harmonic oscillator

$$\frac{dp_n}{dt} = \gamma(\bar{n}+1) \left[(n+1)p_{n+1} - np_n \right] + \gamma \bar{n} \left[np_{n-1} - (n+1)p_{n+1} \right]$$

Problems with the standard formulation

- Not clear how to extend to multiple reservoirs.
- Not clear how to extend to engineered / non-equilibrium reservoirs.
- * Π and Φ diverge when $T \rightarrow 0$.

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

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

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

- Zero temperature limit is extensively used in experiment (vaccum fluctuations).
- * *Everything* is well behaved. Even dS/dt. *Only* Π and Φ diverge.

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.

Rényi-2 and Wigner entropy

- * We propose an alternative to describe the entropy production and entropy flux.
- * We do not attempt to define a *thermodynamic entropy*. Instead, we adopt the pragmatic point of view of choosing one of several *entropic measures* which characterize the disorder in the system.
- Instead of using the von Neumann entropy, we use the Rényi entropy:

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

* When alpha = 1, we recover the von Neumann entropy:

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

 Recently there has been some proposals on how to construct the laws of thermodynamics using the Rényi 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}

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* In the classical limit all Rényi entropies converge to the von Neumann entropy.

* The most convenient entropy is the *Rényi-2*, which is directly related to the *purity* of a quantum state:

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

- * We consider a single bosonic system for simplicity (the extension to several bosonic modes is straightforward).
- * We also work in phase space by defining the Wigner function:

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

* It was shown in *PRL* **109**, 190502 (2012) that for Gaussian states this coincides with the *Wigner entropy*:

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

Quantum Fokker-Planck equation

 ∂_t

 In phase space the Lindblad Eq.
becomes a quantum Fokker-Planck Eq.:

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

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

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

$$\rho_{\rm eq} = \frac{e^{-\beta\omega a^{\dagger} a}}{Z} \qquad \qquad W_{\rm eq} = \frac{1}{\pi(\bar{n}+1/2)} \exp\left\{-\frac{|\alpha|^2}{\bar{n}+1/2}\right\}$$

Wigner entropy production and flux

* Now we define the entropy production rate as:

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

Substituting the Fokker-Planck equation we get

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

The entropy flux rate then becomes

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

* In this model the energy flux is given by

$$\Phi_E = \gamma \omega \left[\langle a^\dagger a \rangle - \bar{n} \right]$$

* Thus the entropy flux and energy flux will be related by

$$\Phi = \frac{\Phi_E}{\omega(\bar{n} + 1/2)}$$

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

$$\Phi = \frac{\Phi_E}{\omega(\bar{n} + 1/2)} \simeq \frac{\Phi_E}{T}$$

* But 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

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

Dephasing bath

- * A dephasing bath is one which does not affect the populations of the energy levels, but eliminates coherences (off-diagonal elements).
- * For the harmonic oscillator the dephasing bath reads:

$$D(\rho) = \lambda \left[a^{\dagger} a \rho a^{\dagger} a - \frac{1}{2} \{ (a^{\dagger} a)^2, \rho \} \right]$$

* For this bath, applying a similar procedure we find that

$$\Pi = \frac{2}{\lambda} \int \frac{d^2 \alpha}{|\alpha|^2} \frac{|I(W)|^2}{W}, \qquad \Phi = 0$$

$$I(W) = \lambda \alpha (\alpha^* \partial_{\alpha^*} W - \alpha \partial_{\alpha} W)/2$$

- For the dephasing bath there is no entropy flux, only a production.
- Sometimes "dephasing" is defined as a noise for which there is no flow of energy. But that is not always true.
- * Now we find a more general definition: *dephasing is a type of bath for which there is no entropy flux.*
- This also matches with the definition of dephasing as a unital map (a map which has the identity matrix as a fixed point).
- * It is know that the entropy of a unital map can never decrease. This agrees with the idea of no flux.

Squeezed bath

A general dephasing bath can be represented by the dissipator

$$\begin{split} \mathcal{D}_z(\rho) &= \gamma (N+1) \left[a\rho a^{\dagger} - \frac{1}{2} \{ a^{\dagger} a, \rho \} \right] \\ &+ \gamma N \left[a^{\dagger} \rho a - \frac{1}{2} \{ aa^{\dagger}, \rho \} \right] \\ &- \gamma M_t \left[a^{\dagger} \rho a^{\dagger} - \frac{1}{2} \{ a^{\dagger} a^{\dagger}, \rho \} \right] \\ &- \gamma M_t^* \left[a\rho a - \frac{1}{2} \{ aa, \rho \} \right] \end{split}$$

$$N + 1/2 = (\bar{n} + 1/2) \cosh 2r$$

 $M_t = -(\bar{n} + 1/2)e^{i(\theta - 2\omega_s t)} \sinh 2r$

 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

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

Pumped cavity under a squeezed bath

 We consider a cavity pumped by a laser and subject to a squeezed bath at zero temperature.

$$H = \omega_c a^{\dagger} a + i (\mathcal{E} e^{-i\omega_p t} a^{\dagger} - \mathcal{E}^* e^{i\omega_p t} a)$$

* The energy flux is given by

$$\Phi_E = \left\langle \frac{\partial H}{\partial t} \right\rangle = \frac{2\kappa\omega_p |\mathcal{E}|^2}{\kappa^2 + \Delta_{cp}^2}$$

It is zero when there is no pump



* In the steady-state $\Pi = \Phi$ and we get

$$\Pi = \frac{2\kappa\Delta_{sc}^2}{\kappa^2 + \Delta_{sc}^2} \sinh^2(2r) + \frac{4\kappa|\mathcal{E}|^2}{\kappa^2 + \Delta_{cp}^2} \cosh(2r) + 4\kappa \operatorname{Re}\left[\frac{\mathcal{E}^2 e^{-i(2\Delta_{ps}t + \theta)}}{(\kappa + i\Delta_{cp})^2}\right] \sinh(2r)$$

First term remains even when there is no pump

$$\Pi = \frac{2\kappa\Delta_{sc}^2}{\kappa^2 + \Delta_{sc}^2} \sinh^2(2r) \qquad \qquad \Delta_{sc} = \omega_s - \omega_c$$

- This means there is an entropy production even though there is no energy flux.
 - * The system is at a NESS because of a frequency mismatch.
 - * This is a clear exception to the paradigm that non-equilibrium steady-states must be associated with macroscopic currents.

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Wigner Entropy Production Rate

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To appear soon in PRL as an editor suggestion.

Experiment

 We have estimated the total entropy production rate for two experimental systems presenting a NESS

Measurement of irreversible entropy production in mesoscopic quantum systems out of equilibrium

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Optomechanical oscillator

BEC in a high-finesse cavity

group of M. Aspelmeyer, University of Vienna group of T. Esslinger, ETH Zürich

* In both cases one bath describes the loss of photons from the cavity, which is a bath at zero temperature.

 In the steady-state the entropy production rate equals the entropy flux rate.

$$\Pi = \Phi = 4\kappa_a \langle a^{\dagger}a \rangle + \frac{2\gamma_b}{\bar{n}_b + 1/2} (\langle b^{\dagger}b \rangle - \bar{n}_b)$$

* Estimating the entropy production experimentally is not so easy because all parameters are not actually constant.



BEC

Optomechanical oscillator

- * At the time of these experiments we were not able to measure the *individual* contribution to the entropy production.
- * We measured only the individual entropy fluxes.
- To measure each entropy production rate we need to know the entire covariance matrix of the system, which is harder.
 - * But now we know how to do it.
 - Would be very nice to do this experimentally in the future.

Conclusions

- * Irreversibility can be quantified by the entropy production.
- The theory of entropy production for open quantum systems is not complete.
 - * Quantum systems are interesting due to the possibility of constructing engineered/non-equilibrium reservoirs.
- * We have proposed an alternative to this problem based on the *Rényi-2 entropy* and *phase space measures*.
- Our approach works at T = 0 and is applicable to different types of non-equilibrium baths.

Future perspectives

- * We have also constructed a similar theory for spin systems using *spin coherent states*.
- In the future, our goal will be to relate entropy production with loss of coherence and loss of entanglement.
- We also want to investigate the connection between entropy production and non-Markovian dynamics.

