Title: Quantum fluctuation theorems in open systems

Date: Mar 25, 2015 04:00 PM

URL: http://pirsa.org/15030095

Abstract: For isolated quantum systems fluctuation theorems are commonly derived within the two-time energy measurement approach. In this talk we will discuss recent developments and studies on generalizations of this approach. We will show that concept of fluctuation theorems is not only of thermodynamic relevance, but that it is also of interest in quantum information theory. In a second part we will show that the quantum fluctuation theorem generalizes to PT-symmetric quantum mechanics with unbroken PT-symmetry. In the regime of broken PT-symmetry the Jarzynski equality does not hold as also the CPT-norm is not preserved during the dynamics. These findings will be illustrated for an experimentally relevant system ? two coupled optical waveguides. It turns out that for these systems the phase transition between the regimes of unbroken and broken PT-symmetry is thermodynamically inhibited as the irreversible work diverges at the critical point. The discussion will be concluded with an alternative approach to fluctuation theorems and quantum entropy production in quantum phase space.

Classic thermodynamics

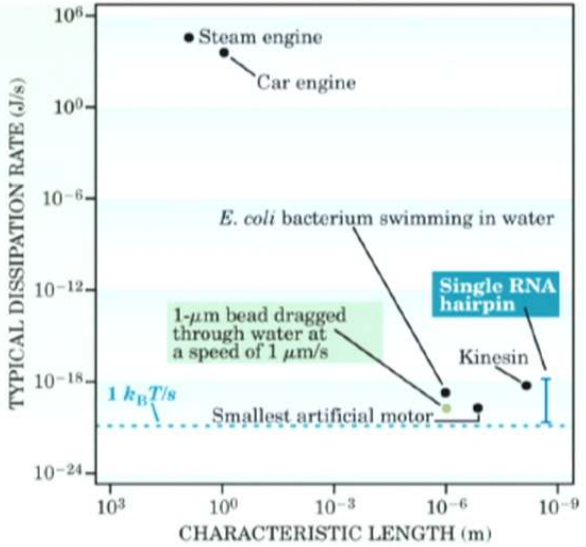
- phenomenological theory for average values of heat and work
- many applications on all length scales:
  phase transitions, chemical reactions, astrophysics...
- only quasistatic processes completely describable
- real processes: characterized by irreversible entropy production Σ

Purpose:

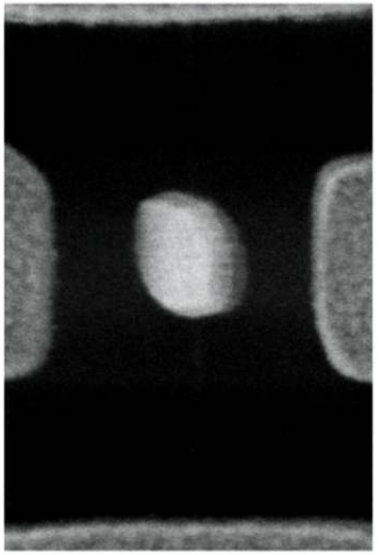
- understand and improve thermodynamic devices
- minimize dissipation in heat engines

Classical nanodevices

Bustamante, Liphardt & Ritort, Phys. Tod. 58, 43 (2005)



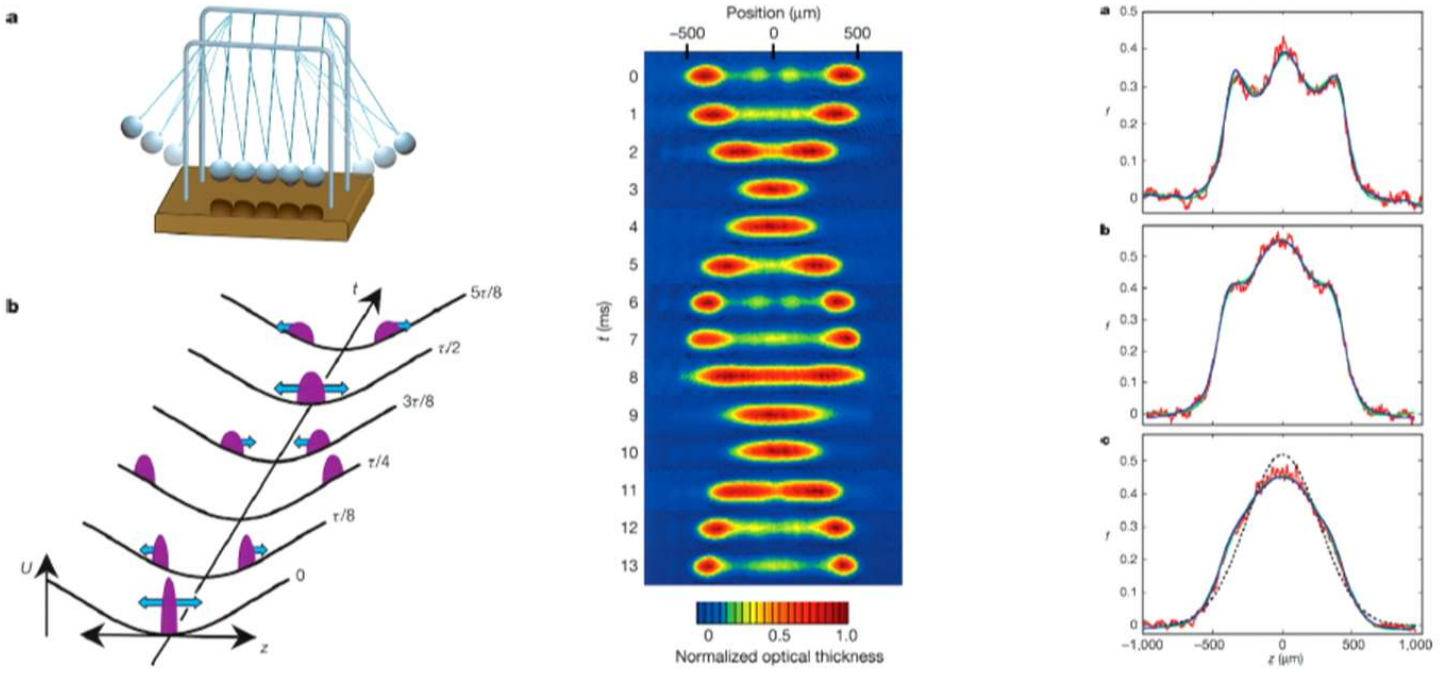
Fennimore *et al.*, Nature 424, 408 (2003)



- dynamics governed by fluctuations
- devices generically out of equilibrium

Quantum nanodevice: Quantum Newton's cradle

Kinoshita, Wenger & Weiss, Nature 440, 900 (2006)



→ **Need:** Thermodynamic description of quantum device operating intrinsically far from equilibrium

Outline

- Jarzynski equality in classical and quantum mechanics
  - Generalized second law for systems far from equilibrium
- Jarzysnki equality in $\mathcal{PT}$-symmetric quantum mechanics
  - Realization of $\mathcal{PT}$-quantum mechanics in optics
- Generalized two-time measurement approach
  - Generalized fluctuation theorem for arbitrary observables
- Quantum entropy production in phase space
  - Entropy production along trajectories in phase space

Classical Jarzynski equality – theory

General form:

Jarzynski, PRL 78, 2690 (1997)

$$\langle \exp\left(-\beta\left(W-\Delta F\right)\right)\rangle = \langle \exp\left(-\beta W_{\rm irr}\right)\rangle = 1$$

W = total work done on the system → fluctuating quantity

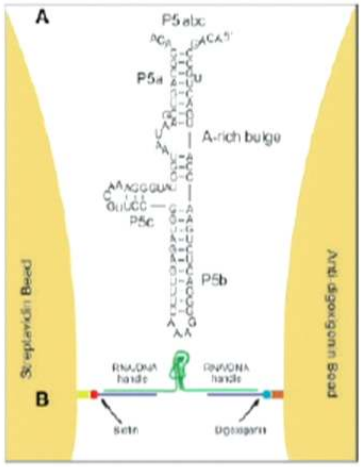
$$\langle \exp\left(-\beta W\right)\rangle = \int \mathrm{d}W\, \mathcal{P}(W)\, \exp\left(-\beta W\right)$$

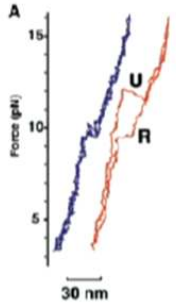
- → calculation of ΔF requires $\mathcal{P}(W)$
- → valid for slow and fast transformations
- → valid for closed and open systems
- → generalization of second law, $\langle W_{\rm irr}\rangle > 0$

Classical Jarzynski equality – experiment

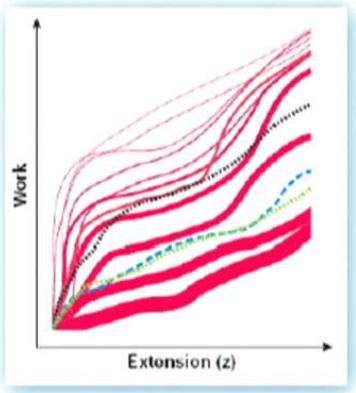
Stretching of single RNA molecule

Liphardt *et al.*, Science **296**, 1832 (2002)





Average over 40 pullings



red: $W(z) = \int_0^z \mathrm{d}x\, f(x)$

green: $\Delta F = \langle W_{\mathrm{rev}} \rangle$

black: $\langle W \rangle > \Delta F$

blue: $\Delta F = -1/\beta \, \ln \langle \exp(-\beta W) \rangle$

Quantum Jarzynski equality

Problem: Notion of classical trajectory not applicable!

Solution: Two-time energy measurements

Campisi, Hänggi & Talkner, RMP 83, 771 (2011)

Quantum work:

$$W_{\rm qm}[|m(\alpha_\tau)\rangle;|n(\alpha_0)\rangle] = E_m(\alpha_\tau) - E_n(\alpha_0)$$

Work distribution:

$$\mathcal{P}_{\rm qm}(W) = \sum_{m,n} \delta\left(W - W_{\rm qm}[|m(\alpha_\tau)\rangle;|n(\alpha_0)\rangle]\right)\, p^\tau_{m,n}\, p^0_n$$

Consequences:

- Jarzynski equality: $\langle \exp\left(-\beta H_{\rm H}(\tau)\right) \exp\left(\beta H(0)\right)\rangle = \exp\left(-\beta \Delta F\right)$
- conceptually simple notion of quantum work

Midterm summary

What we have:

- Generalized second law for classical and quantum system
- Approach for isolated quantum systems

What we want:

- Experimentally relevant, physical theory
- Simplest realization of (quasi)-open systems

Where we start:

- $\mathcal{PT}$-symmetric quantum mechanics
- Thermally isolated systems with balanced loss and gain:
  microwave billards, phontonic lattices, LRC circuits, optical lattices, metamaterials, phonon lasers, optical waveguides...

$\mathcal{PT}$-symmetric quantum systems

Bender & Boettcher, PRL 80, 5243 (1998)

$\mathcal{P}$arity-$\mathcal{T}$ime symmetry:

$$\mathcal{P}\,x\,\mathcal{P} = -x \quad \text{and} \quad \mathcal{P}\,p\,\mathcal{P} = -p$$
$$\mathcal{T}\,x\,\mathcal{T} = x, \quad \mathcal{T}\,p\,\mathcal{T} = -p \quad \text{and} \quad \mathcal{T}\,i\,\mathcal{T} = -i$$

$\mathcal{PT}$-symmetric Hamiltonian: $[\mathcal{PT}, H] = 0$

- unbroken regime: all eigenvalues real
- broken regime: complex and real eigenvalues

Definition of the inner product:

$$\langle\psi_1|\psi_2\rangle_{\mathcal{CPT}} = (\mathcal{CPT}\psi_1)\cdot\psi_2$$

Metric operator (unbroken regime):

$$[\mathcal{C}, H] = 0 \quad \text{and} \quad \mathcal{C}^2 = \mathbb{I}$$

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$\mathcal{PT}$-symmetric Jarzynski equality

Gong & Wang, J. Phys. A 46, 485302 (2013) Deffner & Avadh, arXiv:1501.06545

Generalized time-dependent Schrödinger equation:

$$i\hbar\,\partial_t|\psi_t\rangle = \left[H_t - \frac{i\hbar}{2}\left(\mathcal{C}_t^T\right)^{-1}\partial_t\mathcal{C}_t^T\right]|\psi\rangle$$

Transition probabilities:

$$p_{m\to n} = (\mathcal{C}_\tau\mathcal{PT}\,\phi_n)\cdot(U_\tau\phi_m)\cdot(\mathcal{C}_0\mathcal{PT}\,\phi_m)\cdot(\rho_0\phi_m)\cdot(\mathcal{C}_\tau\mathcal{PT}\,U_\tau\phi_m)\cdot\phi_n$$

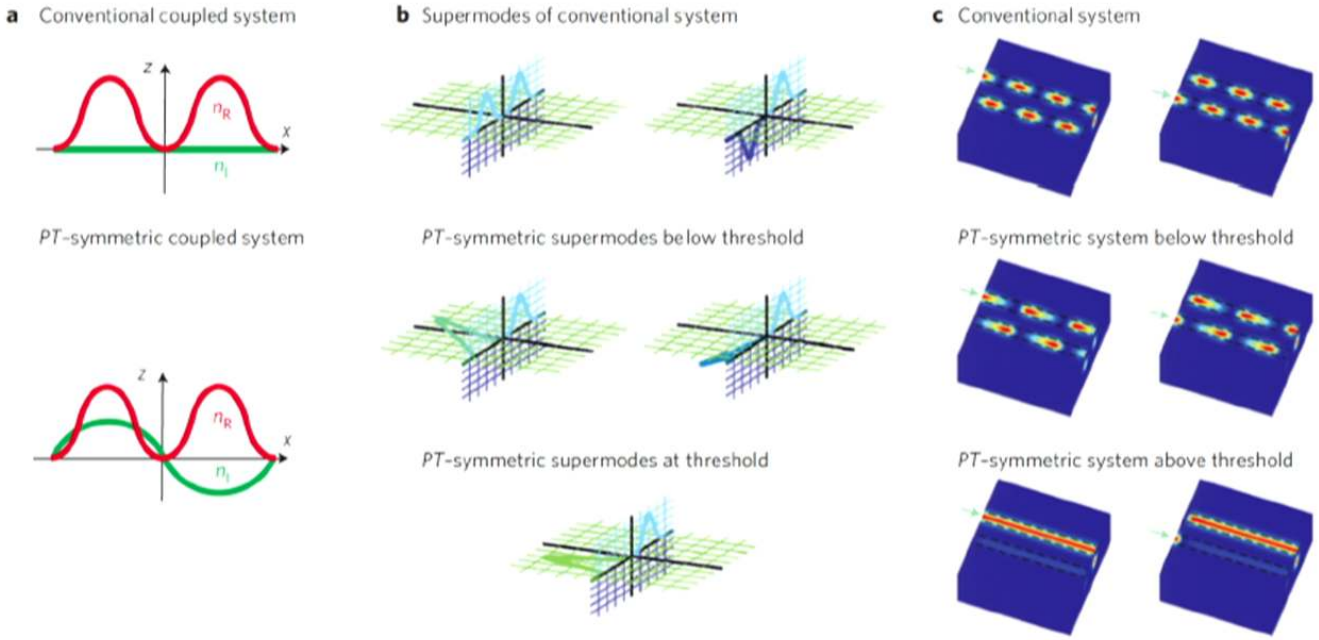
Jarzynski equality for unbroken $\mathcal{PT}$-symmetry:

$$\langle\exp(-\beta W)\rangle = \sum_{m,n}\exp(-\beta E_n+\beta E_m)\,p_{m\to n}$$

$$= (1/Z_0)\sum_{m,n}\exp(-\beta E_n)\,(\mathcal{C}_\tau\mathcal{PT}\,\phi_n)\cdot(U_\tau\phi_m)\cdot(\mathcal{C}_\tau\mathcal{PT}\,U_\tau\phi_m)\cdot\phi_n$$

$\mathcal{PT}$-symmetric quantum mechanics in optics

Rüter *et al.*, Nature Physics 6, 192 (2010)



Two coupled, optically pumped waveguides

$\mathcal{PT}$-symmetric Jarzynski equality in optics

Optical field dynamics:

$$i\,\partial_z E_1 = \frac{i\gamma}{2}\,E_1 - \kappa\,E_2\,,$$
$$i\,\partial_z E_2 = -\frac{i\gamma}{2}\,E_2 - \kappa\,E_1\,,$$

Equivalent, time-independent Hamiltonian: $(\alpha = \gamma/2\kappa)$

$$H(\alpha) = \kappa \begin{pmatrix} i\,\alpha & -1 \\ -1 & -i\,\alpha \end{pmatrix}$$

Energy eigenvalues

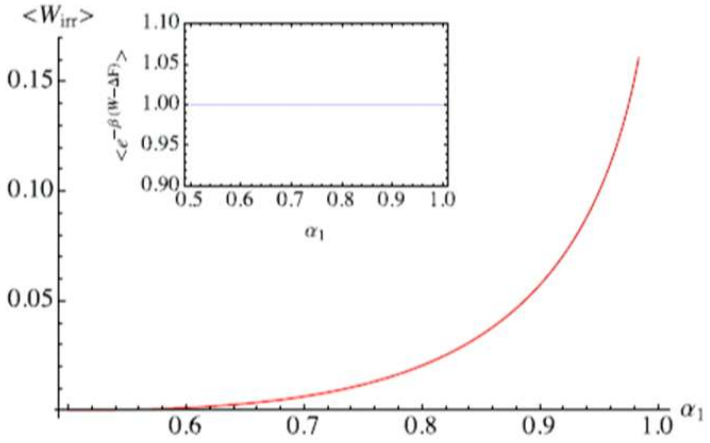
$$\epsilon_{1,2} = \pm\kappa\,\sqrt{1-\alpha^2}$$

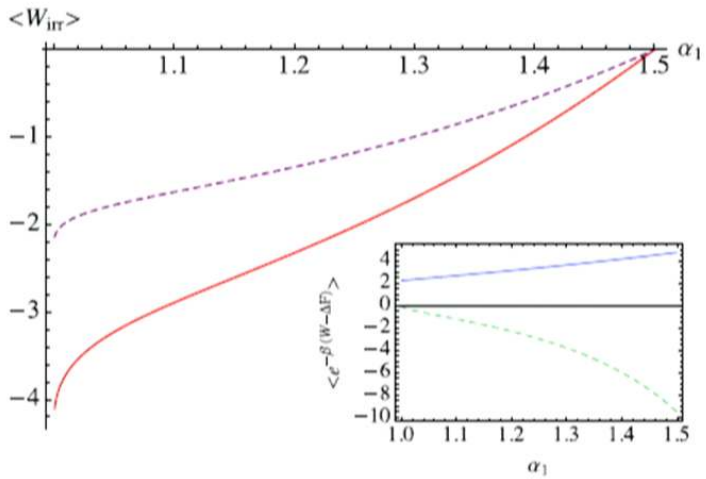
unbroken $\mathcal{PT}$-symmetry: $\alpha \leq 1$ broken $\mathcal{PT}$-symmetry: $\alpha > 1$

Irreversible work at the critical point

Deffner & Avadh, arXiv:1501.06545

$$\alpha_t = \alpha_0 + (\alpha_1 - \alpha_0)\, t/\tau$$





unbroken regime: $\alpha_0 = 1/2$

broken regime: $\alpha_0 = 3/2$

Phase transition thermodynamically inhibited!

Thermodynamics of general open quantum system

Generalizations:

Initial thermal state	→	arbitrary density operator
Unitary dynamics	→	general time evolution
Energy measurements	→	arbitrary observables
Work and energy	→	entropy and information

General quantum measurements

- Quantum observable: $A = \sum_m a_m \Pi_m$, with Π_m orthogonal projector
- Measuring a_m: $\rho \to \Pi_m \rho \Pi_m / p_m$ with $p_m = \mathrm{tr}\{\Pi_m \rho \Pi_m\}$
  - Density operator ρ projected into eigenspace of A
  - collapse of wavefunction for pure ρ
- Statistics of measured quantum system: $M(\rho) = \sum_m \Pi_m \rho \Pi_m$
  - accounting for all possible measurement outcomes

Note: If and only if ρ and A commute, then $M(\rho) = \rho$!

Trace preserving, completely positive maps

Properties of $\mathbb{E}$:

- Any linear quantum transformation
- Maps density operators onto density operators
  - trace preserving and completely positive
- Measurement performed by environment on system
- Dynamics not necessarily reducible to differential equation
- Kraus operator representation: $\mathbb{E}(\rho) = \sum_\nu K_\nu \, \rho \, K_\nu^\dagger$

General quantum fluctuation theorem (GQFT)

System initially prepared in arbitrary density operator ρ_0

equilibrium or non-equilibrium, stationary or transient, pure or mixed

Quantum procedure:

(1) Measurement of A^{i}
(2) System evolves under $\mathbb{E}$
(3) Measurement of A^{f}

- Random variable: $\Delta a_{n,m} = a_n^{\mathrm{f}} - a_m^{\mathrm{i}}$
- Transition probability: $p_{m\to n} = p_m \cdot p_{n|m} = \mathrm{tr}\left\{\Pi_n^{\mathrm{f}}\,\mathbb{E}\left(\Pi_m^{\mathrm{i}}\rho_0\Pi_m^{\mathrm{i}}\right)\right\}$
- Probability distribution: $\mathcal{P}(\Delta a) = \sum_{m,n}\delta\left(\Delta a - \Delta a_{n,m}\right)\,p_{m\to n}$

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GQFT – Quantum efficacy

Kafri & Deffner, PRA **86**, 044302 (2012)

$$\langle \exp(-\Delta a) \rangle = \gamma$$

Quantum efficacy: $\gamma = \mathrm{tr}\left\{\exp\left(-A^{\mathrm{f}}\right)\mathbb{E}\left(M^{\mathrm{i}}(\rho_0)\exp\left(A^{\mathrm{i}}\right)\right)\right\}$

- Similar fluctuation theorems in the context of classical feedback

$$\langle \exp(-\Sigma) \rangle = \gamma_{\mathrm{cl}}$$

- γ_{cl} commonly called (classical) efficacy of the feedback protocol

Sagawa & Ueda, PRL **104**, 090602 (2010)

- Jensen's inequality: $\langle \Delta a \rangle \geq -\ln(\gamma)$

Shortcomings of two-time measurements

Issues:

- for open quantum systems stationary state not Gibbs

  Gelin & Thoss, PRE **79**, 051121 (2009)

- two-time energy measurements on system not sufficient

  Kafri & Deffner, PRA **86**, 044302 (2012)

Solutions and Generalizations:

- measure energy of system AND environment

  Deffner & Lutz, PRL **107**, 140404 (2011)

- find better definition for quantum entropy production

  Subaşı & Hu, PRE **85**, 011112 (2012) Horowitz, PRE **85**, 031110 (2012) Leggio *et al.*, PRA **88**, 042111 (2013)

  Campisi, NJP **15**, 115008 (2013) Deffner, EPL **103**, 30001 (2013) Allahverdyan, PRE **90**, 032137 (2014)

Quantum entropy production in Wigner space

Deffner, EPL 103, 30001 (2013)

Wigner distribution:

$$\mathcal{W}_t(x,p) = \frac{1}{2\pi\hbar}\int \mathrm{d}y\, \exp\left(-i/\hbar\, py\right) \langle x + y/2|\rho_t|x - y/2\rangle$$

Quantum master equation:

$$\partial_t\, \mathcal{W}(\Gamma,t) = \mathcal{L}_\alpha\, \mathcal{W}(\Gamma,t)$$

Define entropy production:

$$\Sigma[\Gamma_\tau;\, \alpha_\tau] = -\int_0^\tau \mathrm{d}t\, \dot{\alpha}_t\, \frac{\partial_\alpha \mathcal{W}_{\mathrm{stat}}(\Gamma_t,\alpha_t)}{\mathcal{W}_{\mathrm{stat}}(\Gamma_t,\alpha_t)}$$

- mathematical construct "like trajectories" in path integral
- assign physical meaning to average $\langle\Sigma\rangle$

Integral fluctuation theorem

Joint distribution:

$$\partial_t P(\Gamma, \sigma, t) = [\mathcal{L}_\alpha - j_{\rm stat}(\Gamma, \alpha_t)\,\partial_\sigma]\; P(\Gamma, \sigma, t)$$

(Quasi-)Probability flux:

$$j_{\rm stat}(\Gamma, \alpha_t) = \dot{\alpha}_t \, \frac{\partial_\alpha \mathcal{W}_{\rm stat}(\Gamma, \alpha_t)}{\mathcal{W}_{\rm stat}(\Gamma, \alpha_t)}$$

Exponentially weighted marginal:

$$\Psi(\Gamma, t) = \int \mathrm{d}\sigma \, P(\Gamma, \sigma, t) \, \exp(-\sigma) \quad \rightarrow \quad \Psi(\Gamma, t) = \mathcal{W}_{\rm stat}(\Gamma, \alpha_t)$$

Fluctuation theorem:

$$1 = \int \mathrm{d}\Gamma \, \mathcal{W}_{\rm stat}(\Gamma, \alpha_\tau) = \int \mathrm{d}\Gamma \, \Psi(\Gamma, \tau) = \langle \exp(-\Sigma) \rangle$$

Take-home-message

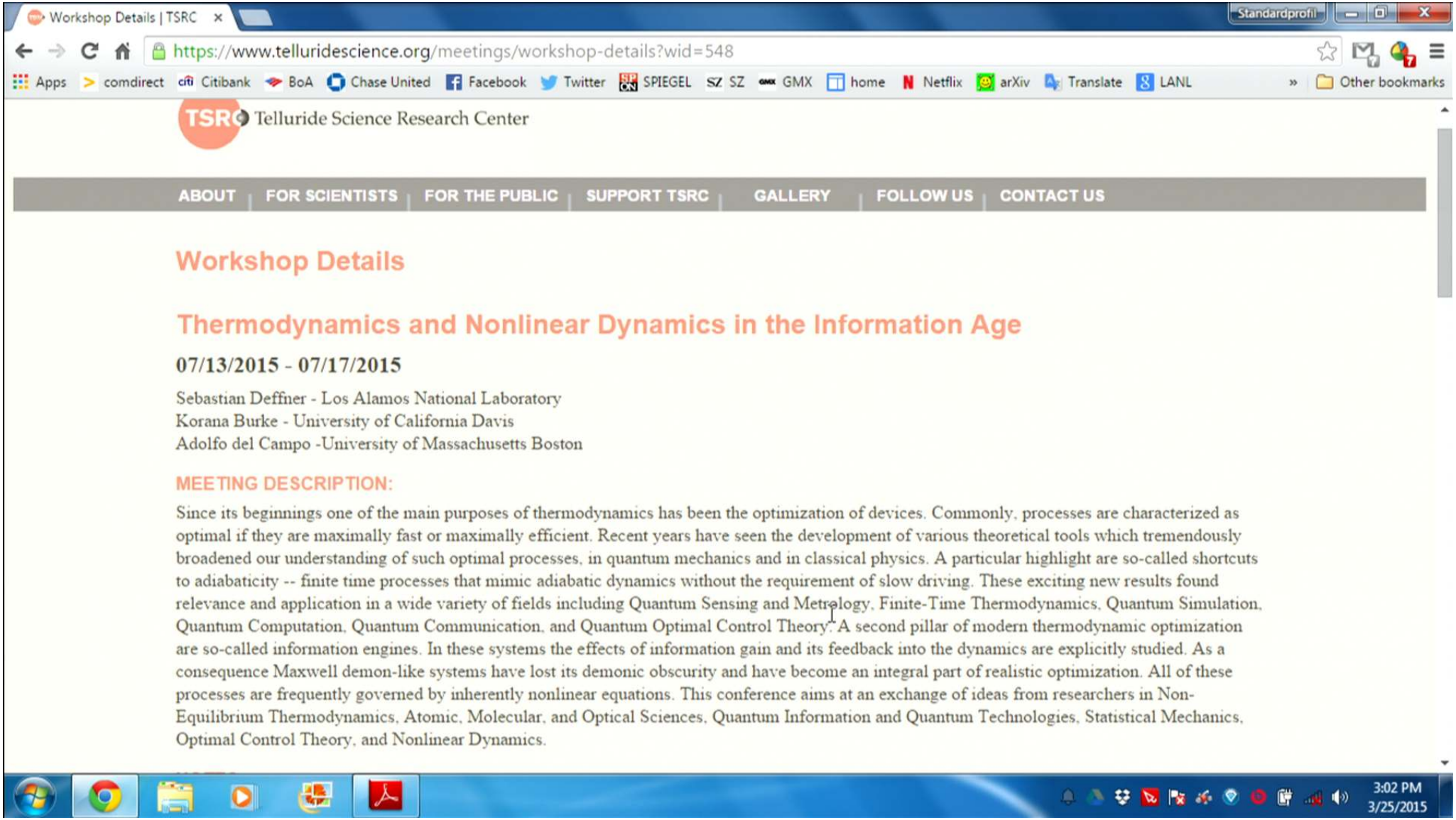
- Fluctuation theorems as generalization of the second law
- Two-time measurements for isolated and open quantum systems
- Quantum entropy production in phase space

Deffner & Lutz, PRL **107**, 140404 (2011)

Kafri & Deffner, PRA **86**, 044302 (2012)

Deffner, EPL **103**, 30001 (2013)

Deffner & Avadh, arXiv:1501.06545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Thermodynamics and Nonlinear Dynamics in the Information Age
07/13/2015 - 07/17/2015
Sebastian Deffner - Los Alamos National Laboratory
Korana Burke - University of California Davis
Adolfo del Campo -University of Massachusetts Boston
MEETING DESCRIPTION:
Since its beginnings one of the main purposes of thermodynamics has been the optimization of devices. Commonly, processes are characterized as optimal if they are maximally fast or maximally efficient. Recent years have seen the development of various theoretical tools which tremendously broadened our understanding of such optimal processes, in quantum mechanics and in classical physics. A particular highlight are so-called shortcuts to adiabaticity -- finite time processes that mimic adiabatic dynamics without the requirement of slow driving. These exciting new results found relevance and application in a wide variety of fields including Quantum Sensing and Metrology, Finite-Time Thermodynamics, Quantum Simulation, Quantum Computation, Quantum Communication, and Quantum Optimal Control Theory. A second pillar of modern thermodynamic optimization are so-called information engines. In these systems the effects of information gain and its feedback into the dynamics are explicitly studied. As a consequence Maxwell demon-like systems have lost its demonic obscurity and have become an integral part of realistic optimization. All of these processes are frequently governed by inherently nonlinear equations. This conference aims at an exchange of ideas from researchers in Non-Equilibrium Thermodynamics, Atomic, Molecular, and Optical Sciences, Quantum Information and Quantum Technologies, Statistical Mechanics, Optimal Control Theory, and Nonlinear Dynamics.
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