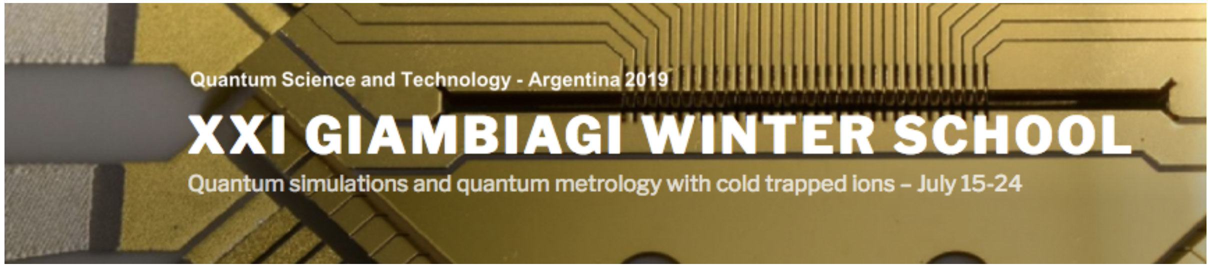


XXI Giambiagi Winter School
July 2019
University of Buenos Aires
Argentina

Quantum Thermodynamics

Janet Anders
University of Exeter, UK

joint work with :
Philipp Kammerlander
Sai Vinjanampathy
Harry Miller
....

UNIVERSITY OF EXETER

Quantum Advantages

Quantum Computing

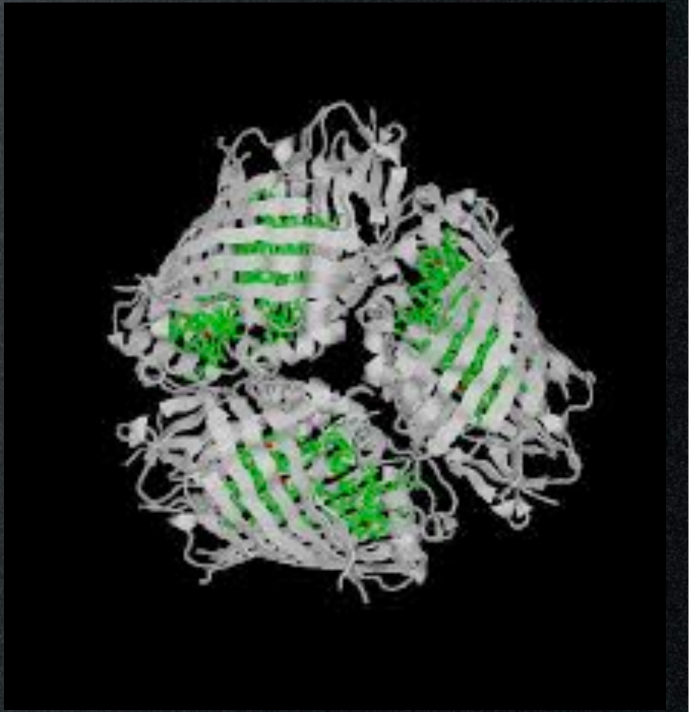
➤ exponential speed up

Quantum Cryptography

➤ non-breakable secret key distribution

Quantum Metrology

➤ increased accuracy



Quantum Simulation

➤ faster predictions

Quantum Biology

➤ increased transfer efficiency

Quantum thermodynamics - Motivation

MICROSCOPIC WORLD

- atoms, electrons, photons

MACROSCOPIC WORLD

- gases, fluids, solids
- pistons and weights

1nm/1amu

1m/1kg

Quantum thermodynamics

- include small ensemble sizes
- include non-equilibrium properties
- include quantum properties

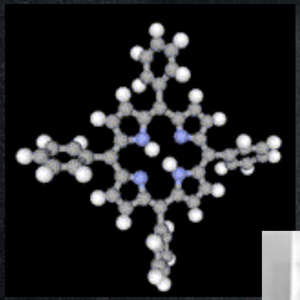
Quantum Mech

- superposition
- quantum correlations

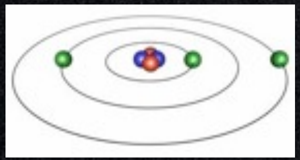
cs

- ork, heat, entropy
- 1st law, 2nd law, 3rd law
- Carnot efficiency, engines

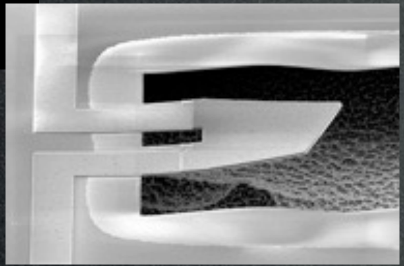
photon



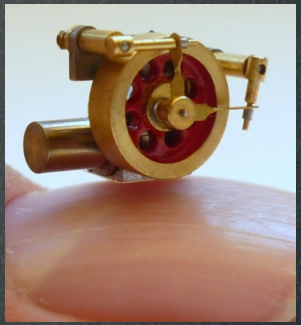
bio-molecule



atom



micro-meter resonator

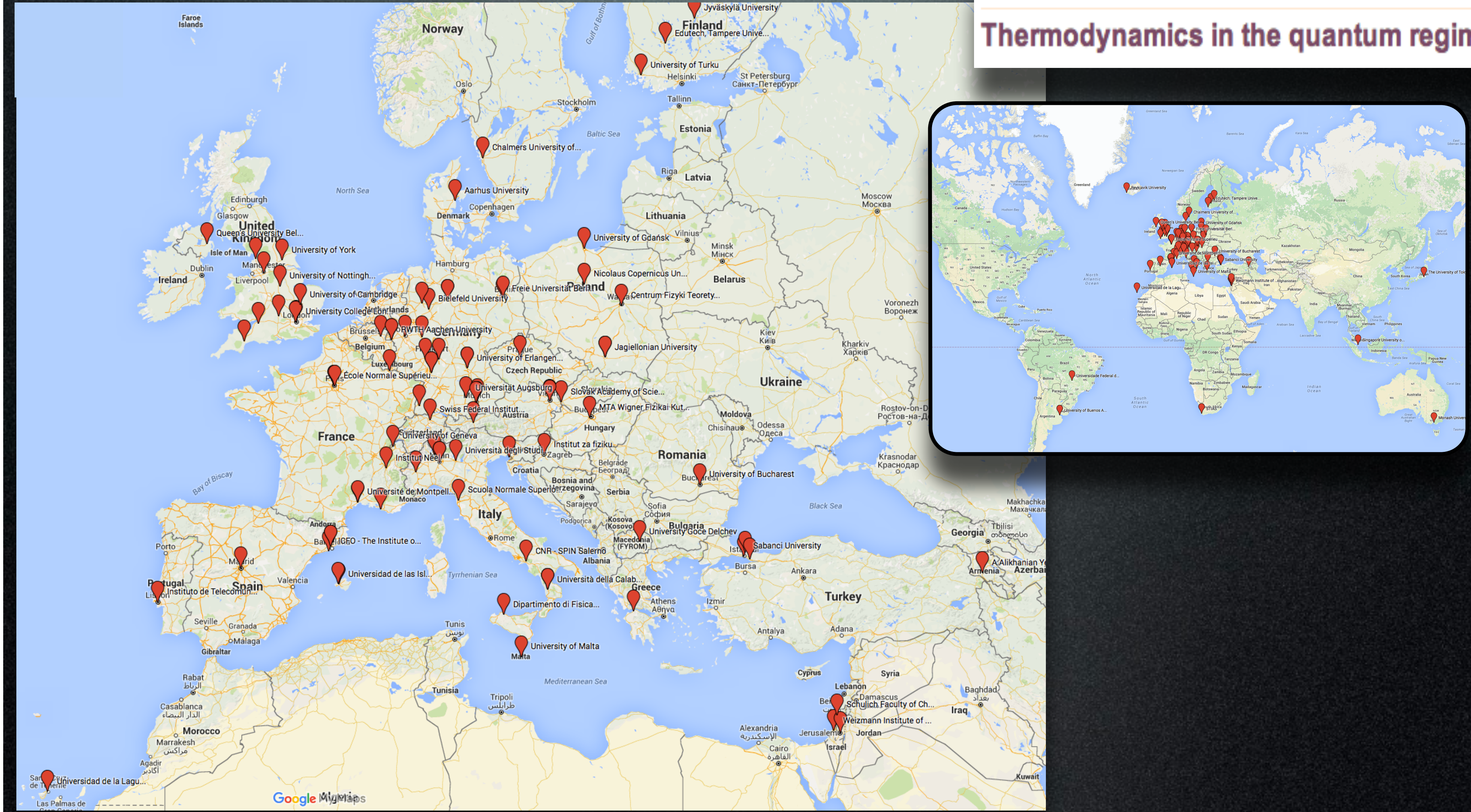


COST network (2013-2017)

EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY

MPNS COST Action MP1209

Thermodynamics in the quantum regime



QTD announcements: https://qtd.ifisc.uib-csic.es/

Quantum Thermodynamics Conference QTD2020

Barcelona - Spain
20 - 24 April 2020

check QTD webpage http://qtd.ifisc.uib-csic.es/ for updates

Col·legi Major Sant Jordi

Lecture overview

I - Work extraction from quantum coherences

II - Maxwell’s demon and his exorcism - experimental evidence

III - Thermodynamics beyond the weak coupling limit

Outline - I

- Laws of Thermodynamics
- Landauer’s principle
- Quantum Jarzynski equality
- Thermodynamic resource theory
- Work from quantum coherences
- Implications

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- Laws of Thermodynamics
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from ca 1800 engines

thermodynamics

1st: $\Delta U = \langle Q_{abs} \rangle - \langle W_{ext} \rangle$

2nd: $T \Delta S_{th} \geq \langle Q_{abs} \rangle$

microscopic
description of
macroscopic
thermodynamics

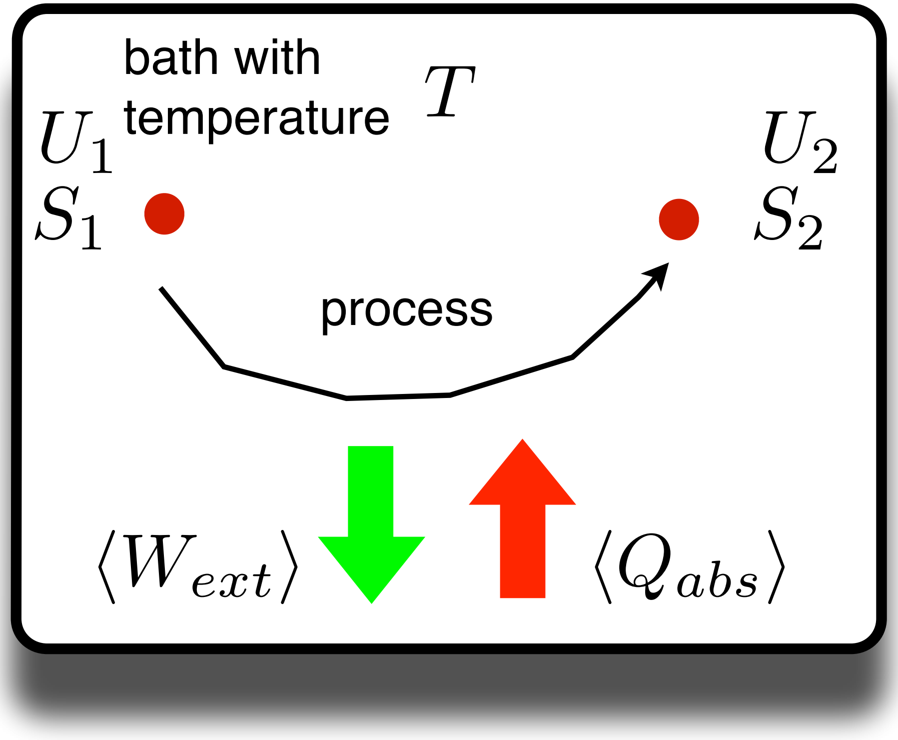
statistical physics

ideal gas

N k T = p V

Boltzmann 1880

macroscopic quantities



internal energy, U

heat, Q

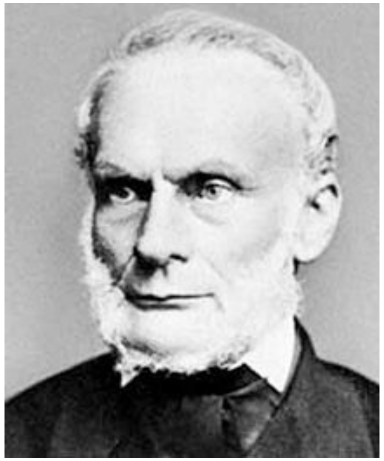
work, W

temperature, T

entropy, S

pressure, p

volume, V



Clausius 1865

from ca 1800 engines

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microscopic
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statistical physics

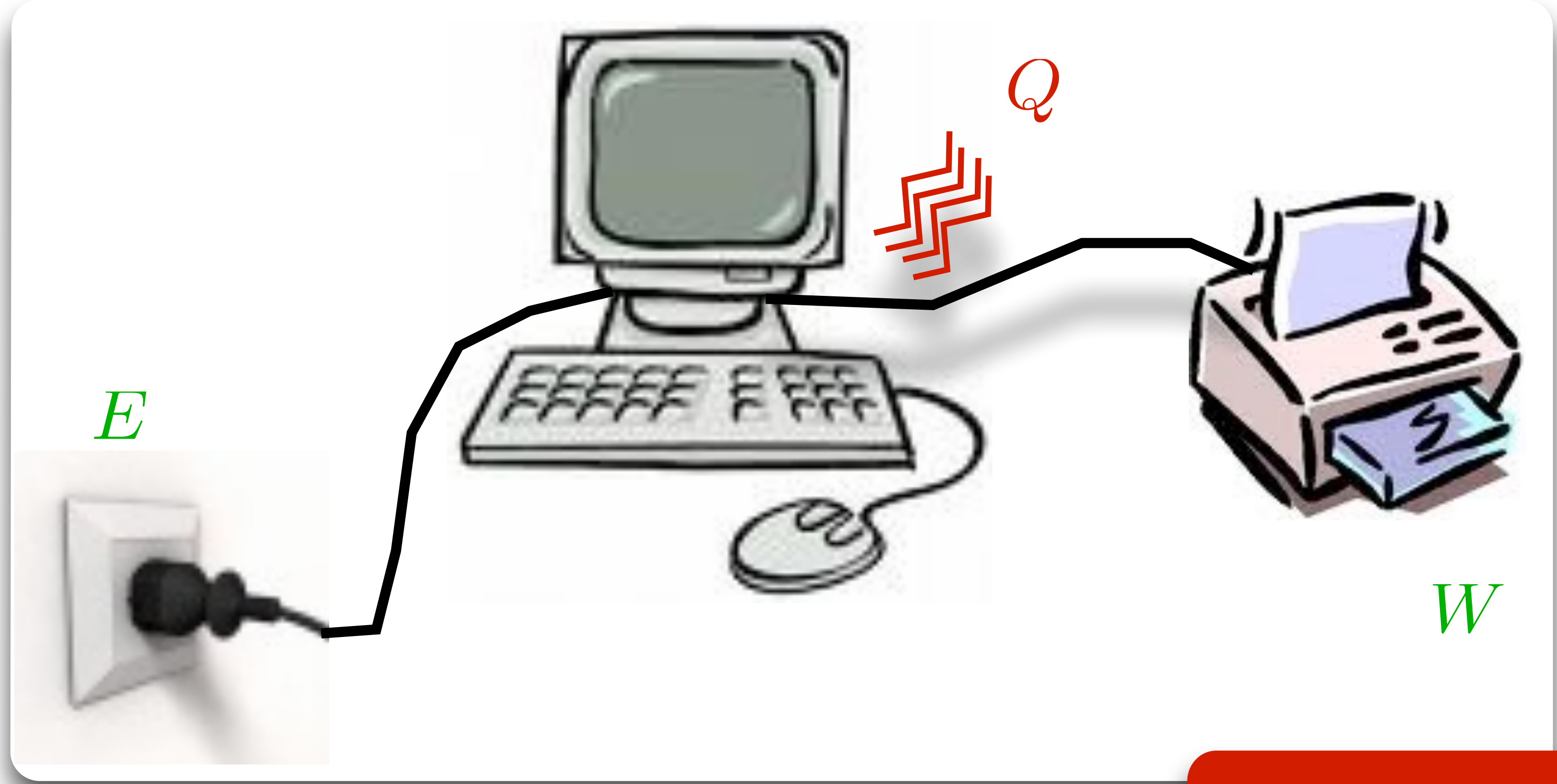
from ca 1950
computers

information theory

information: $S_{Sh} > 0$

Shannon 1948

Landauer’s erasure principle



energy conservation: $\Delta E = W + Q$

can heat be reduced to 0?

erasure of bits (at finite operating temperature) **dissipates heat**

Landauer 1960ties

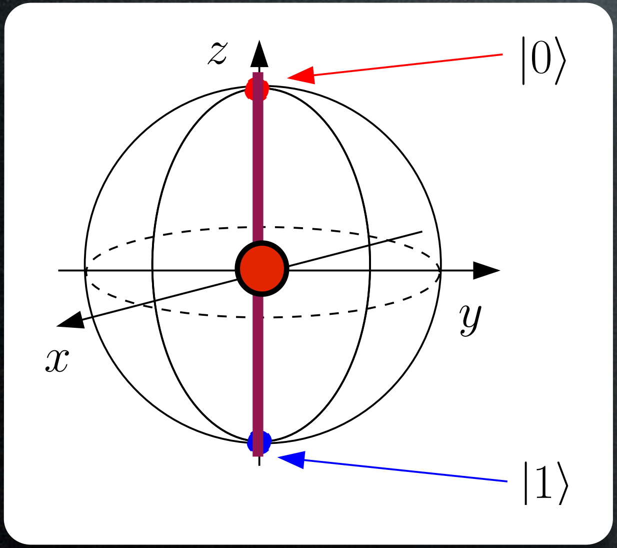
(i.e. resetting bits in your computer to 0)

Landauer's principle

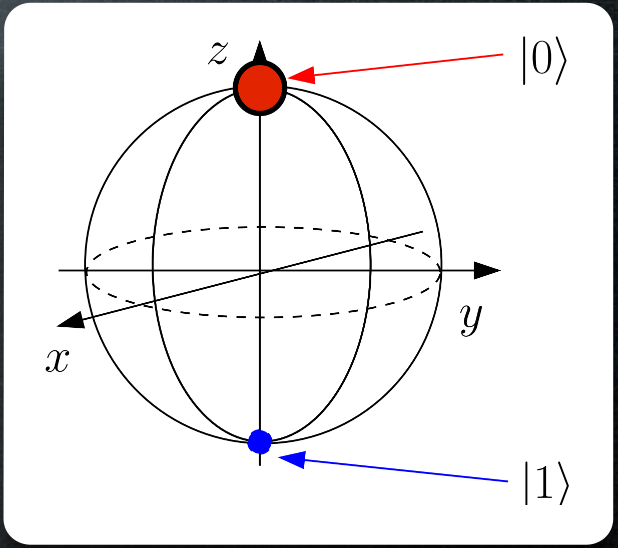
classical or quantum bit

erasure of 1 bit of information = state transfer

$$\rho^{(1)} = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| \quad \Longrightarrow \quad \rho^{(2)} = |0\rangle\langle 0|$$



$$\begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \qquad \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$



$$S(\rho^1) = \ln 2 \qquad S = -tr[\rho \ln \rho] \qquad S(\rho^2) = 0$$

2nd law

$$T\,\Delta S \geq Q_{\text{abs}} \longrightarrow Q_{gen} \geq k_B T \ln 2$$

link

Landauer's erasure principle

erasure of 1 bit of information results in **dissipation** of heat:

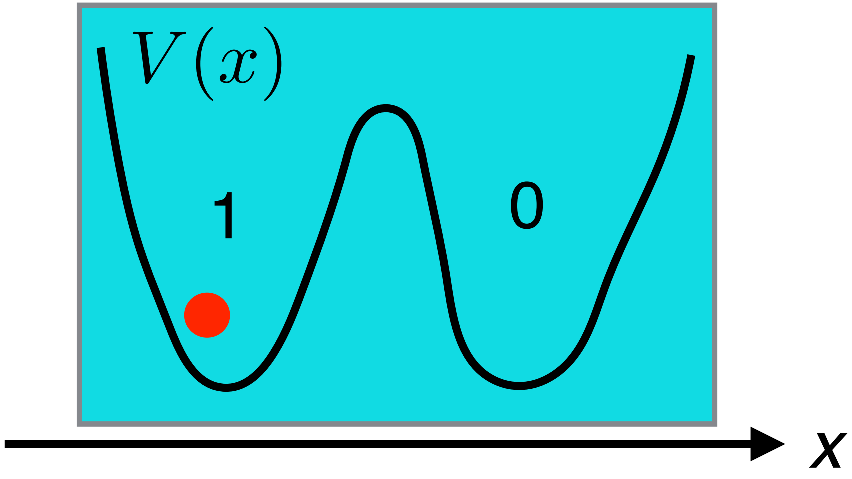
$$Q_{diss} \geq k_B T \ln 2$$

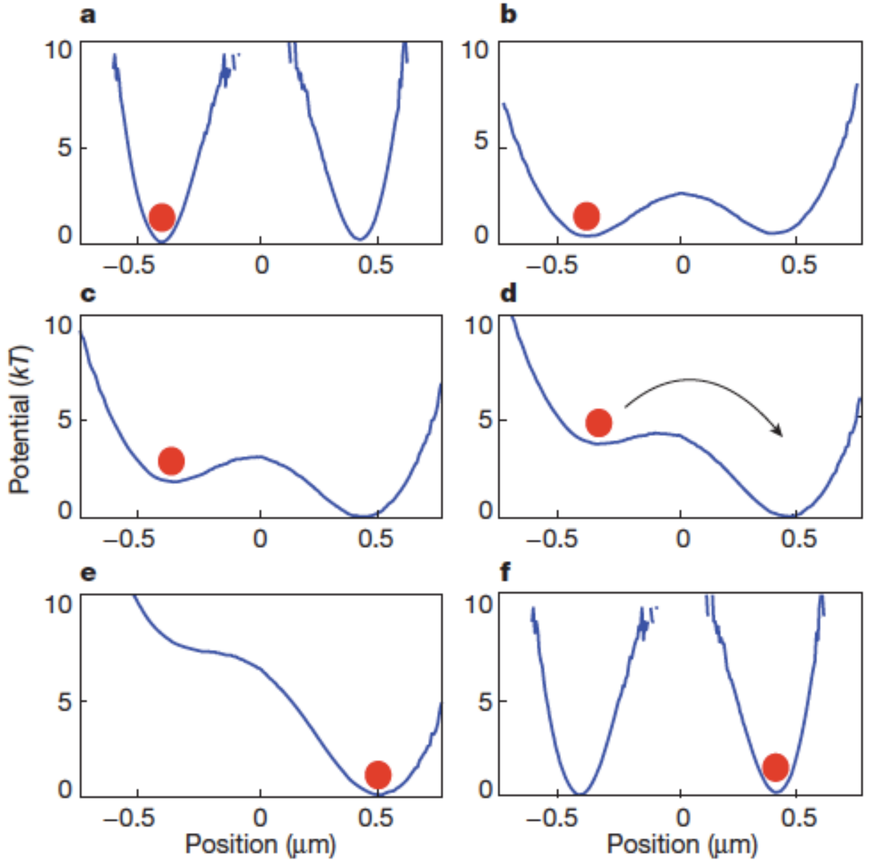
minimum dissipated heat

Boltzmann constant

operating temperature in Kelvin

Experimental realisation of Landauer erasure:





Particle (silicon bead) swimming in water in equilibrium at T.

Trapped in double-well potential.

Berut et al, Nature 483, 187 (2012)

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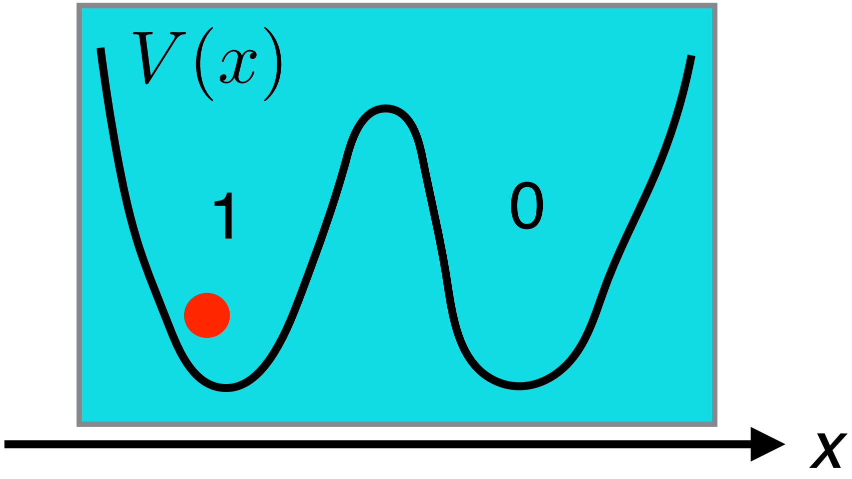

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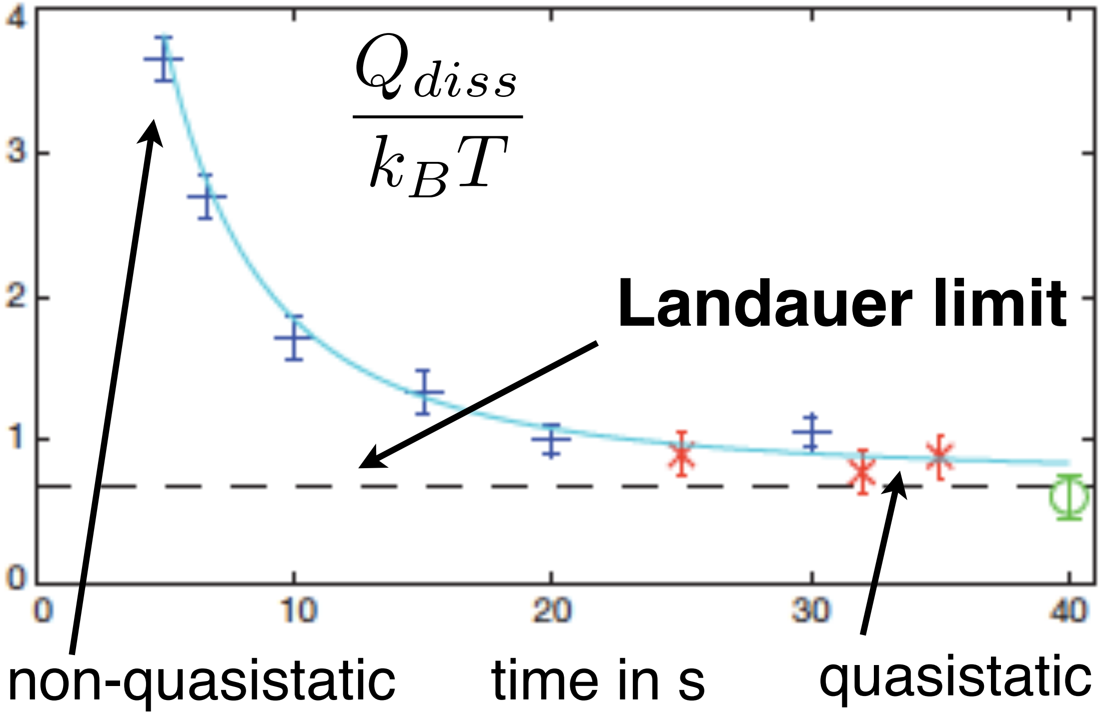
Dissipated heat in units $k_B T$ plotted over time taken to implement erasure.



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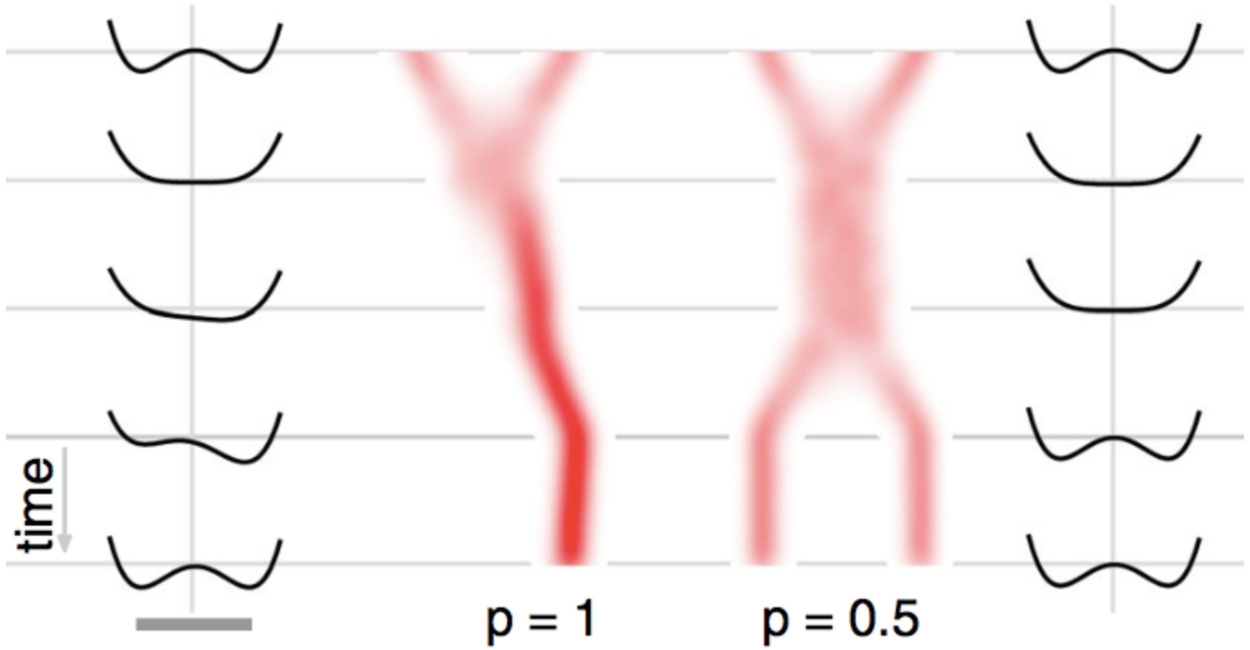
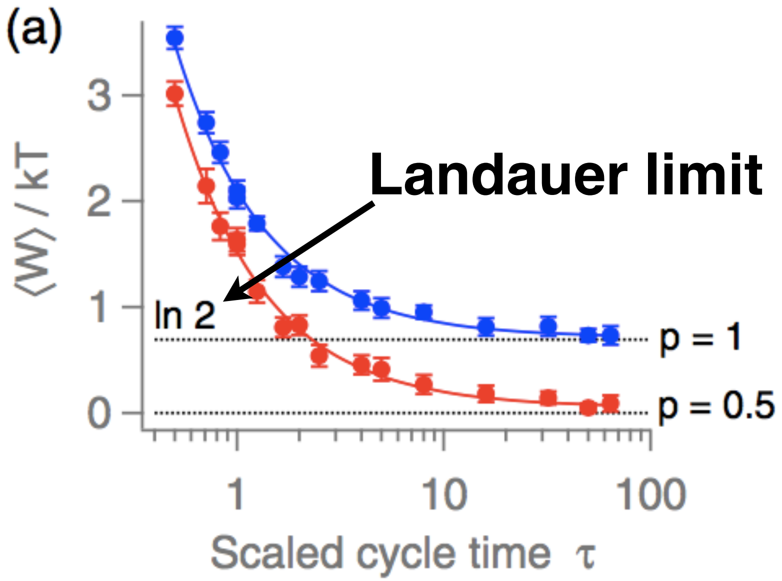
Another **experimental** realisation of Landauer erasure:



erasure no erasure

work required for erasure:



Jun et al, PRL 113, 190601 (2014)

from ca 1800 engines

thermodynamics

1st: $\Delta U = \langle Q_{abs} \rangle - \langle W_{ext} \rangle$

2nd: $T \Delta S_{th} \geq \langle Q_{abs} \rangle$

microscopic description of macroscopic thermodynamics

statistical physics

- information is physical

$$S_{Sh} = S_{th}$$

- information erasure causes heat dissipation

Landauer 1961

erasure: state transfer

$$\rho = \frac{1}{2}\,|0\rangle\langle 0| + \frac{1}{2}\,|1\rangle\langle 1| \to |0\rangle\langle 0|$$

generated heat

$$\langle Q_{gen} \rangle \geq k_B T \,\ln 2$$

from ca 1950

computers

information theory

information: $S_{Sh} > 0$

from ca 1800 engines

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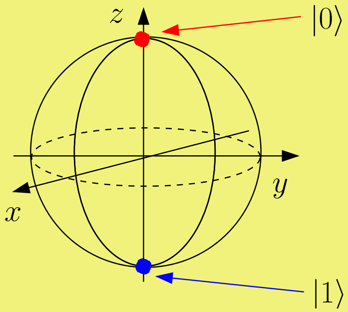

from ca 1980
qubit

quantum information theory

qu. superpositions ➤ **no-cloning theorem** ➤ secure qkd

qu. correlations ➤ **non-locality** ➤ qu. computing

from ca 1800 engines

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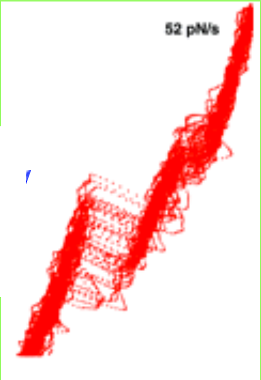
$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$$



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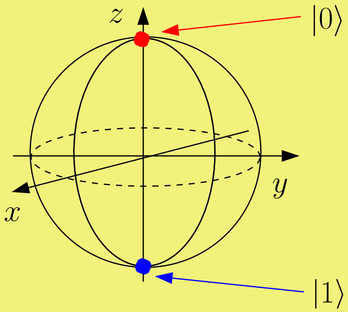

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qubit

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Stochastic thermodynamics & classical fluctuation relations

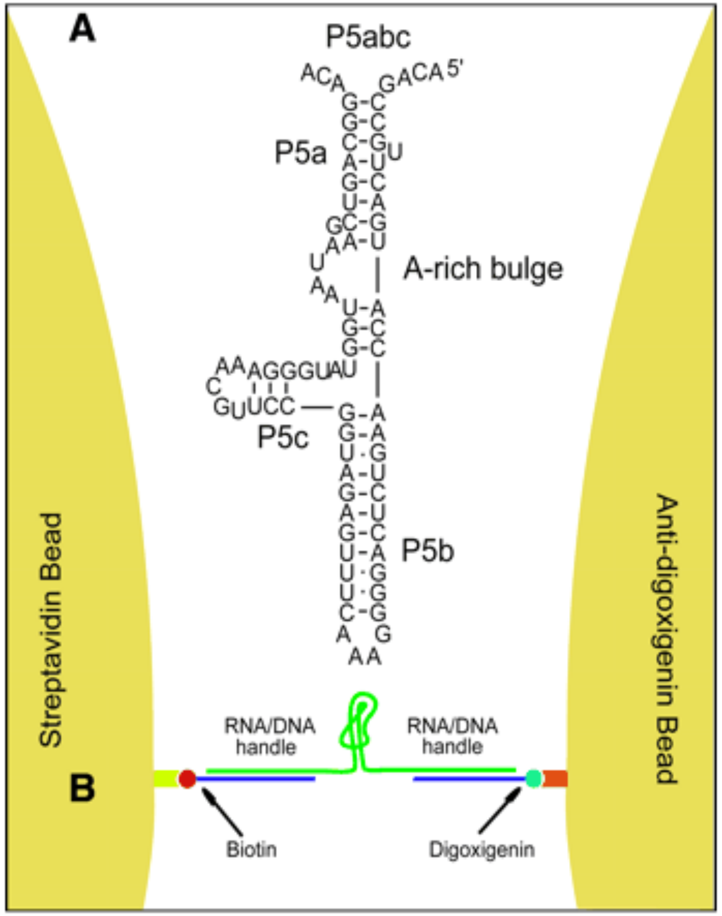
Jarzynski equality Jarzynski, PRL (1997)

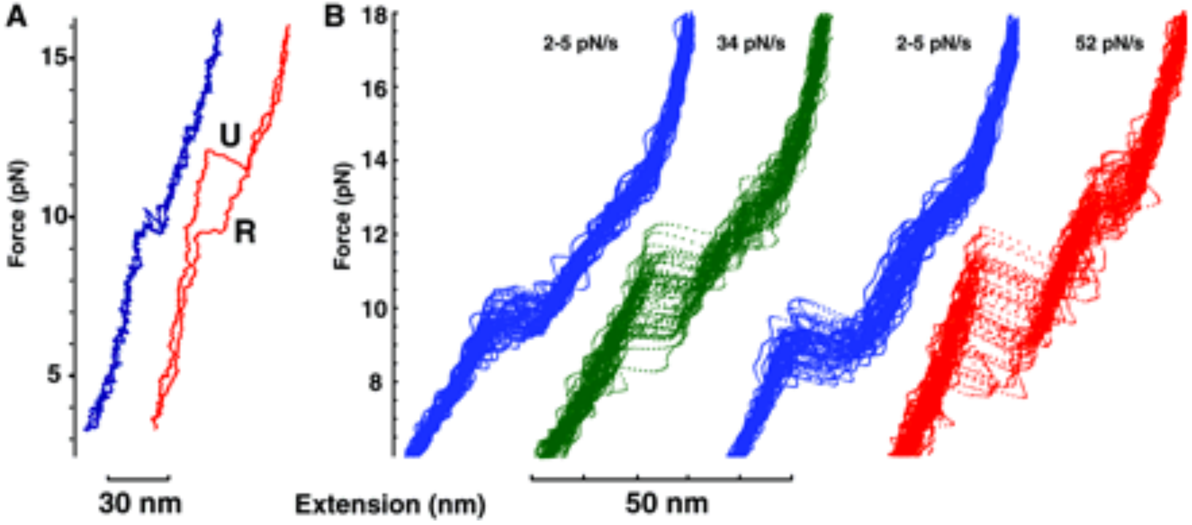
$$\langle e^{-\beta W}\rangle = e^{-\beta \Delta F}$$

non-equilibrium work

inverse temperature

equilibrium free energy





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

Crooks relation Crooks, PRE (2000)

from ca 1800 engines

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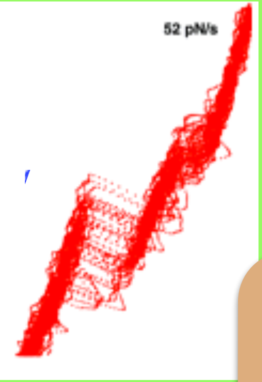
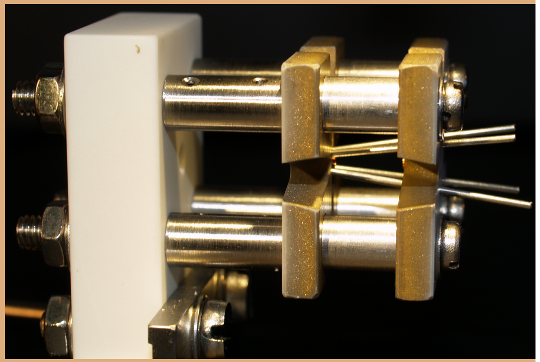


stochastic thermodynamics

quantum fluctuation relations

single ion engine - Singer group



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from ca 1950
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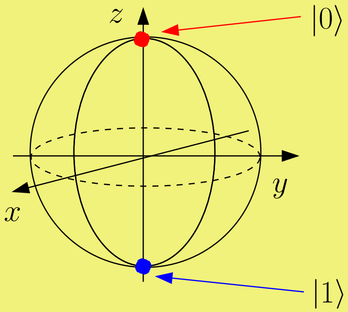

from ca 1980
qubit

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Quantum Jarzynski equality

Tasaki (2000), Kurchan (2000), Mukamel (2003)

2M: Talkner, Lutz, Hänggi PRE (2007)

1M: Mazzola, DeChiara, Paternostro, PRL (2013)

isolated system

thermal initial state

$$\rho_0 = \frac{e^{-\beta H_0}}{Z_0}$$

$$H_0 = \sum_k E_k^0 \, \Pi_k^0$$

$$V$$

protocol = changing Hamiltonian H_t in specific way generates unitary

final non-equilibrium state

$$\rho_\tau = V \, \rho_0 \, V^\dagger$$

$$H_\tau = \sum_n E_n^\tau \, \Pi_n^\tau$$

- to establish a Jarzynski relation need to define fluctuating work W
- there is no observable (if there was, work would be a state variable)
- but one can measure the energy at **beginning** and **end**
- because evolution is unitary, there is no dissipation and energy change is entirely work
- fluctuating work is $W_{k,n} = E_n^\tau - E_k^0$ occurring with probability
- and exponentiated average is

same as classical

$$p_{k,n} = tr[\Pi_n^\tau \, V \, \Pi_k^0 \, \rho_0 \, \Pi_k^0 \, V^\dagger \Pi_n^\tau]$$

$$= \frac{e^{-\beta E_k^0}}{Z_0} \, tr[V \, \Pi_k^0 \, V^\dagger \Pi_n^\tau]$$

$$\langle e^{-\beta W} \rangle = \sum_{n,k} p_{k,n} \, e^{-\beta W_{k,n}} = \frac{Z_\tau}{Z_0} = e^{-\beta \Delta F}$$

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same as classical

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$$\boxed{\langle e^{-\beta W} \rangle} = \sum_{n,k} p_{k,n} \, e^{-\beta W_{k,n}} = \frac{Z_\tau}{Z_0} = \boxed{e^{-\beta \Delta F}}$$

from ca 1800 engines

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from ca 1995

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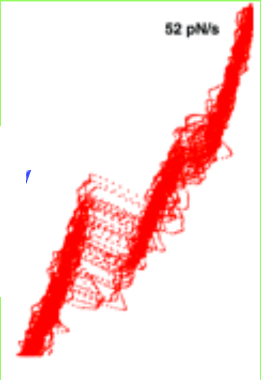

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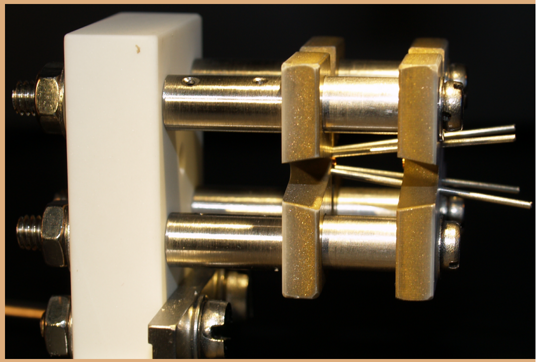

quantum thermodynamics

resource theory

from ca 1950
computers

information theory

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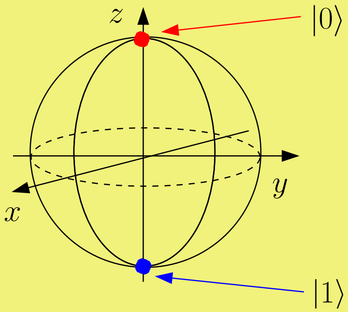

from ca 1980
qubit

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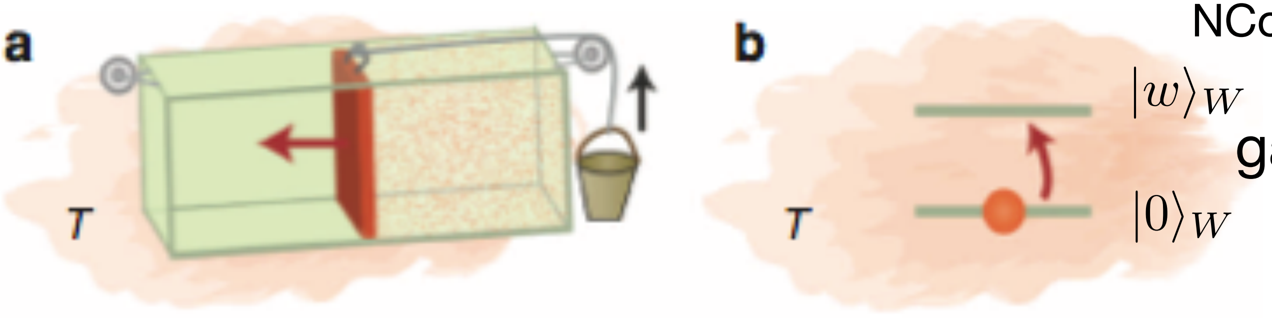
Resource theory: Single shot extractable work

Horodecki+Oppenheim
NComm (2013)



Aberg, Nature Comm.
4 1925 (2013)

Gemmer, Anders,
NJP **17**, 085006 (2015)

Global unitary on system, bath and work storage system

$$tr_{SB}[V\,(\rho_S \otimes \tau_B \otimes |0\rangle_W\langle 0|)\,V^\dagger] \approx |w\rangle_W\langle w|$$

ρ_S diagonal in energy
V commutes with global H

What is **maximum** w so that this outcome happens with probability $1-\epsilon$

single shot work	instead of **average work**
$w_\epsilon^{\max} \leq F_\epsilon^{\min}(\rho_S) - F(\tau_S)$	$\langle W\rangle \leq F(\rho_S) - F(\tau_S)$

Valid for running experiment on one system, but it is *not* the fluctuating work.

For many copies, $\rho_S \rightarrow \rho_S \otimes \rho_S \otimes \rho_S \dots$ this converges $w_\epsilon^{\max} \rightarrow \langle W\rangle$
for $\epsilon \rightarrow 0$

Single shot extractable work

Global unitary on system, bath and work storage system

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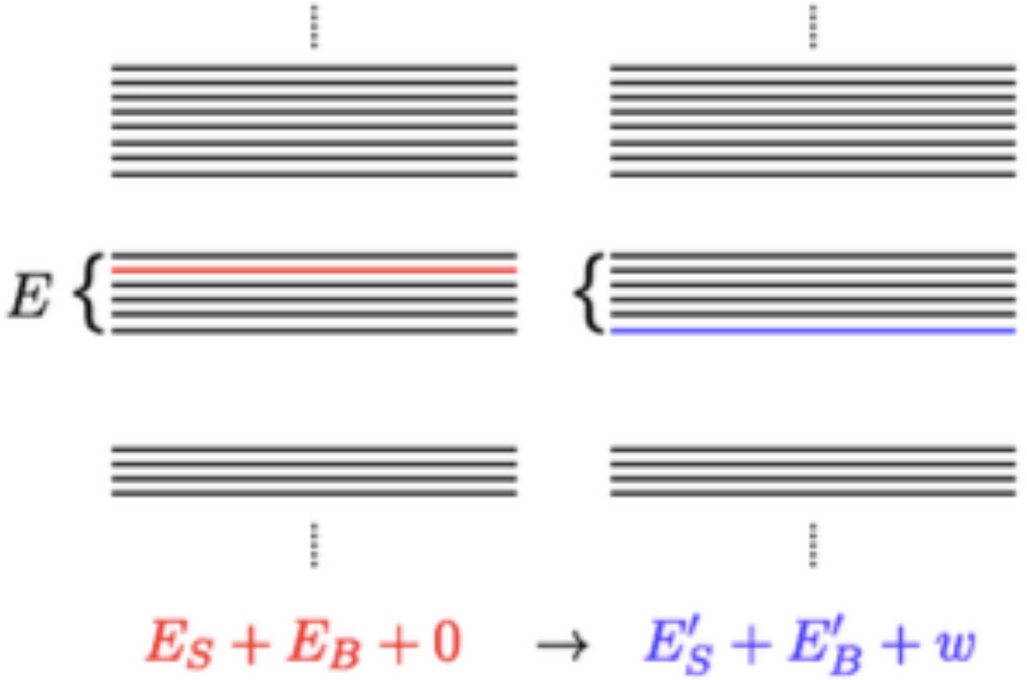
ρ_S diagonal in energy

V commutes with global H

stay in same global energy subspace



Vinjanampathy, Anders, Contemporary Physics (2016)

Single shot extractable work

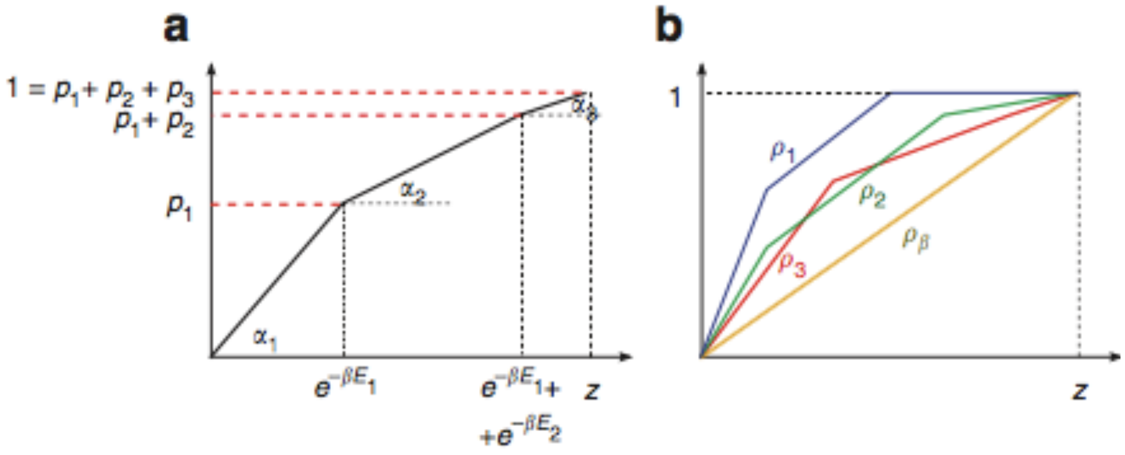
single shot work

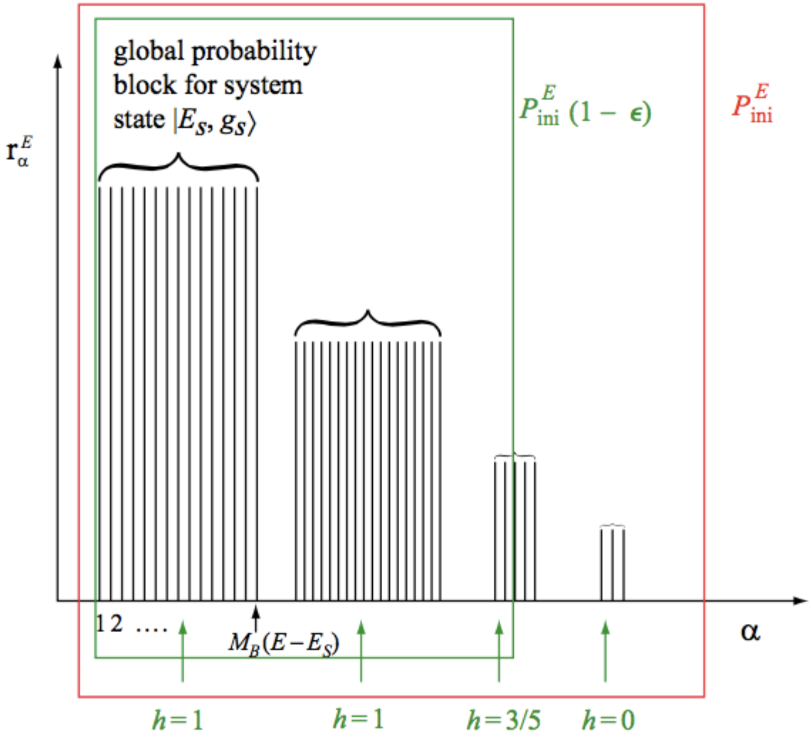
$$w_\epsilon^{\max} \leq F_\epsilon^{\min}(\rho_S) - F(\tau_S)$$

$$F_\epsilon^{\min}(\rho_S) := -\frac{1}{\beta} \ln \sum_{E_S, g_S} e^{-\beta E_S} h(E_S, g_S, \epsilon).$$

$$F_0^{\min}(\rho_S) = -\frac{1}{\beta} \ln tr[\Pi_{\rho_S} \tau_S] + F(\tau_S)$$

Horodecki+Oppenheim
Nature Comm. **4** 2059 (2013)





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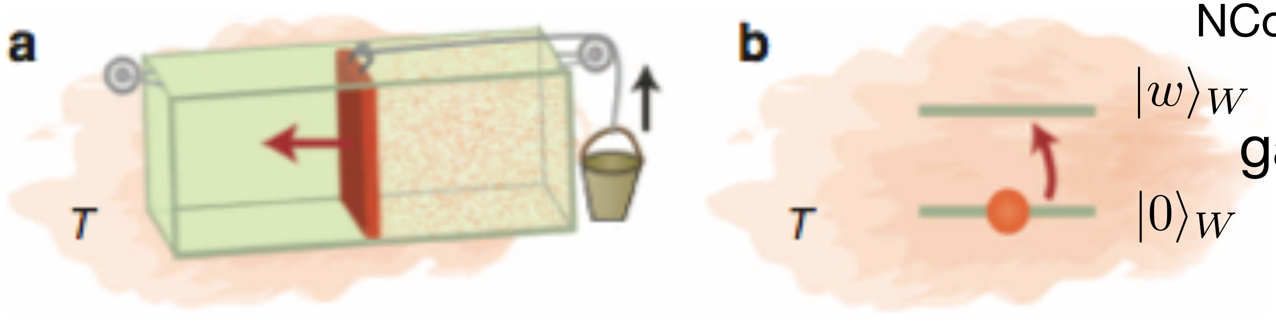
Resource theory: Single shot extractable work

Horodecki+Oppenheim
NComm (2013)



$|w\rangle_W$

gap= w

$|0\rangle_W$

Aberg, Nature Comm.
4 1925 (2013)

finite size effect -
not quantum effect

Global unitary on system, bath and work storage system

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Jarzynski, PRL (1997)
Qu: Talkner, Lutz, Hänggi PRE (2007)

Classical fluctuation relation

Jarzynski non-equilibrium work equality

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$$

non-equilibrium work

inverse temperature

equilibrium free energy

Quantum fluctuation relation:

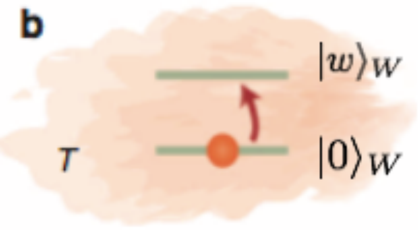
make energy measurements to obtain energetic fluctuations

Quantum Jarzynski relation: same as classical

Because measurements **destroy coherences** between energies.

Horodecki, Oppenheim
Nat. Comm (2013)

Quantum resource theory



gap= w

$$tr_{SB}[V\,(\rho_S \otimes \tau_B \otimes |0\rangle_W\langle 0|)\,V^\dagger] \approx |w\rangle_W\langle w|$$

Obtain bounds on work *w* that can be extracted to a qubit in single shot rather than on average.

Finite size effect - not a quantum effect

ρ_S **diagonal** in energy

V **commutes** with global H

from ca 1800 engines

thermodynamics

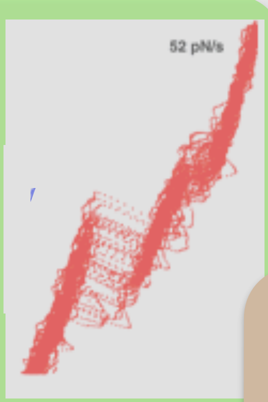
1st: $\Delta U = \langle Q_{abs} \rangle - \langle W_{ext} \rangle$

2nd: $T \Delta S_{th} \geq \langle Q_{abs} \rangle$

microscopic description of macroscopic thermodynamics

from ca 1995

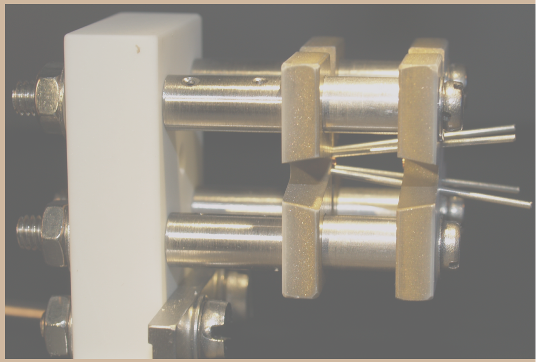
$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$$



stochastic thermodynamics

quantum fluctuation relations

single ion engine - Singer group



quantum thermodynamics

resource theory

- information is
  $S_{Sh} = S$
- information er
  causes heat d

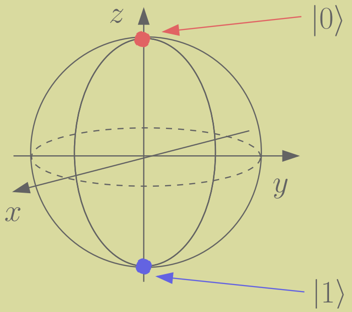
Neither identifies a quantum advantage.

from ca 1950
computers

information theory

information: $S_{Sh} > 0$

$$S_{Sh} \to S_{vN}$$



from ca 1980
qubit

quantum information theory

qu. superpositions ➤ **no-cloning theorem** ➤ secure qkd

qu. correlations ➤ **non-locality** ➤ qu. computing

What is **quantum** in quantum thermodynamics?

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- Idea: consider a *quantum* information process
- Recall: Landauer’s thermodynamic analysis of a classical information process: “erasure” $\rho \to |0\rangle\langle 0|$.

Landauer 1961

What is **quantum** in quantum thermodynamics?

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- Recall: Landauer’s thermodynamic analysis of a classical information process: “erasure” $\rho \rightarrow |0\rangle\langle 0|$.

- Projections of quantum states (unselective measurements)

projection = state transfer $\rho \rightarrow \sum_k \hat{\Pi}_k \, \rho \, \hat{\Pi}_k =: \eta_O$

initial quantum state

projectors on energy eigenstates

quantum state after the process

Sci. Rep. 6, 22174 (2016)

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Sci. Rep. 6, 22174 (2016)

What is **quantum** in quantum thermodynamics?

Example: equal superposition of two energy eigenstates

$$|\psi\rangle = \frac{|e_0\rangle + |e_1\rangle}{\sqrt{2}} \quad \Rightarrow \quad \eta = \frac{1}{2}(|e_0\rangle\langle e_0| + |e_1\rangle\langle e_1|)$$

$$\rho = \begin{pmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{pmatrix} \qquad \eta = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix}$$

- Projections of quantum states (unselective measurements)

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Sci. Rep. 6, 22174 (2016)

What is **quantum** in quantum thermodynamics?

- Optimal implementation can extract maximal work

energy basis projection
$\Delta U = 0$

$$\langle W_{ext}^{max} \rangle = k_B T \left(S(\eta_H) - S(\rho) \right)$$

> 0
for initial states with coherences

- Projections of quantum states (unselective measurements)

projection = state transfer $\rho \to \sum_k \hat{\Pi}_k \, \rho \, \hat{\Pi}_k =: \eta_O$

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Sci. Rep. 6, 22174 (2016)

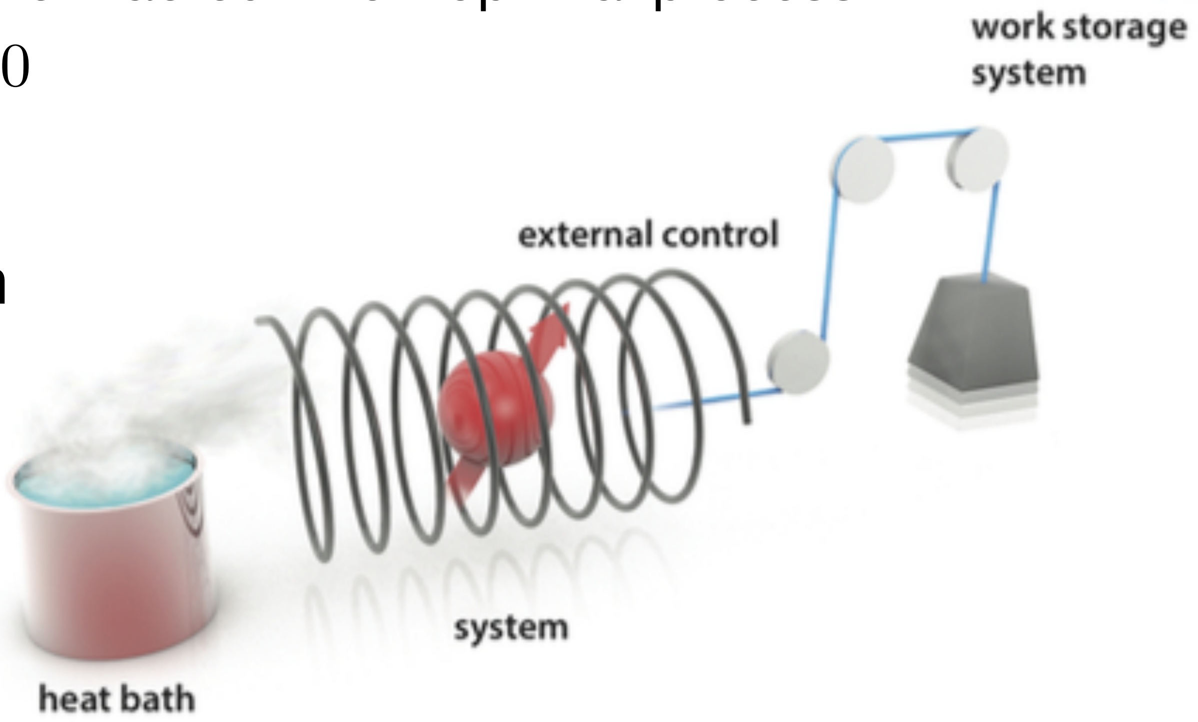
How to perform the optimal thermodyn. process?

- desired state transfer: $\rho \rightarrow \eta$

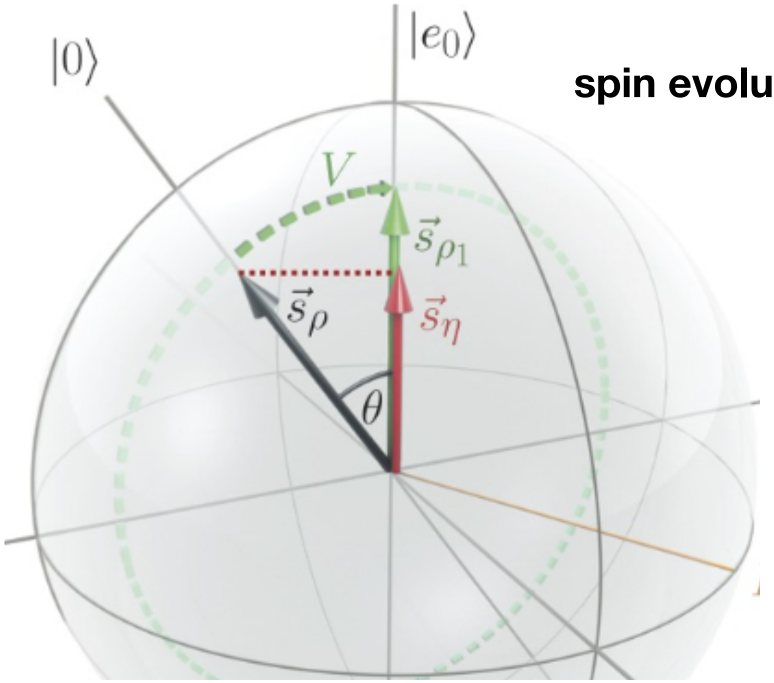
Decoherence:

- This state transfer is achieved by letting system interact with environment in an uncontrolled fashion for a long enough time.
- No work is extracted - non-optimal process. $\langle W_{\text{ext}} \rangle = 0$

- optimal implementation in thermodynamic setting?



Optimal work extraction from coherences



spin evolution

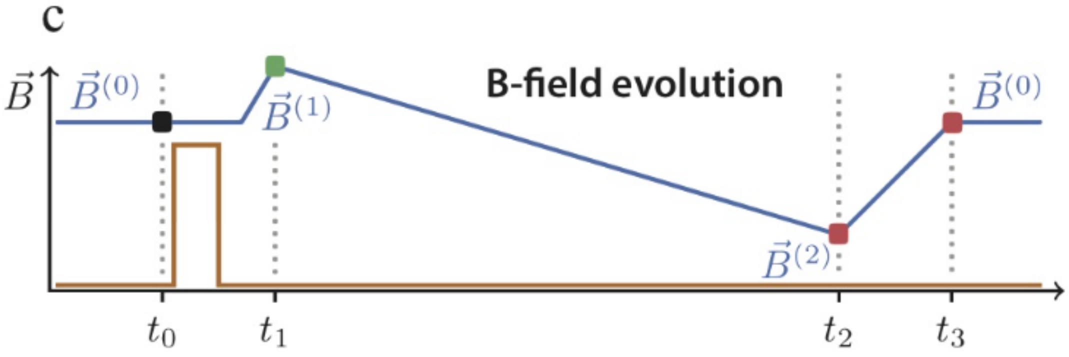
Qubit example $\sigma_z = |e_0\rangle\langle e_0| - |e_1\rangle\langle e_1|$

0) start with $(\rho, H = E\sigma_z)$

1) change B-field and evolve state unitarily ending in $(\rho_1 = V\,\rho\,V^\dagger, H_1 = E_1\sigma_z)$ such that this pair is thermal

2) connect system to bath, thermalise and quasi-statically decrease B-field to end in $(\rho_2 = \eta, H_2 = E_2\sigma_z)$ choosing H such that this pair is thermal

3) disconnect system from bath, then quench B-field to initial strength leading to (η, H)



B-field evolution

Optimal work extraction from coherences

equilibrium free energy

$$F(\rho) := U(\rho) - T\,S(\rho)$$

process isolated, energy change = work

$$\langle W^1_{ext} \rangle = -tr[\rho_1\, H_1 - \rho\, H]$$

isothermal, quasi-static process,
work = free energy change

$$\langle W^2_{ext} \rangle = -(F(\eta) - F(\rho_1))$$

process isolated, energy change = work

$$\langle W^3_{ext} \rangle = -tr[\eta\, H - \eta\, H_2]$$

sum of work contributions

$$\langle W_{ext} \rangle = k_B T\,(S(\eta) - S(\rho))$$

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Work from coherences

- a **quantum** system that has **coherences** (eg. in energy basis) can be brought into a state where these coherences have been removed - by realisable thermodynamic steps.
- no change of the energy expectation value has occurred $\Delta U = 0$
- but the quantum (vN) **entropy** of the state has been modified
$$S(\eta) \neq S(\rho)$$
- work is extracted from this **entropic** change
- So - work can be extracted from both: energy **populations** that are non-thermal (cl) and also from energetic **superpositions** (qu)
- the extracted work is done on the field and may be **measured**

Jarzynski, PRL (1997)
Qu: Talkner, Lutz, Hänggi PRE (2007)

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Tasaki (2000), Kurchan (2000), Mukamel (2003)

2M: Talkner, Lutz, Hänggi PRE (2007)

1M: Mazzola, DeChiara, Paternostro, PRL (2013)

Quantum Jarzynski equality

isolated system

V

thermal
initial state

$$\rho_0 = \frac{e^{-\beta H_0}}{Z_0}$$

$$H_0 = \sum_k E_k^0 \, \Pi_k^0$$

protocol = changing Hamiltonian H_t in specific way generates unitary

$$\rho_\tau = V \, \rho_0 \, V^\dagger$$

$$H_\tau = \sum_n E_n^\tau \, \Pi_n^\tau$$

final non-
equilibrium
state

- to establish a Jarzynski relation need to define fluctuating work W
- there is no observable (if there was, work would be a state variable)
- but one can measure the energy at **beginning** and **end**
- because evolution is unitary, there is no dissipation and energy change is entirely work
- fluctuating work is $W_{k,n} = E_n^\tau - E_k^0$ occurring with probability
- and exponentiated average is

same as classical

$$p_{k,n} = tr[\Pi_n^\tau \, V \, \Pi_k^0 \, \rho_0 \, \Pi_k^0 \, V^\dagger \Pi_n^\tau]$$

$$= \frac{e^{-\beta E_k^0}}{Z_0} \, tr[V \, \Pi_k^0 \, V^\dagger \Pi_n^\tau]$$

$$\langle e^{-\beta W} \rangle = \sum_{n,k} p_{k,n} \, e^{-\beta W_{k,n}} = \frac{Z_\tau}{Z_0} = e^{-\beta \Delta F}$$

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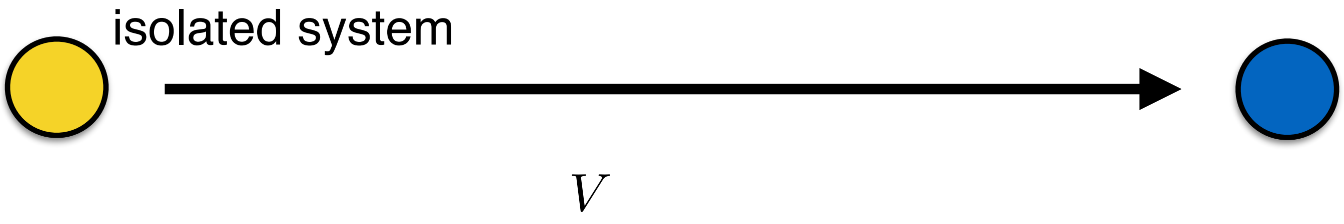
Quantum Jarzynski equality



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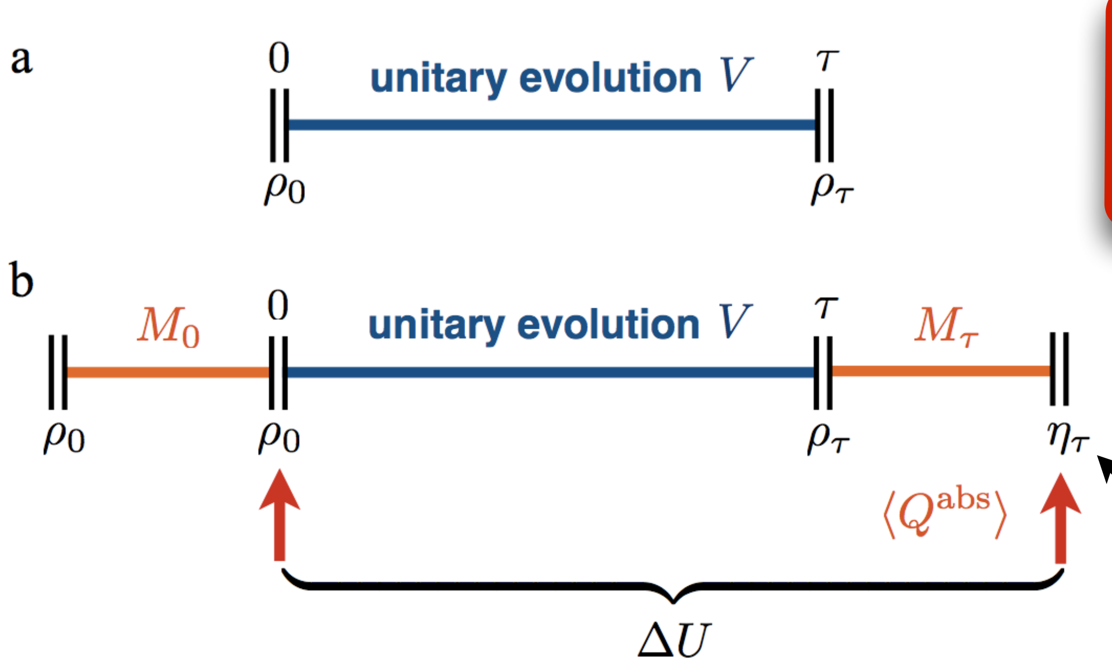

measurement changes entropy & makes process open

$$\langle Q^{opt}_{abs} \rangle > 0$$

projected state after measurement (average)

~~same as classical~~

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$$p_{k,n} = tr[\Pi^\tau_n \, V \, \Pi^0_k \, \rho_0 \, \Pi^0_k \, V^\dagger \Pi^\tau_n]$$

$$= \frac{e^{-\beta E^0_k}}{Z_0} \, tr[V \, \Pi^0_k \, V^\dagger \Pi^\tau_n]$$

$$\boxed{\langle e^{-\beta W} \rangle} = \sum_{n,k} p_{k,n} \, e^{-\beta W_{k,n}} = \frac{Z_\tau}{Z_0} = \boxed{e^{-\beta \Delta F}}$$

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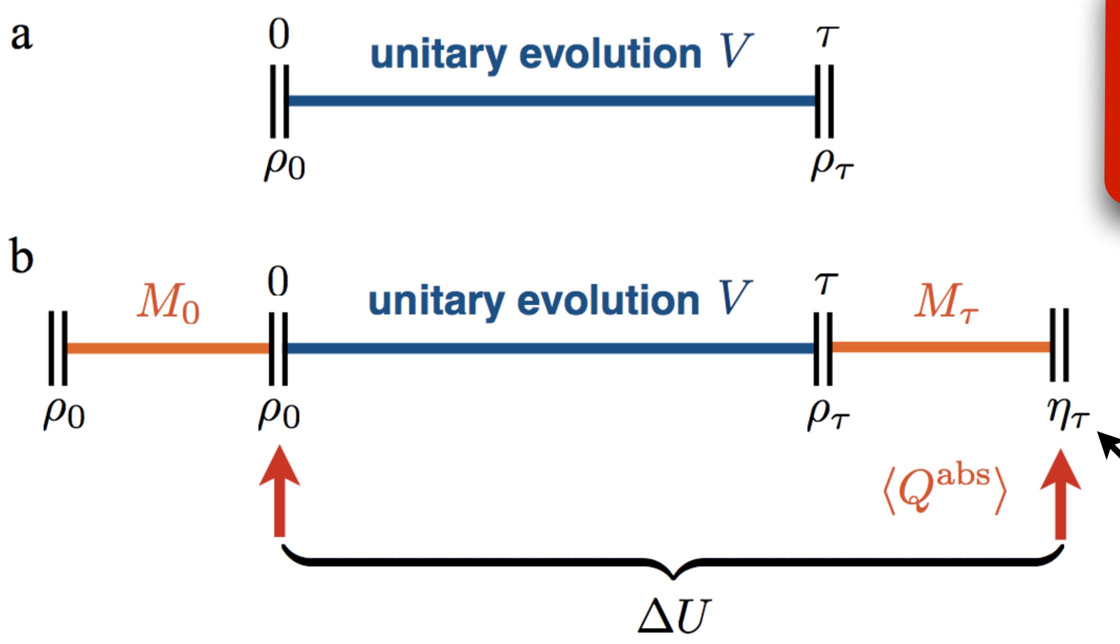

measurement changes entropy & makes process open

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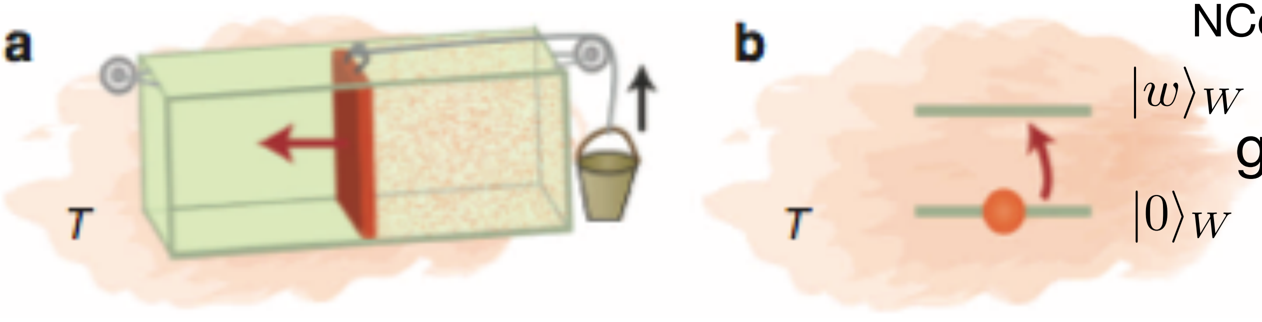
$$= \frac{e^{-\beta E^0_k}}{Z_0}\, tr[V\, \Pi^0_k\, V^\dagger \Pi^\tau_n]$$

$$\langle e^{-\beta\Delta E}\rangle = \sum_{n,k} p_{k,n}\, e^{-\beta W_{k,n}} = \frac{Z_\tau}{Z_0} = e^{-\beta\Delta F}$$

Resource theory: Single shot extractable work



Horodecki+Oppenheim
NComm (2013)

Aberg, Nature Comm.
4 1925 (2013)

Gemmer, Anders,
NJP **17**, 085006 (2015)

Global unitary on system, bath and work storage system

$$tr_{SB}[V\left(\rho_S\otimes\tau_B\otimes|0\rangle_W\langle 0|\right)V^\dagger]\approx|w\rangle_W\langle w|$$

ρ_S diagonal in energy
V commutes with global H

What is **maximum** w so that this outcome happens with probability $1-\epsilon$

single shot work	instead of **average work**
$w_\epsilon^{\max}\leq F_\epsilon^{\min}(\rho_S)-F(\tau_S)$	$\langle W\rangle\leq F(\rho_S)-F(\tau_S)$

Valid for running experiment on one system, but it is *not* the fluctuating work.

For many copies, $\rho_S\to\rho_S\otimes\rho_S\otimes\rho_S\dots$ this converges $w_\epsilon^{\max}\to\langle W\rangle$
for $\epsilon\to 0$

Quantum Thermo: Single shot extractable work

ρ_S **diagonal in energy**

single shot work

$$w_\epsilon^{\max} \leq F_\epsilon^{\min}(\rho_S) - F(\tau_S)$$

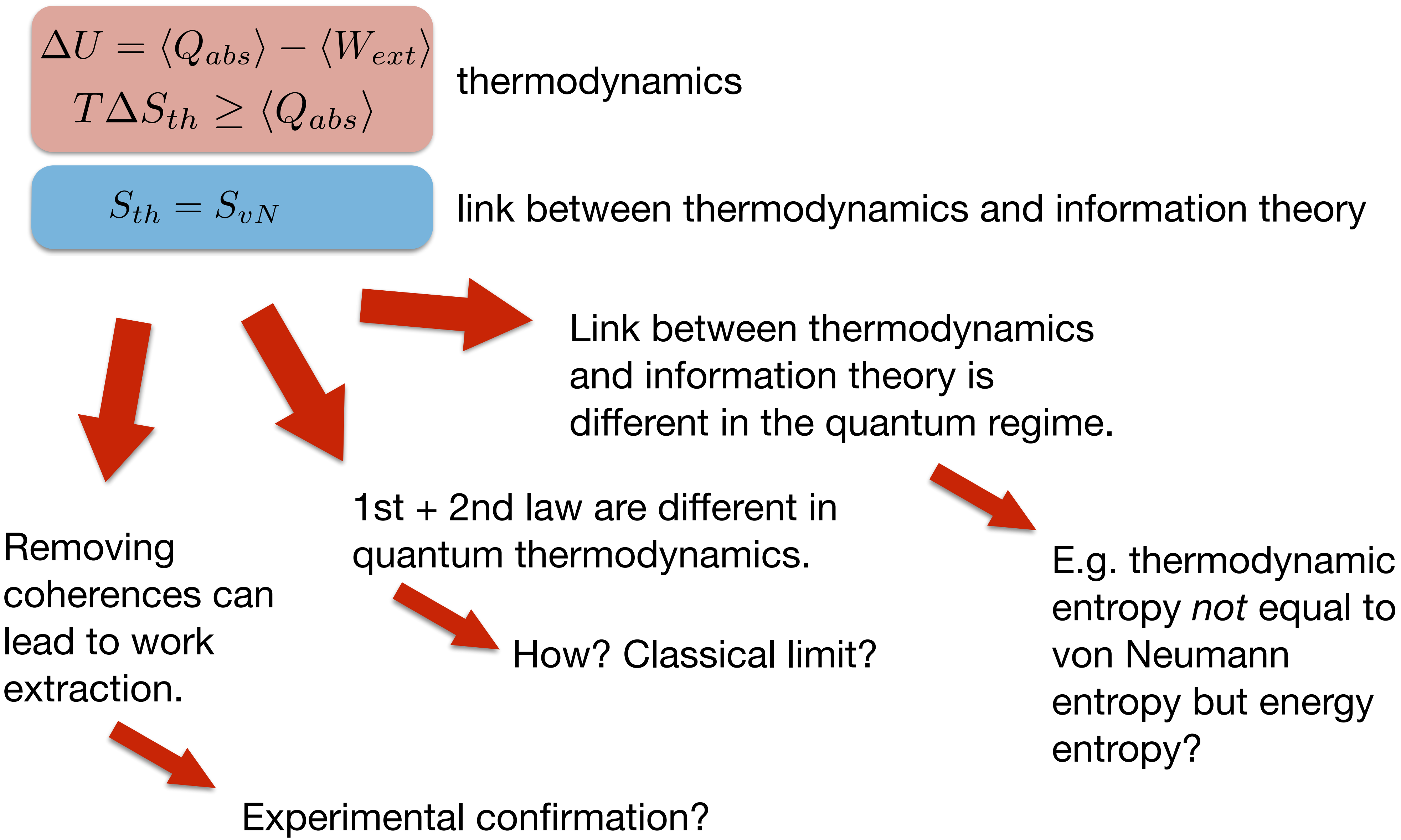
not the maximum?

ρ_S **not diagonal in energy**

Decohere first then extract work

in general $\langle W_{ext}^{opt} \rangle = k_B T \left(S(\eta) - S(\rho) \right)$

Implications



$$\Delta U = \langle Q_{abs} \rangle - \langle W_{ext} \rangle$$
$$T \Delta S_{th} \geq \langle Q_{abs} \rangle$$

thermodynamics

$$S_{th} = S_{vN}$$

link between thermodynamics and information theory

Link between thermodynamics and information theory is different in the quantum regime.

E.g. thermodynamic entropy *not* equal to von Neumann entropy but energy entropy?

1st + 2nd law are different in quantum thermodynamics.

How? Classical limit?

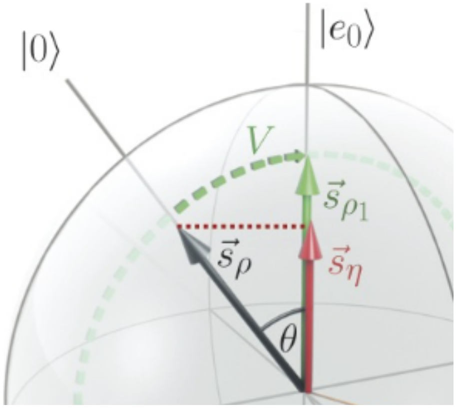
Removing coherences can lead to work extraction.

Experimental confirmation?

Summary: Work from coherences

Landauer found that the only information processing task that has an optimal non-trivial thermodynamic aspect is **erasure**.

Same result for classical and quantum information.

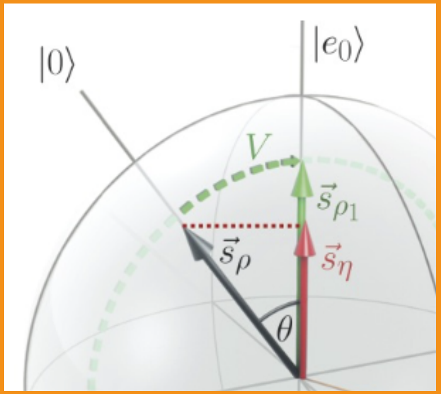


Scientific Reports 6:22174 (2016)

Projections are a second kind of information processing task with an associated work.

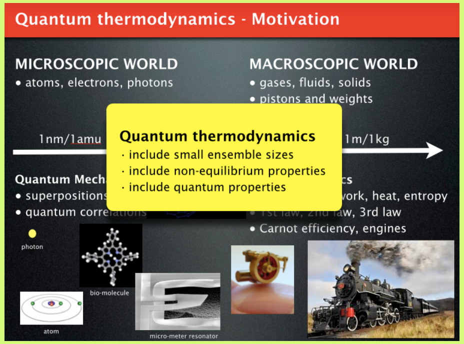
Work only from quantum states with **coherences.**

Coherence work can be important for analysis of thermodynamic **experiments** that involve measurement.



Work from Coherences
Sci. Rep. **6**, 22174 (2016)

Philipp Kammerlander
ETH Zurich



Quantum thermodynamics - Motivation

MICROSCOPIC WORLD
- atoms, electrons, photons

MACROSCOPIC WORLD
- gases, fluids, solids
- pistons and weights

1nm/1amu

Quantum thermodynamics
· include small ensemble sizes
· include non-equilibrium properties
· include quantum properties

1m/1kg

Quantum Mech
- superpositions
- quantum correlations

cs
- work, heat, entropy
- 1st law, 2nd law, 3rd law
- Carnot efficiency, engines

Quantum Thermodynamics
Contemporary Physics
57, 545 (2016)

Sai Vinjanampathy
IITB Bombai

Further reading:

Uzdin, et al, PRX **5**, 031044 (2015)

Solinas, et al, PRX **92**, 042150 (2015)

Klatzow, et al, PRL **122** 110601 (2019)

EPSRC
Engineering and Physical Sciences Research Council

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EUROPEAN COOPERATION IN SCIENCE AND TECHNOLOGY
MPNS COST Action MP1209
Thermodynamics in the quantum regime

Thank you!