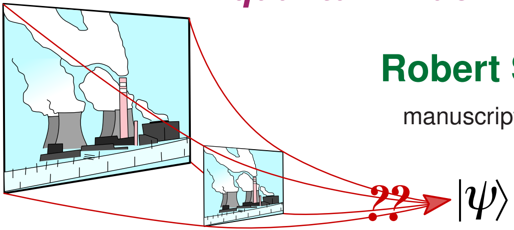
Laboratoire de Physique et Modélisation des Milieux Condensés
Univ. Grenoble Alpes & CNRS, Grenoble, France

Second law of thermodynamics for non-markovian quantum machines



Robert S. Whitney

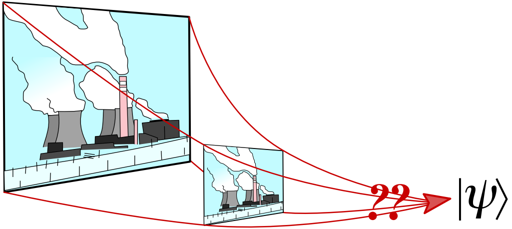
manuscript in preparation

New Trends in Quantum Heat and Thermoelectrics, Trieste — 23 Aug 2016

OVERVIEW

♣ Fluctuation theorems : *better than* 2nd law

♣ Quantum machine: *heat* $\Rightarrow$ *electrical power*



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- non-markovian = strong coupling to reservoirs
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  ... but non-interacting reservoirs
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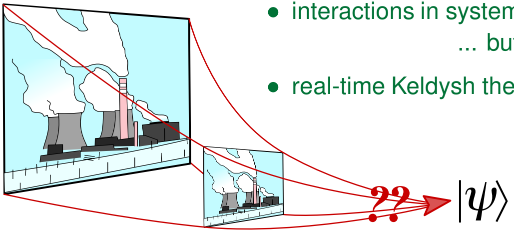

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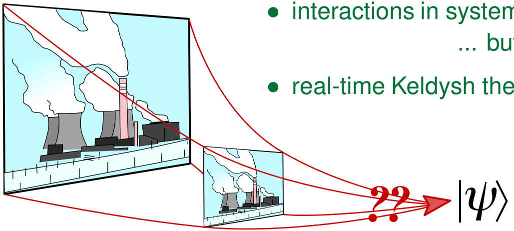


♣ Conclusion: $\mathit{Quantum}$ fluctuation theorems & 2nd law
= classical fluctuation theorems & 2nd law

CLASSICAL FLUCTUATION THEOREMS & 2nd LAW

Throw all bricks in air!

$$P_{\mathrm{good}} = \frac{\text{N}^\circ \text{ of “good” states}}{\text{Total N}^\circ \text{ states}}$$

Entropy:

$$S_{\mathrm{good}} = \ln \left[\text{N}^\circ \text{ of “good” states} \right]$$

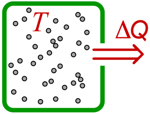
$$S_{\mathrm{bad}} = \ln \left[\text{N}^\circ \text{ of “bad” states} \right]$$

$$P_{\mathrm{bad}\to\mathrm{good}} = P_{\mathrm{good}\to\mathrm{bad}} \times \exp\left[-\Delta S_{\mathrm{good}\to\mathrm{bad}} \right]$$

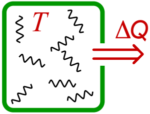
CLASSICAL FLUCTUATION THEOREMS & 2nd LAW

Seifert (2005)

electrons

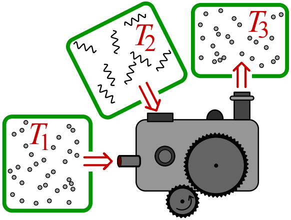


photons/phonons



Any large reservoir
at thermal equilibrium

$$\Delta S = \frac{\Delta Q}{k_{\rm B} T}$$



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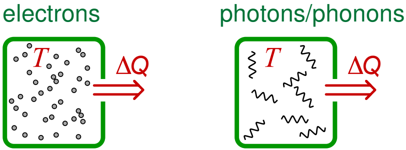

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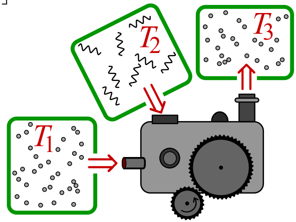
Fluctuation theorems:

- Under right conditions Evans-Searles (1994), Crooks (1998)

$$\overline{P}(-\Delta S) = P(\Delta S)\ \exp\left[\,-\Delta S\,\right]$$



$\Rightarrow$ 2nd law *on average* $\langle \Delta S \rangle \geq 0$

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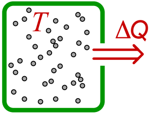

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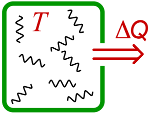

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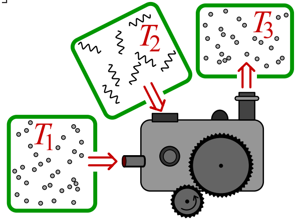
- Universal : Kawasaki (1967), Seifert (2005)

$$\left\langle \exp\left[\, -\, \Delta S \,\right] \right\rangle \; = \; 1$$

- Other relations: Jarzynski (1997), etc

$\Rightarrow$ 2nd law *on average* $\langle \Delta S \rangle \; \geq \; 0$



PROOF via CLASSICAL "STOCHASTIC TRAJECTORIES"

Proof of fluctuation theorem
& hence 2nd law

Reviews: Seifert (2012), van den Broeck (2013),
Benenti-Casati-Saito-Whitney (2016)

INGREDIENTS:

(i) a classical Markov rate equation (master equation)

$$\frac{\mathrm{d}}{\mathrm{d}t} P_b(t) \;=\; \sum_a \Big(\Gamma_{ba}\, P_a(t) \;-\; \Gamma_{ab}\, P_b(t) \Big)$$

where P_b = prob. system is in state b
& $\Gamma^{(i)}_{ba} =$ rate $a \to b$ due to reservoir i

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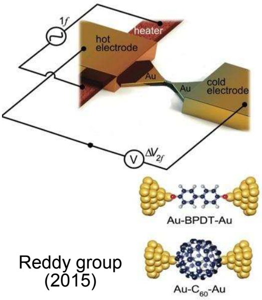
(ii) local detailled balance (microreversibility)

$$\Gamma^{(i)}_{ab} \;=\; \Gamma^{(i)}_{ba}\, \exp\Big[-\Delta S^{(i)}_{ba}\Big]$$

where $\Delta S^{(i)}_{ba}$ =entropy change in i
due to $a \to b$

EXAMPLES: EXISTING NANOSCALE MACHINES

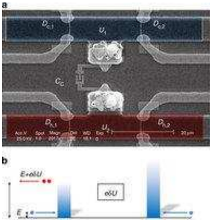
TWO reservoirs



Reddy group (2015)

THREE reservoirs 1 for heat & 2 for current

Glattli group (2015)



2 reservoir theory (& older expts) = Molenkamp group, Mahan-Sofo, Linke group

3 reservoir theory = Entin-Wohlmann et al, Sánchez & Büttiker

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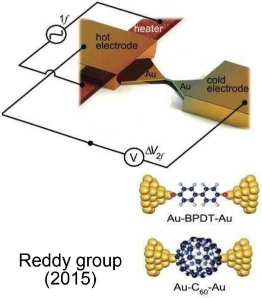

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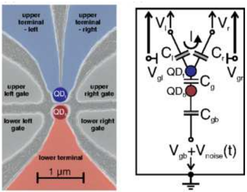

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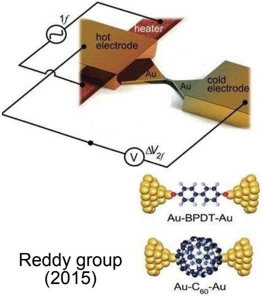

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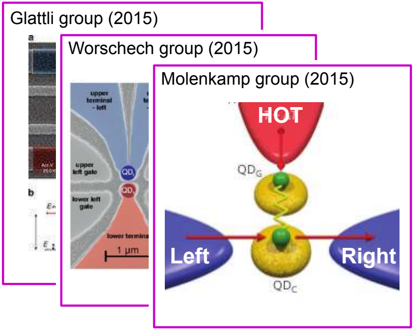

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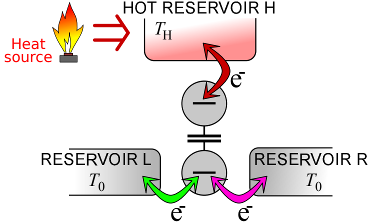
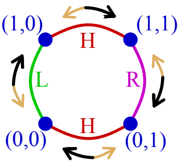
CLASSICAL (stochastic) TRAJECTORIES

Sanchez-Büttiker (2011)

Strasberg-Schaller-Brandes-Esposito (2013)





$$\left.\begin{array}{l}\text{Rate}(0 \to 1) \propto \text{Fermi} \\ \text{Rate}(1 \to 0) \propto 1 - \text{Fermi}\end{array}\right\} \Rightarrow$$

local detailed balance

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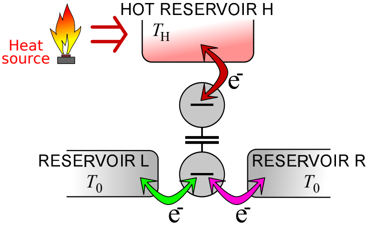
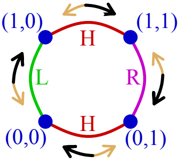
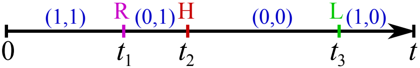




Evolution with time:

Trajectory ζ =



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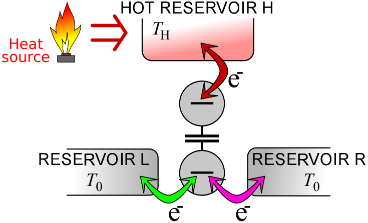
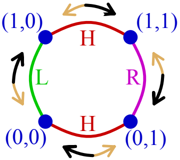
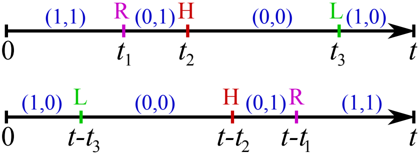




Evolution with time:

Trajectory ζ =

time-reverse $\bar{\zeta}$ =



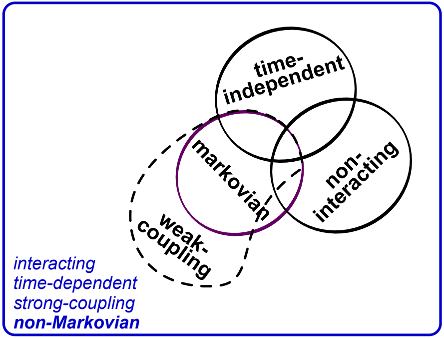
Prob. of $\bar{\zeta}$ = (Prob. of ζ) $\times$ exp $\left[-\Delta S_{\mathrm{res}}(\zeta) \right]$ $\Rightarrow$ Fluctation theorem

completely *quantum*

SUPERPOSITIONS, ENTANGLEMENT, etc

& GENERAL : strong-coupling, time-dependence, etc

PREVIOUS PROOFS OF 2nd LAW FOR QUANTUM MACHINES



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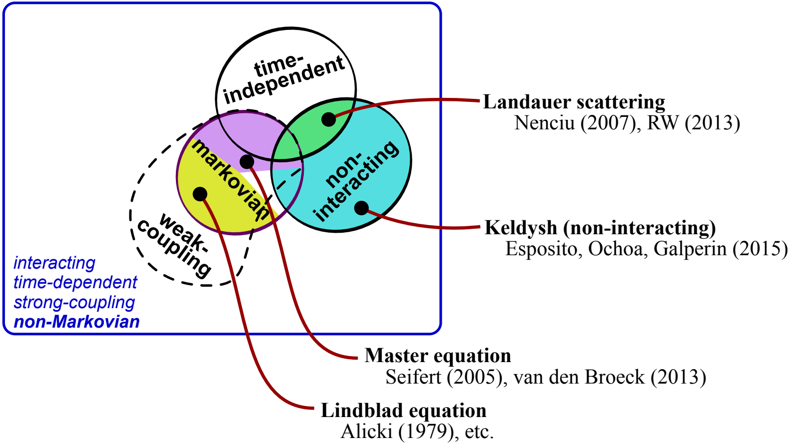

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REAL-TIME KELDYSH APPROACH

quantum + non-markov + interactions + far from equilibrium

Schoeller-Schön (1994)

♣ big simplifications:

- interactions in system but NOT in reservoirs

  $\Longrightarrow$ many-body eigenbasis for system

  $\Longrightarrow$ free-particle eigenbasis for reservoirs

- infinite N° of reservoir modes k

  $\Longrightarrow$ coupling to lowest (2nd) order for each k

Example Hamiltonian:

$$\hat{\mathcal{H}} = \underbrace{\hat{\mathcal{H}}_{\rm sys}\left(\hat{d}_n^\dagger, \hat{d}_n\right)}_{\text{interacting system}} + \sum_k V_{n,k} \underbrace{\left(\hat{d}_n^\dagger \hat{c}_k + \hat{d}_n \hat{c}_k^\dagger\right)}_{\text{coupling}} + \underbrace{\sum_k E_k \hat{c}_k^\dagger \hat{c}_k}_{\text{electron reservoirs}}$$

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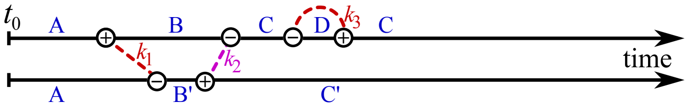

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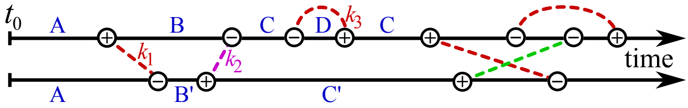
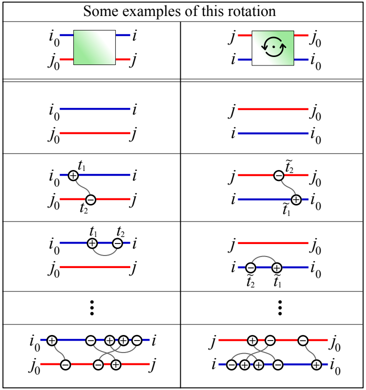


ENTROPY CHANGE IN RESERVOIRS (rotating double-paths)



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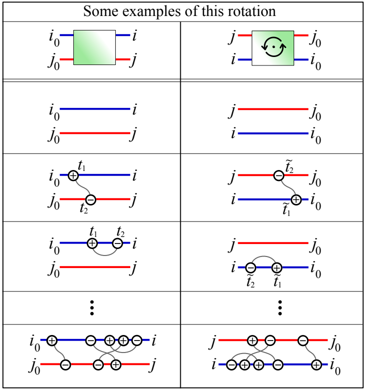

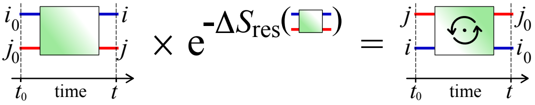

ENTROPY CHANGE IN RESERVOIRS (rotating double-paths)

- *Initial* system density-matrix

$$\hat{\rho}_{\rm sys}(t_0) = \hat{\mathcal{W}}_0\, \hat{\mathbf{p}}^{(0)}\, \hat{\mathcal{W}}_0^\dagger \quad \Leftarrow \text{diagonal } \hat{\mathbf{p}}^{(0)}$$

- *Final* (reduced) system density-matrix

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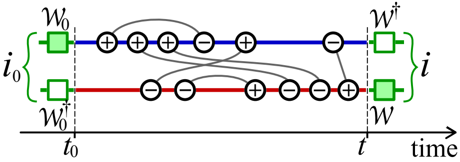
$$\hat{\rho}_{\rm sys}(t) = \hat{\mathcal{W}}\, \hat{\mathbf{p}}\, \hat{\mathcal{W}}^\dagger \qquad \Leftarrow \text{diagonal } \hat{\mathbf{p}}$$

Define "probability-weight" of double path, ζ,
from state i_0 of $\hat{\mathbf{p}}^{(0)}$ to state i of $\hat{\mathbf{p}}$

$P(\zeta) =$  + Complex Conj.

Result : $\overline{P}(\overline{\zeta}) = P(\zeta) \times \exp\left[-\Delta S_{\rm reservoirs}(\zeta)\right]$

ENTROPY CHANGE IN SYSTEM

$$\Delta S_{\rm sys} \;=\; S_{\rm sys}(t) \;-\; S_{\rm sys}(t_0)$$

with von Neumann

$$S_{\rm sys}(\tau) = {\rm Tr}\Big[\hat{\rho}_{\rm sys}(\tau)\ln\Big(\hat{\rho}_{\rm sys}(\tau)\Big)\Big]$$

Seifert (2005) $\Rightarrow$ **QUANTUM**

Assign entropy to *each* state in diagonal basis
of system's (reduced) density matrix, $\hat{\rho}_{\rm sys}$,
at beginning (t_0) and end (t)

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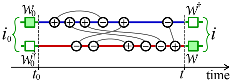
$$\Delta S_{\rm sys}^{i_0 \to i} = p_i \ln p_i - p_{i_0}^{(0)} \ln p_{i_0}^{(0)}$$

where $p_{i_0}^{(0)}$ is prob. initial state is i_0 in diag. basis of $\hat{\rho}_{\rm sys}(t_0)$
& p_i is prob. final state is i in diag. basis of $\hat{\rho}_{\rm sys}(t)$

QUANTUM FLUCTUATION THEOREM



quantizing Seifert

DEFINE $\Delta S_{\text{total}}^{i_0 \to i} = \Delta S_{\text{res}}^{i_0 \to i} + \Delta S_{\text{sys}}^{i_0 \to i}$

+ some algebra

$\Longrightarrow$ *ALL CLASSICAL FLUCTUATION THEOREMS*

Crook's, Jarzynski, Kawasaki, etc

$\Longrightarrow$ 2nd LAW

♣ neglected entropy of entanglement between system & reservoirs

PROOF or just RECIPE ??

WHY assume we can NEGLECT:

- ♣ Entropy of entanglement between system & reservoirs
- ♣ Non-zero *off-diagonal* trajectories

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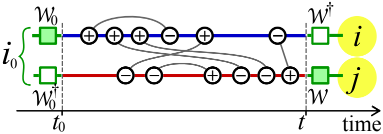

has *no* time-reverse for $j \neq i$

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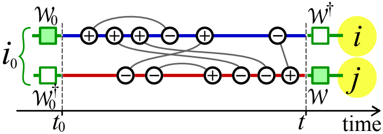

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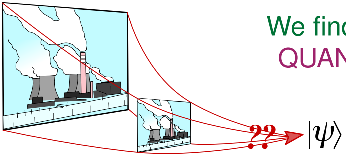
ASSUMPTIONS seem reasonable
if **no** *Maxwell demons*

i.e. assume cannot use knowledge
of *microscopic* state of reservoir
to get *extra work* from system

CONCLUSIONS

warning: work only just finished



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QUANTUM FLUCTUATION THEOREMS

for *arbitrary* quantum machine

interacting, NON-MARKOVIAN,
time dependent, etc

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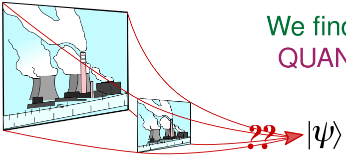

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$\Rightarrow$ proof of 2 nd LAW

CONCLUSIONS

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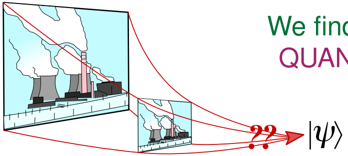

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time dependent, etc

... *identical* to CLASSICAL FLUCTUATION THEOREMS

$\Rightarrow$ proof of 2nd LAW

Assumption: **no** Maxwell demons

for specific definition of “Maxwell demon”