Title: On the logical complexity of tiny heat engines -- and whether they can really be reversible

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Abstract: I consider systems that consist of a few hot and a few cold two-level systems and define heat engines as unitaries that extract energy. These unitaries perform logical operations whose complexity depends on both the desired efficiency and the temperature quotient. I show cases where the optimal heat engine solves a hard computational task (e.g. an NP-hard problem) [2]. Heat engines can also drive refrigerators and use the temperature difference between two systems for cooling a third one. I argue that these triples of systems define a classification of thermodynamic resources [1]. All the above assumes that unitaries are implemented by an external controller. To get a thermodynamically reversible process, the joint process on system and controller must be reversible. Then, the implementation of the joint process requires a "meta-controller", and so on. To study thermodynamic limits without such an infinite sequence of controllers, I introduce the model of "physically universal cellular automata", in which the boundary between system and controller can be shifted (in analogy to the Heisenberg-cut for the quantum measurement problem). I show that this model raises a lot of fundamental questions [3]. Literature: [1] Janzing et al: Thermodynamic cost of reliability and low temperatures: Tightening Landauer's principle and the second law, J. Stat. Phys. 2000 [2] Janzing: On the computation power of molecular heat engines, J. Stat. Phys. 2006 [3] Janzing: Is there a physically universal cellular automaton or Hamiltonian? arXiv:1009.1720

On the logical complexity of tiny heat engines – and whether they can really be reversible

Dominik Janzing

MPI for Intelligent Systems, Tübingen, Germany

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- definitely about thermodynamics
- don't consider quantum superpositions
- "quantum" only in the sense of discrete energy levels

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Why I started to think about quantum heat engines in 1999...

- to understand thermodynamics – I found two qubits easier to understand than steam engines.

- to teach thermodynamics to students of computer science

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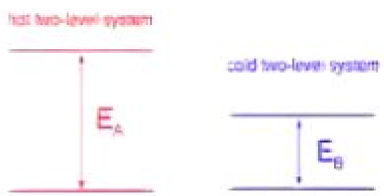

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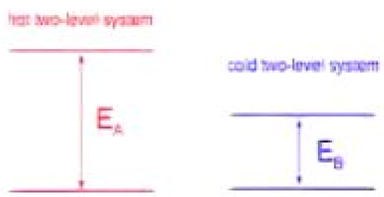

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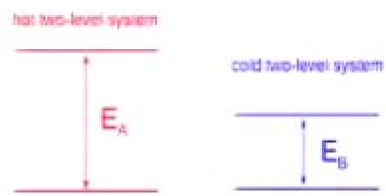

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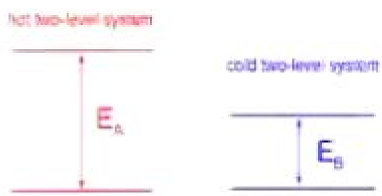

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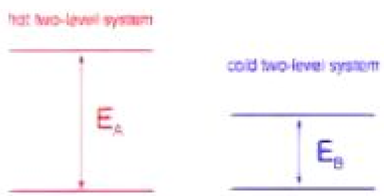

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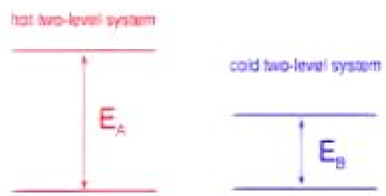

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This talk

- is far from applications
- like a game that teaches thermodynamics
- game with simple rules, but challenging questions

Unitary work extraction

(Allahverdyan, Balian, Nieuwenhuizen 2004)

Given a quantum system with state ρ and Hamiltonian H

- unitary U extracts the work

$$\Delta W := \mathrm{tr}(\rho H) - \mathrm{tr}(U\rho U^\dagger H)\,.$$

- U is optimal if is maximizes ΔW

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Passive systems and Gibbs equilibrium

(Lenard 1978)

- ρ is called **passive** if no unitary can extract energy ($\Leftrightarrow$ ρ diagonal in the energy basis and eigenvalues are ordered according to the energy)

- ρ is called **completely passive** iff $\rho^{\otimes n}$ is passive for all $n \in \mathbb{N}$ ($\Leftrightarrow$ ρ is a Gibbs state to some temperature $T \in [0, \infty]$)

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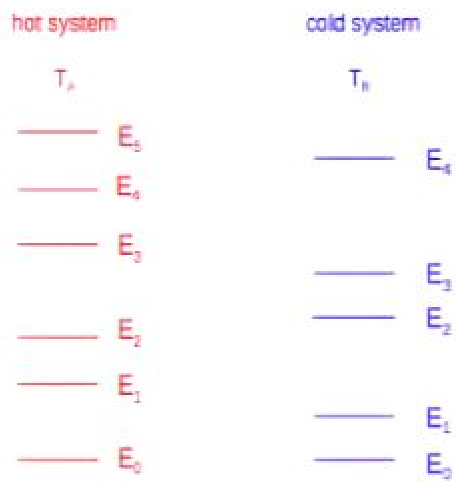
Toy Model of Molecular Heat Engine

quantum systems as hot and cold reservoirs



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- optimal heat engine: unitary that maximizes ΔW

(many quantum heat engines have been constructed meanwhile, I focus on the relation to computation)

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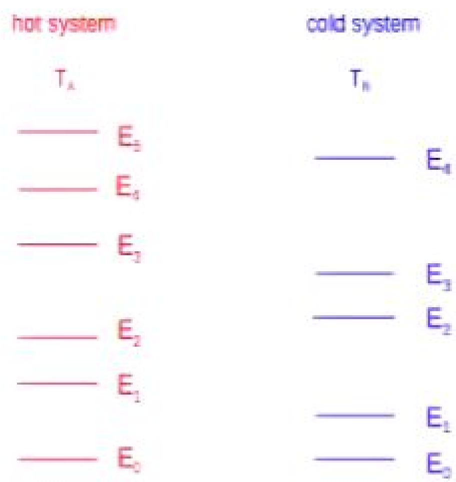

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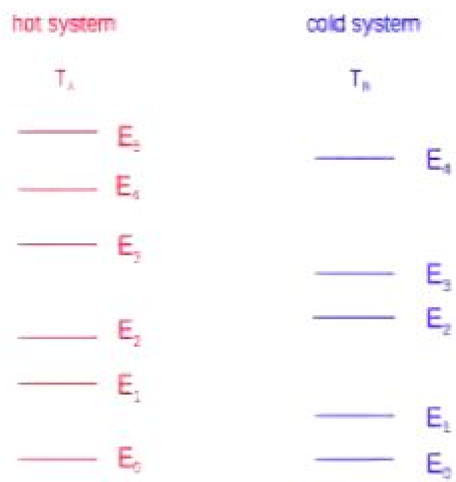

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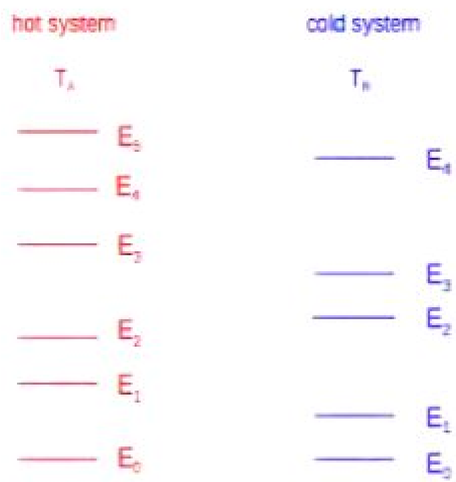

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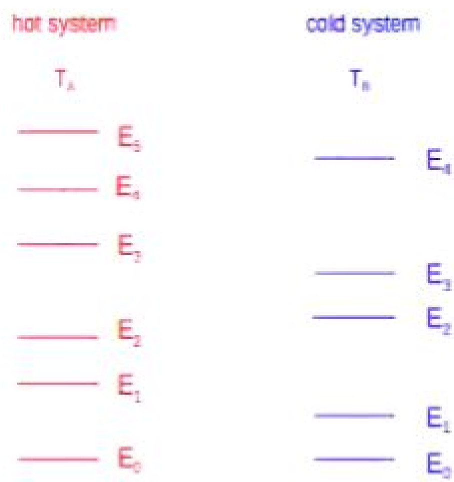

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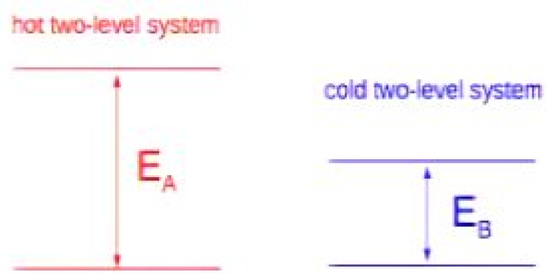
Simplest Heat Engine: SWAP gate

Two 2-level systems with energy gaps $E_B < E_A < E_B \frac{T_A}{T_B}$.



- $|10\rangle$ more likely than $|01\rangle$ although its energy is larger.
- $|01\rangle \leftrightarrow |10\rangle$ releases the energy $(p_{10} - p_{01})(E_A - E_B)$.
- **SWAP gate is the unique optimal heat engine.**

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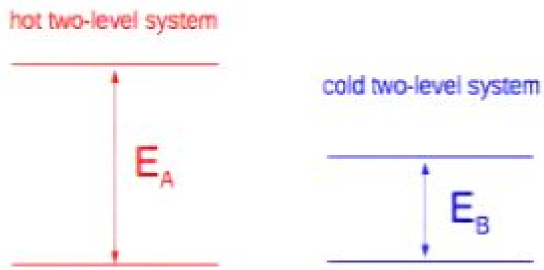

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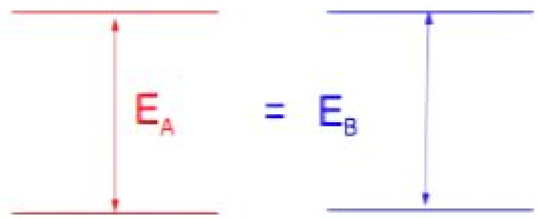
This already shows...

whether or not a heat engine exists depends on

- the energy level structure of both systems
- their temperature ratio

Two qubits with equal energy gap



- no enery release – SWAP permutes states with equal energy
- state of the joint system is passive
- not completely passive because the joint state is not Gibbs ($\Rightarrow$ many copies of this pair allow for a heat engine)

Qubits with equal energy gaps

require more complex gates

Simplest example:

- 2 hot and 1 cold qubit with $T_A > 2T_B$.
- $|110\rangle$ more likely than $|001\rangle$ although its energy is larger.
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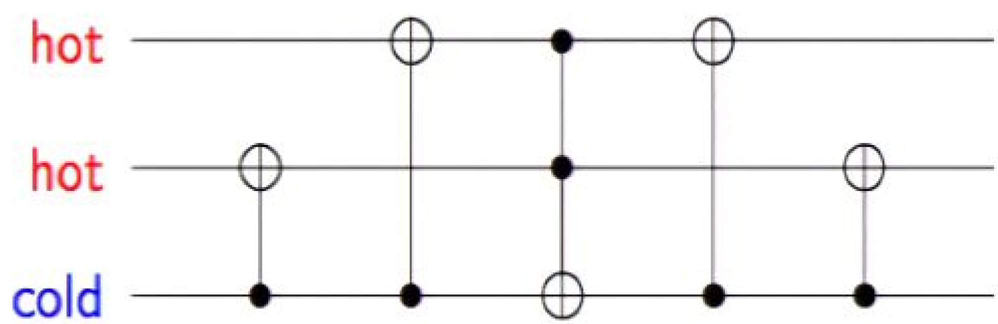
Implemented by



(Note: for $T_A = T_B$ the circuit is a refrigerator)

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(Janzing, 2006)

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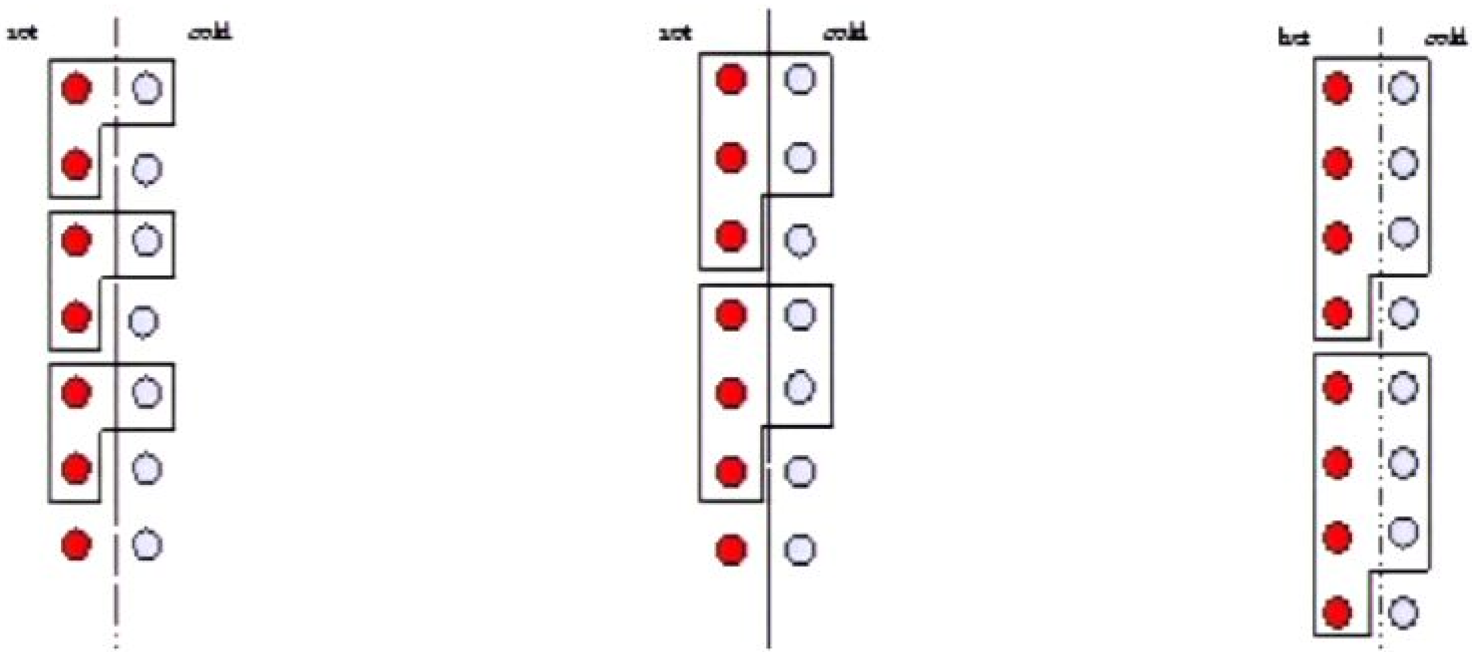

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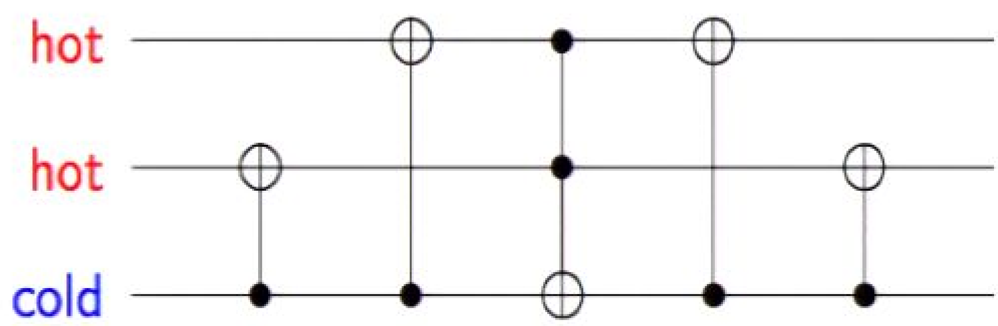

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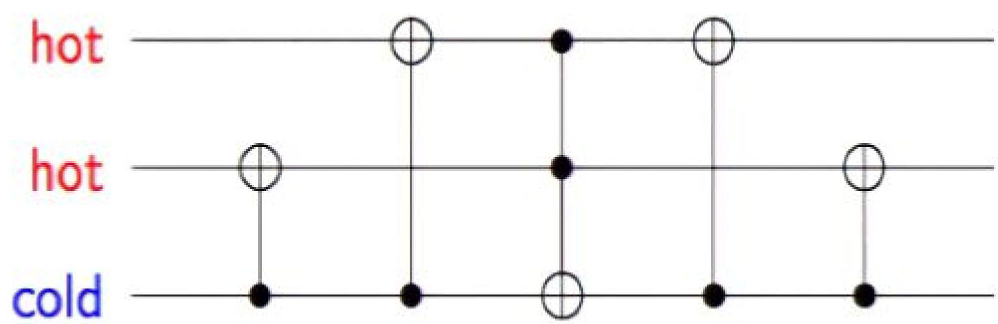

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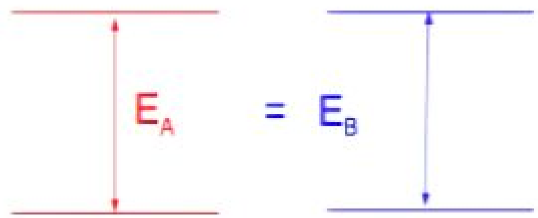

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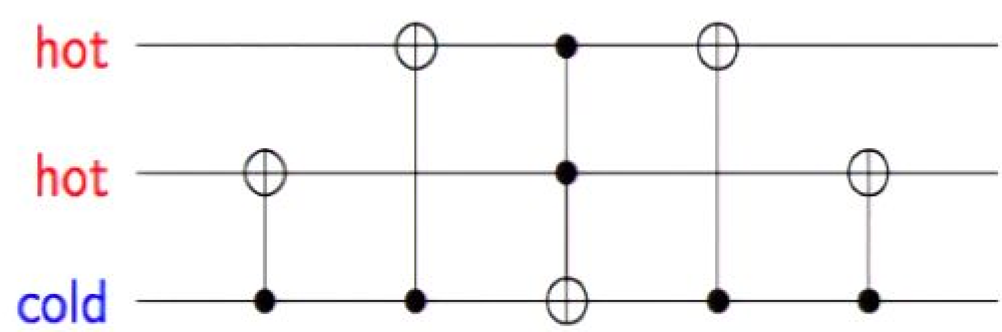

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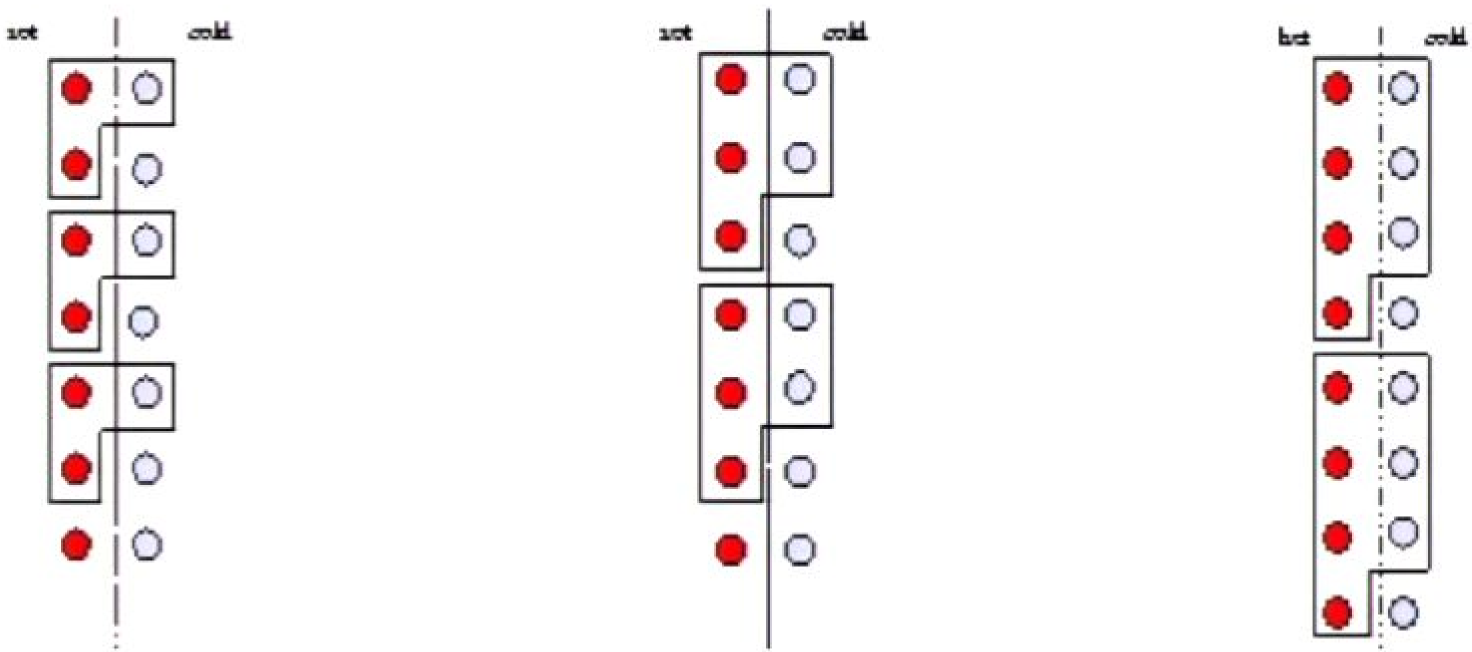

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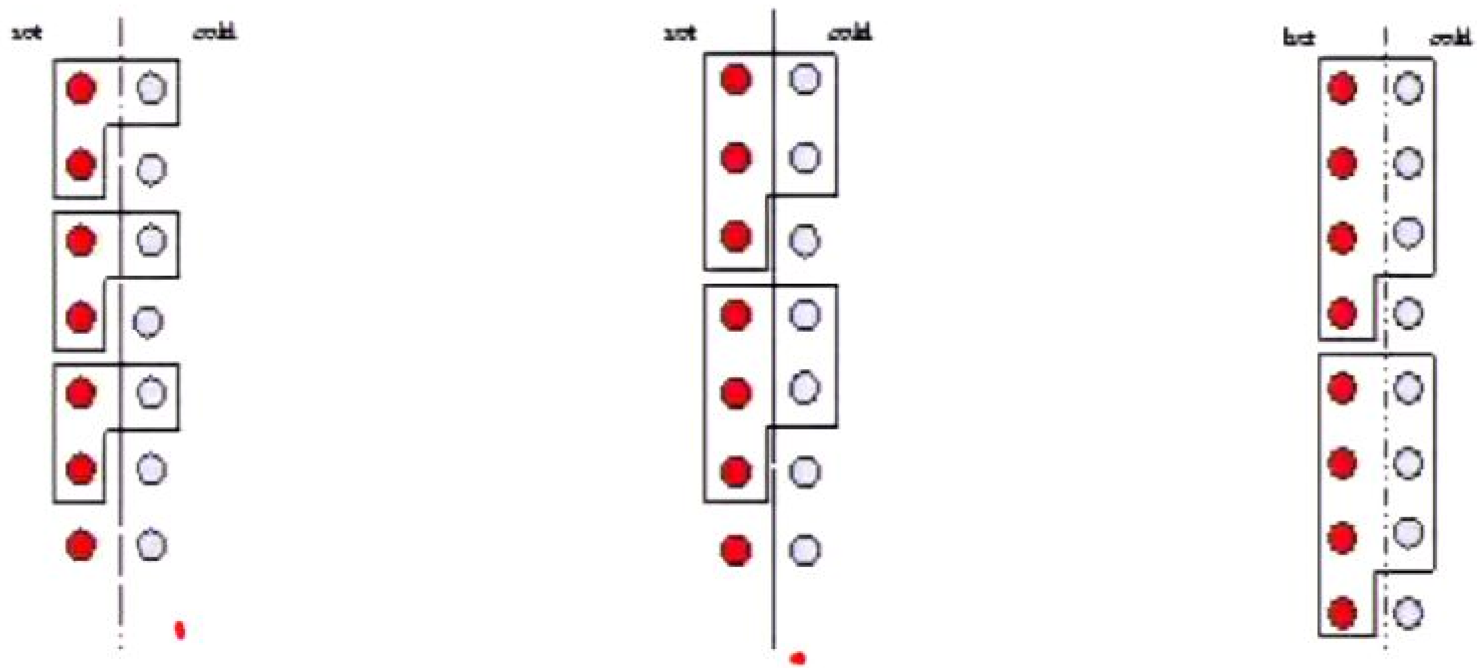

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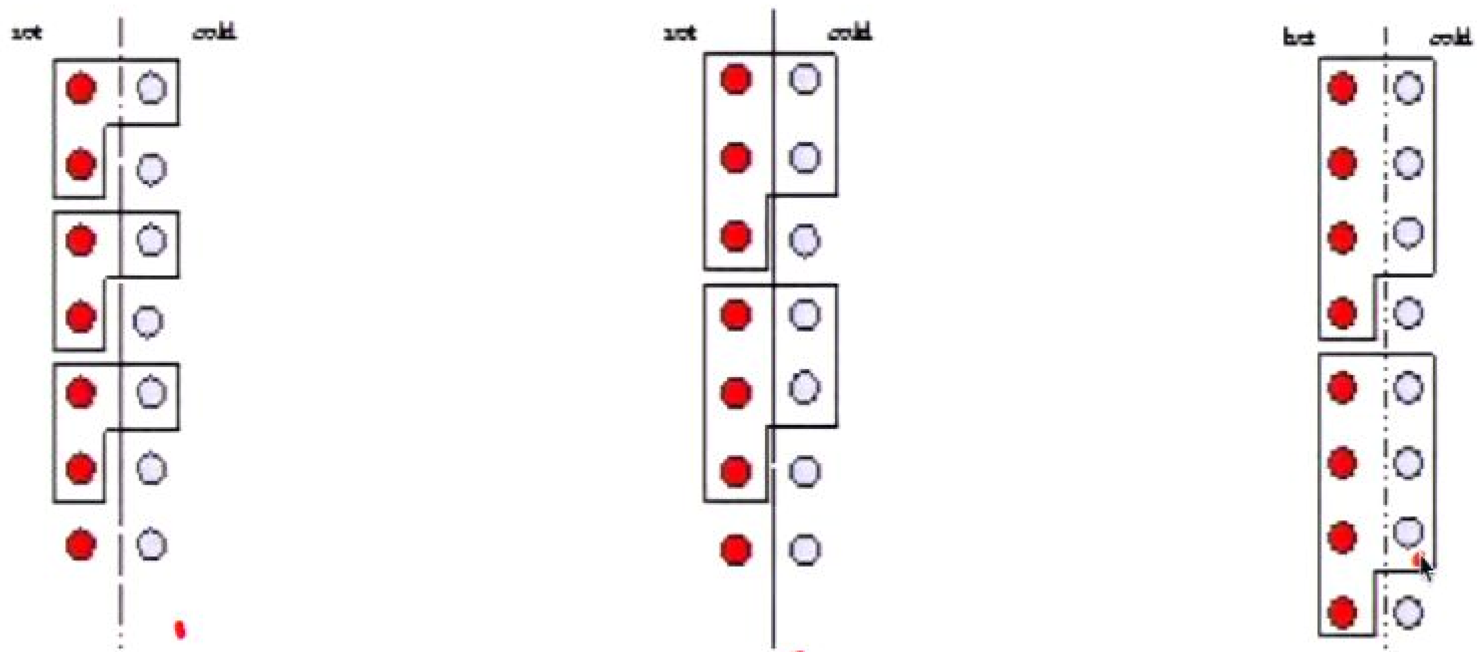
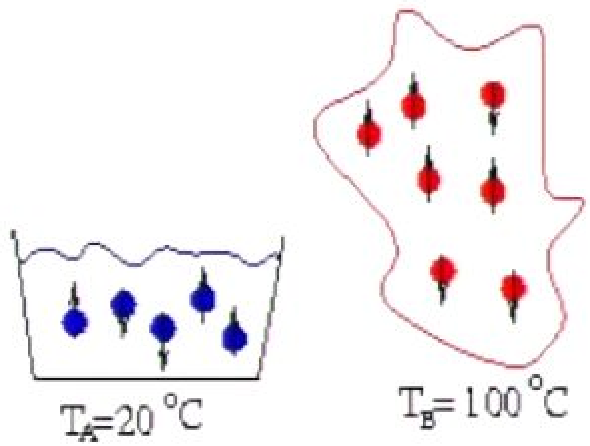
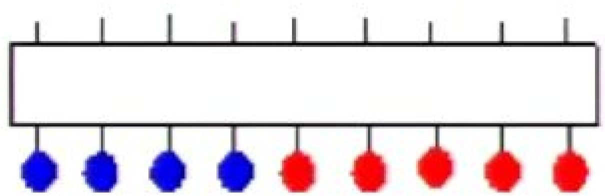


Example:

$T_A := 100^o\ C$ (vapor)
$T_B := 20^o\ C$ (room temperature)



requires 9-Qubit gate (4 cold and 5 hot qubits).



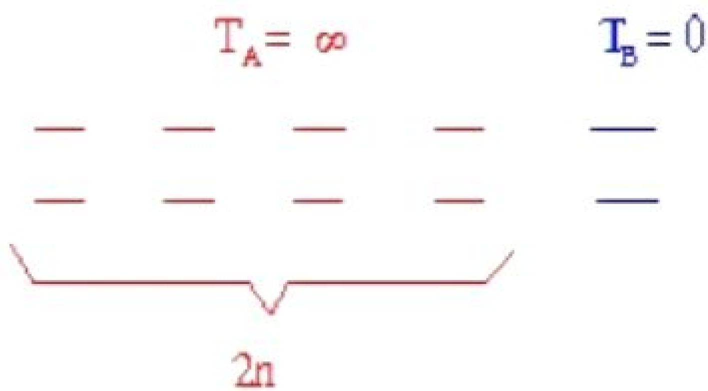
Heat engines are non-trivial multi-qubit gates –

what's their computational power?

(SWAP is not too exciting as a logical gate)

Heat Engine whose inverse computes

Given $2n$ hot and 1 cold qubits:



- optimal U maps all words with suffix 0 to words with Hamming weight at most n
- Hence, U^{-1} computes MAJORITY
- logical depth of U is at least $\log_2(2n+1)$.

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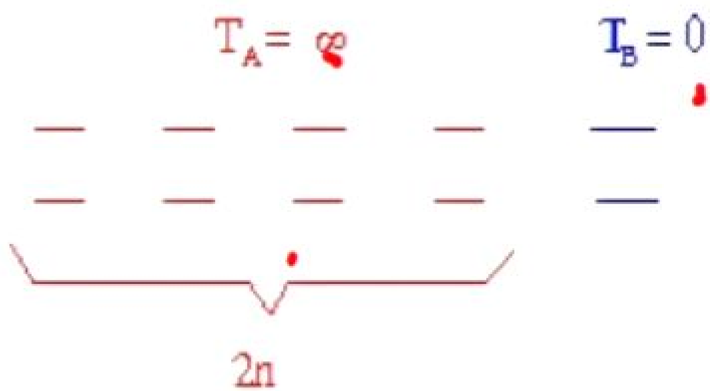

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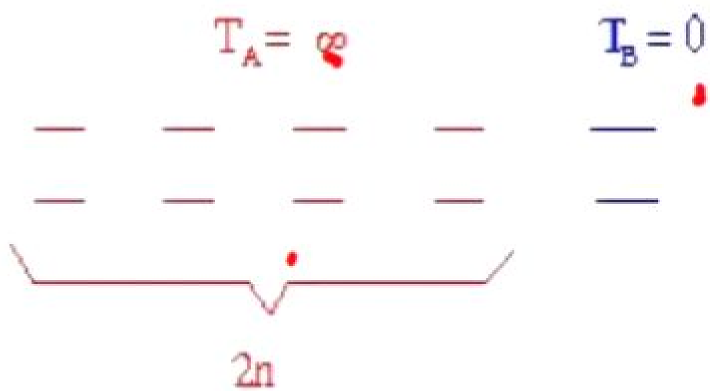

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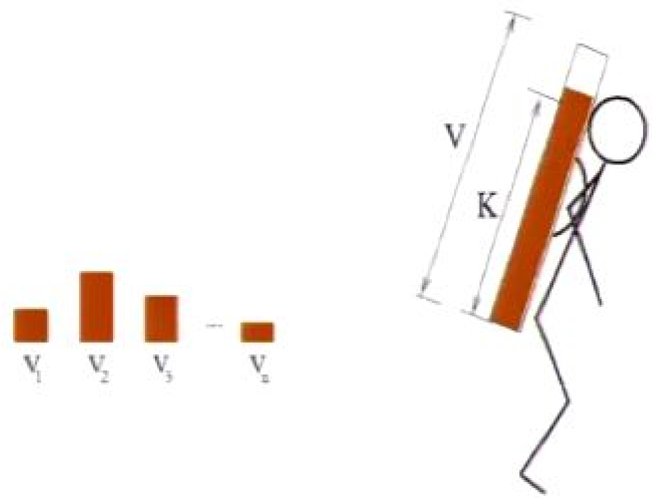
which hard computational problems

can be solved by heat engines?

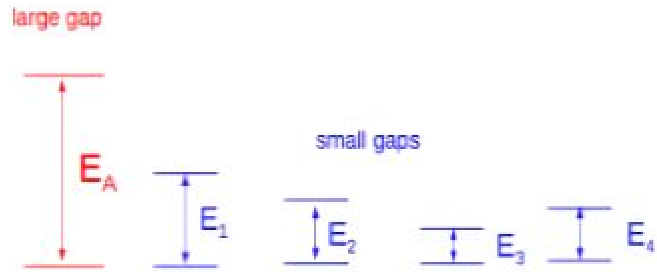
NP-complete problem KNAPSACK

Special instance (still NP-hard, see Papadimitrou: Computational Complexity):

- Given n items with volumes $V_1, \ldots, V_n$.
- Given a knapsack with volume V
- Given some $K \leq V$, is there a subset of items whose total volume is at least K?



Optimal heat engine solves KNAPSACK



- volume of knapsack $= E_A$, volumes of items $= E_1, \ldots, E_n$
- $K = \frac{T_B}{T_A} E_A$
- heat engine exists iff there is a subset S such that

$$E_A > \sum_{j \in S} E_j > K \, .$$

- if the answer is "yes", the heat engine finds the proof:

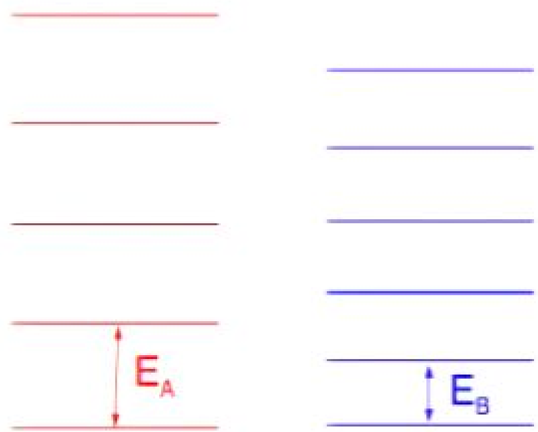
$$U(|1\rangle \otimes |0 \cdots 0\rangle) \in |0\rangle \otimes \mathcal{H}_s \, ,$$

where $\mathcal{H}_s$ is the space of solutions.

admittedly, this example was a bit artificial

let's go back to more physical systems...

Optimal heat engine on two harmonic oscillators



Assume

$$\frac{E_A}{E_B} \notin \mathbb{Q} \quad \text{and} \quad \frac{T_A/E_A}{T_B/E_B} \notin \mathbb{Q}$$

such that joint density operator and joint Hamiltonian are non-degenerate.

$\Rightarrow$ Optimal heat engine is a unique permutation of basis states, i.e., permutation on $\mathbb{N}_0 \times \mathbb{N}_0$

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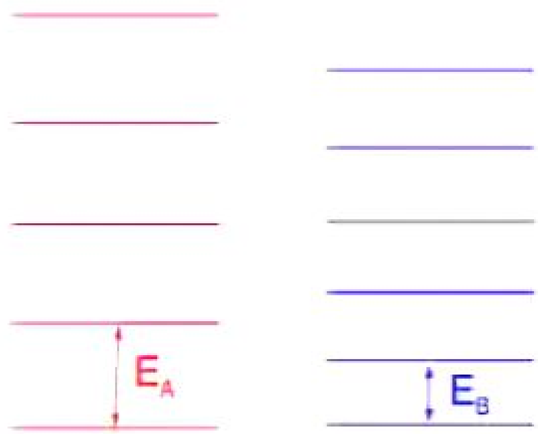

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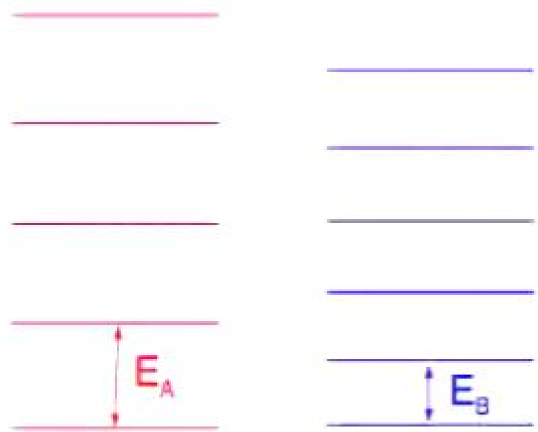

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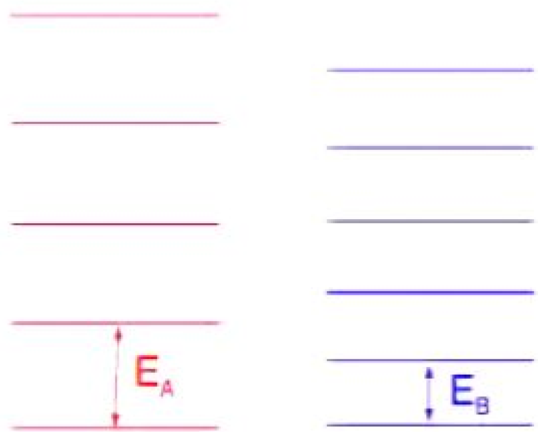

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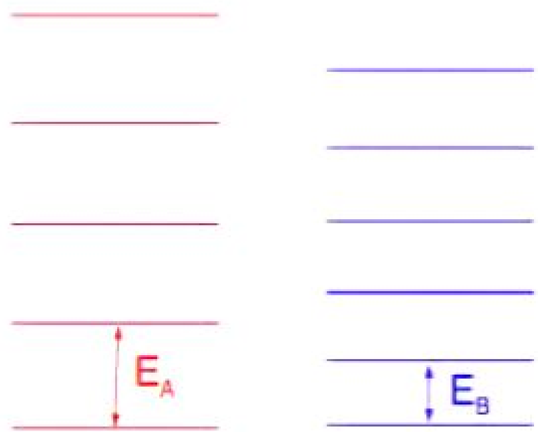

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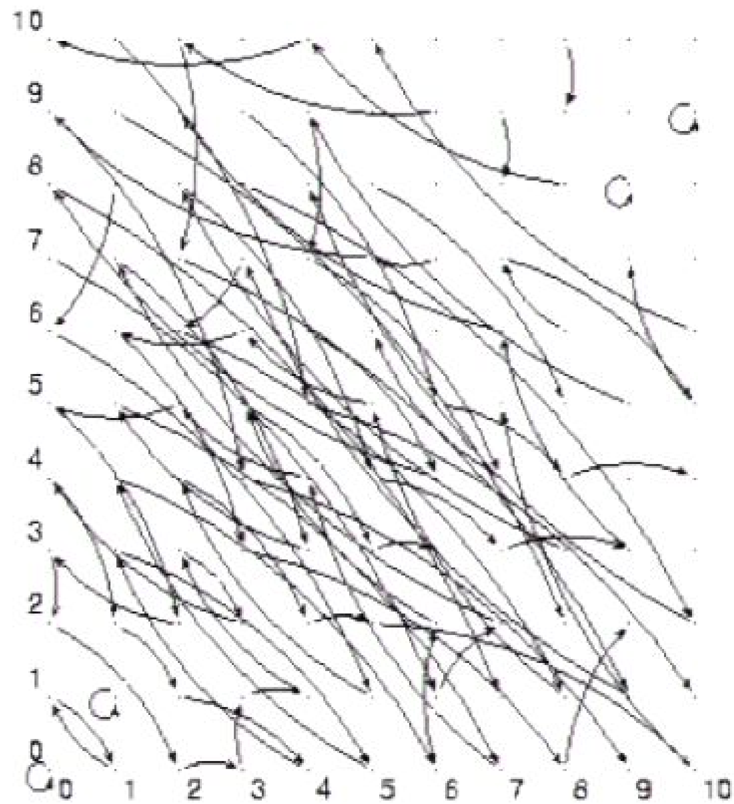
Example with $E_A/E_B = \sqrt{2}$ and $T_B/T_A = E_B/(\sqrt{3}E_A)$



rather complex map on $\mathbb{N}_0 \times \mathbb{N}_0$

Example with $E_A/E_B = \sqrt{2}$ and $T_B/$

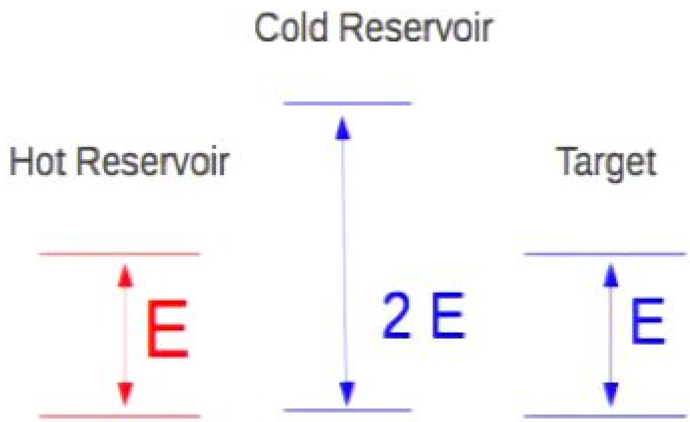
Our toy heat engines show that...

- having different temperatures is necessary for work extraction (derive and "feel" second law from first principles)
- ...but not sufficient (additional constraints for micro-systems)
- more thermodynamic laws for micro-physics yet to be discovered

What was missing...

how can we use the extracted energy?

Using heat for cooling: "quantum absorption heat pump"



- permutation $|010\rangle \leftrightarrow |101\rangle$ reduces temperature of system 3
- implementation does not require energy because it acts on a degenerate subspace
- temperature difference between hot and cold reservoir is used for cooling the target

this inspired a new framework

for thermodynamics at the nanoscale...

Idea (Janzing et al, 2000)

- Assume the whole world is full of quantum systems with uniform temperature T
- except for a few systems called "resources" (resources can be hotter or colder or be in a non-Gibbs state)
- "processes" can transform resources into other resources
- processes are unitaries that commute with the uncoupled joint Hamiltonian

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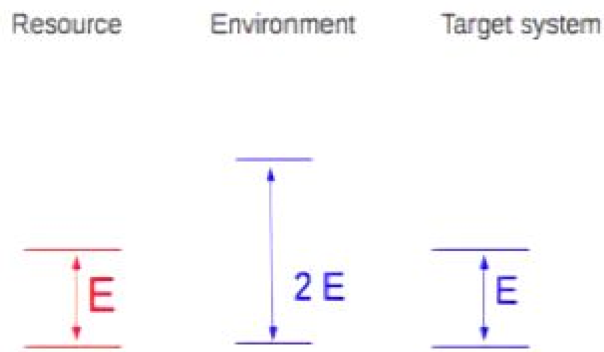
Hamiltonian

Quasi-order of resources



- process $|010\rangle \leftrightarrow |101\rangle$ generates a cold resource from a hot one
- perfect cooling of a single qubit requires infinitely many copies of the resource
- perfect erasure of a qubit requires infinitely large resources ("Tightening Landauer's principle", Janzing et al 2000)

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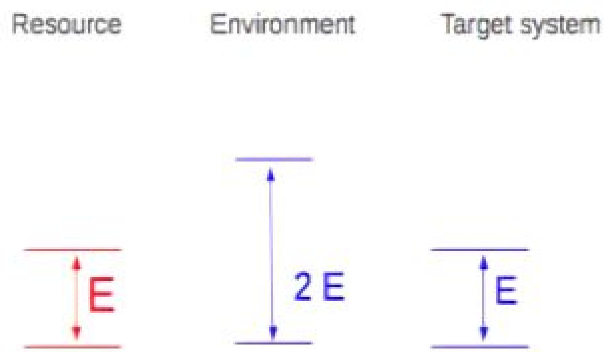

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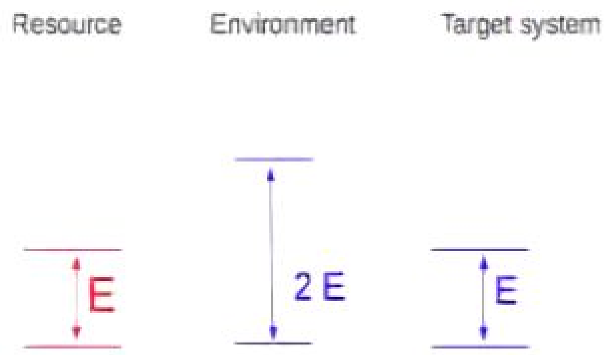

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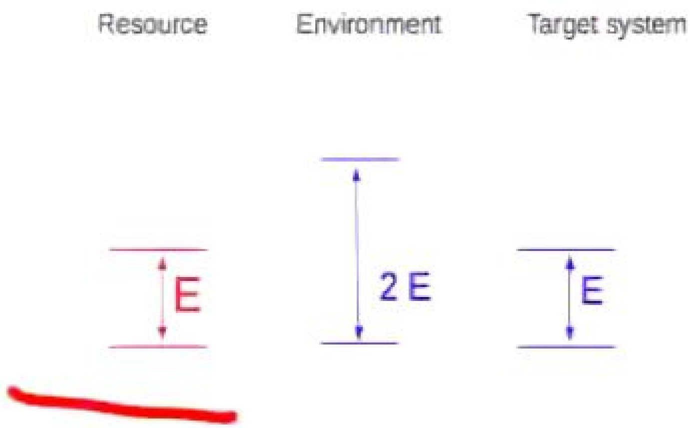

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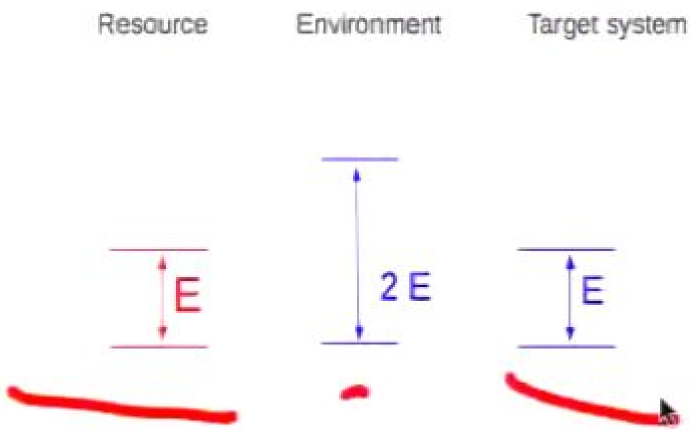

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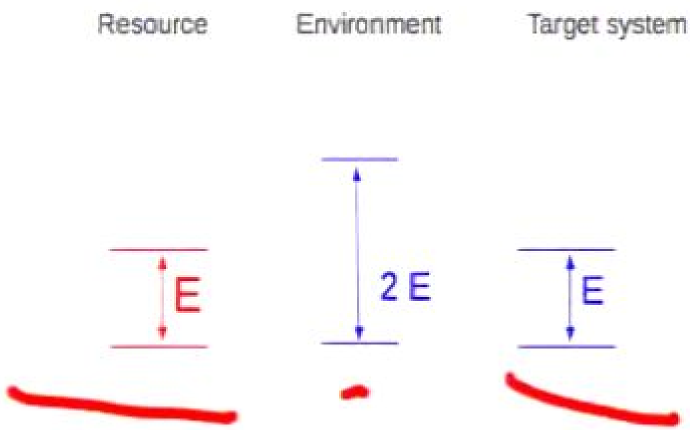

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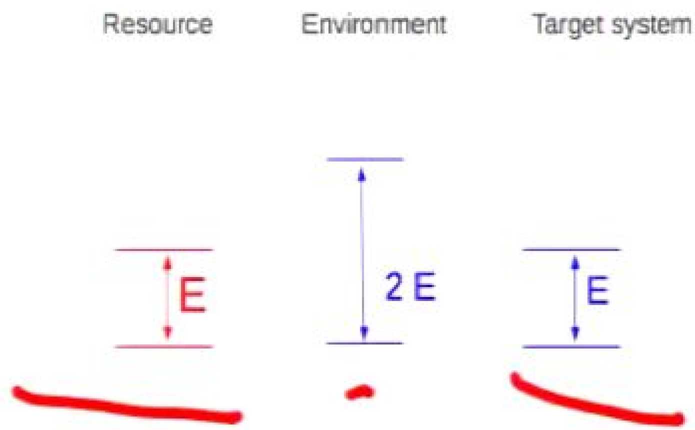

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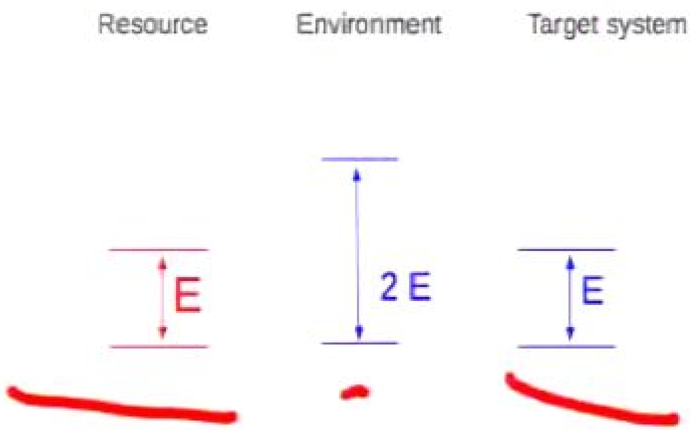

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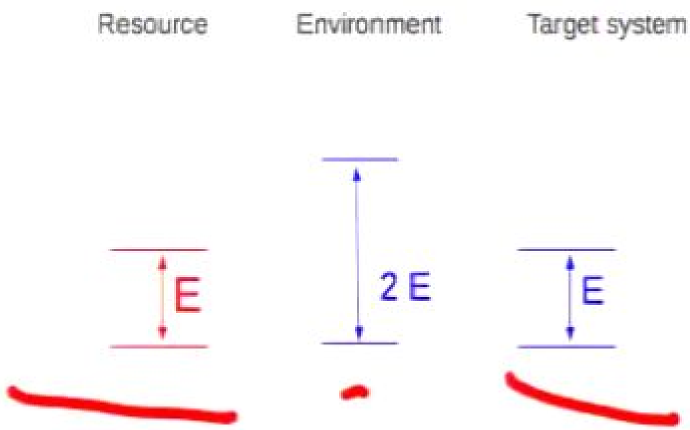

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Quasi-order formally

- Characterize every system by a pair

$$(\rho, H) = (\text{density matrix, Hamiltonian}).$$

- Define an order relation:

$$(\rho, H) \geq (\tilde{\rho}, \widetilde{H})$$

if there is an environment $(\hat{\gamma}, \widehat{H})$ and a unitary U with $[U, H + \widehat{H} + \widetilde{H}] = 0$ such that

$$\mathtt{tr}_{12}\left(U(\rho \otimes \hat{\gamma} \otimes \tilde{\gamma})U^{\dagger}\right) = \tilde{\rho}.$$

- restricted to diagonal states, quasi-order given by a majorization-like criterion

Are these processes thermodynamically reversible?

- formally, every unitary U has an inverse U^{-1}
- but the macroscopic controller implementing U or U^{-1} may consume a lot of work
- try to avoid external controllers

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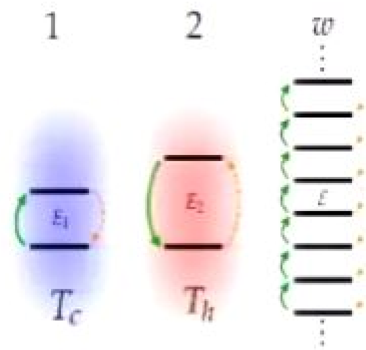
Closed system as heat engine (Linden, Popescu, and Skrzypczyk, 2010)



- consists of 2 qubits and a multi-level system ("weight to be lifted")
- qubits are coupled to hot and cold reservoirs
- tripartite interaction Hamiltonian H lifts the weight without external energy source or control operation

Sounds pretty much "reversible" because $-H$ implements the reverse process...

...but who turns H into $-H$?

actually, we cannot change Hamiltonians,

they are just given and we can only

change *effective* Hamiltonians

by changing the states of matter...

Limits of thermodynamic reversibility?

these questions remain:

- are there thermodynamic costs of switching from one effective Hamiltonian to another?
- all systems are coupled to the environment, are there thermodynamic costs of effectively isolating them?

I don't have an answer, but I propose the following approach to address these questions...

Hamiltonian or cellular automaton model of quantum control

(informal version, for details see arXiv:1009.1720)

- the world W consists of a lattice $\mathbb{Z}^d$ of cells, each cell containing a quantum system
- dynamics of the world: group (α_t)
  ($t \in \mathbb{Z}$: cellular automaton, $t \in \mathbb{R}$: translation invariant finite range Hamiltonian)
- consider a region R consisting of finitely many cells
- depending on the state of $W \setminus R$, the dynamics implements a family of completely positive maps G_t on R

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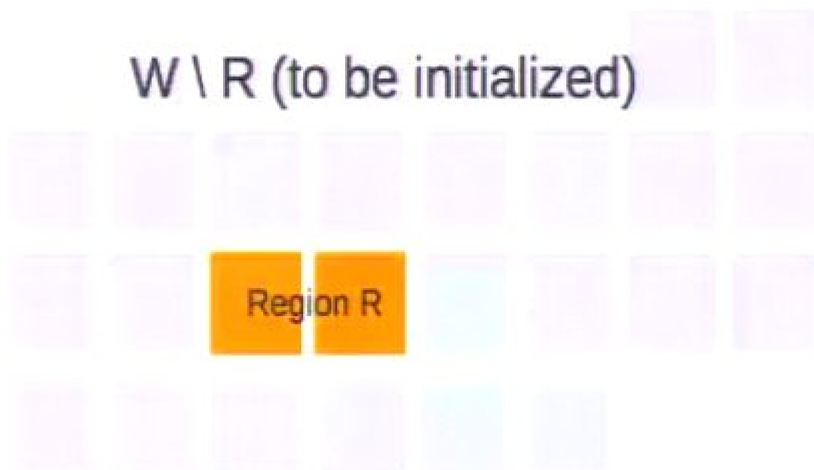
Physically universal CAs or Hamiltonians

dynamics α_t is called physically universal if

the set of all G_t generated by all possible initializations of $W \setminus R$ is dense in the set of completely positive trace preserving maps.



(do they exists? I don't know...)

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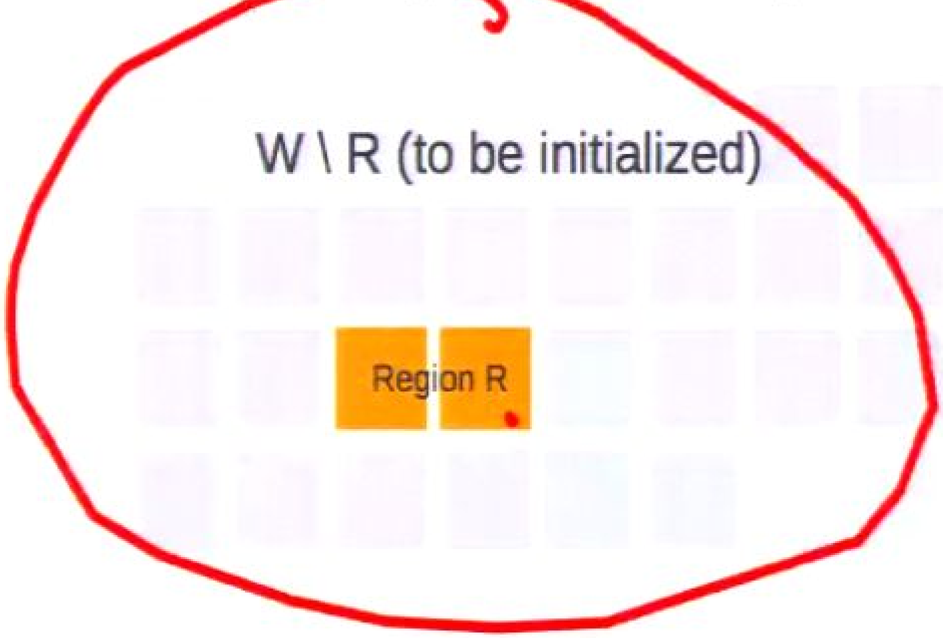

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Note...

Hamiltonians and CAs are known that are **computationally** universal

- they consist of program and data space
- they can implement any desired transformation on the **data** space

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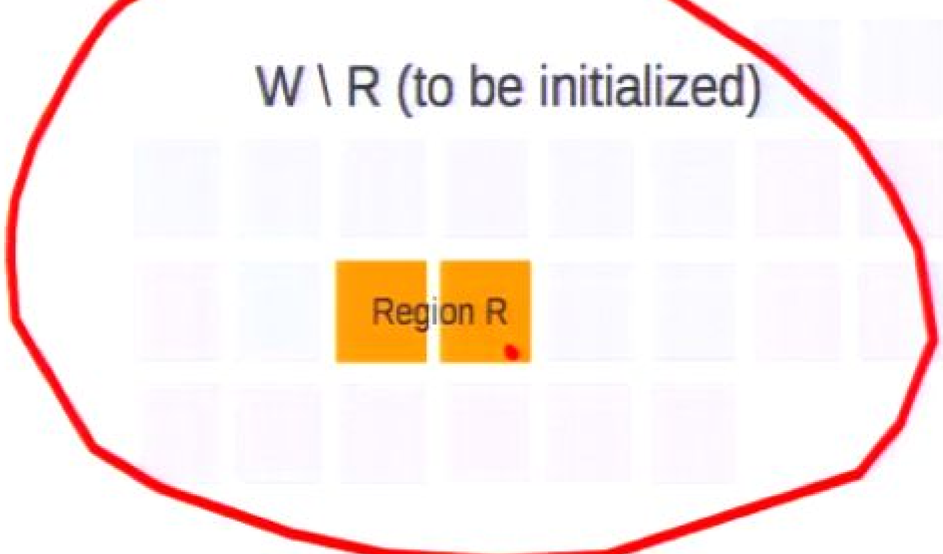

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Physically universal CAs or Hamiltonians...

- provide a model of quantum control where the controller is not external
- boundary between system R and its controller $W \setminus R$ can be shifted (like Heisenberg cut for quantum measurement)
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I would be delighted if
someone could prove existence or non-existence
of physically universal Hamiltonians!

Both would have interesting implications
for the foundations of physics

Thanks for your attention!

Although this talk was only a game –
energy conversion at nanoscale
could become even more relevant in the future

I just read about recent progress
in storing solar energy via artificial photosynthesis
http://www.sciencemag.org/content/321/5892/1072.abstract