In Search of the Holy Grail: how to Reduce the Second Law

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The second law of thermodynamics

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- What is the scope of thermodynamics?
- Can thermodynamics be reduced?

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- Thermodynamics reduces to statistical mechanics: done and dusted?
- But Sklar and Batterman are sceptical: “it is almost surely the case that thermodynamics does not reduce to statistical mechanics according to the received view of the nature of reduction in the philosophical literature” Batterman (2010, p.159).

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  1. Nagel
  2. Thermodynamics (TD) and *Boltzmannian* statistical mechanics (SM)

Thermodynamics: the paradigmatic example of a reduced theory?

- But whether a particular case of reduction is convincing depends on
  1. the account of reduction
  2. the two theories in question
- In what follows:
  1. I'll discuss how functionalism can be helpful for securing reductions.
  2. *Gibbsian* SM and I'll emphasise the importance of equilibrium in TD.

Functionalism

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- An archetypal example of a functional property: ‘being locked’
- ‘Being locked’ can be realised by a variety of mechanisms, D-locks, padlocks, combination locks.

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- Menon and Callender: temperature and entropy are multiply realised functional kinds.

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- Albert and Wallace want to recover the behaviour of macroscopic objects described by classical theory, from the underlying quantum description.
- Spacetime functionalism aims to compare candidate spacetimes across different theories.

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Sklar

The 'temperature equals mean molecular kinetic energy' bridge law *identifies* a fundamentally non-statistical quantity with a fundamentally *statistical quantity*. How is this supposed to work?' (Sklar, p. 161, as quoted by Batterman).

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- Provided that real behaviour can be modelled by both theories, other differences may not matter.

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- **So if you are allergic to 'functionalist' talk, every time I say 'realiser', think 'reductive basis'.**

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Equilibrium is at the heart of thermodynamics, and it is a presupposition of the theory that systems will end up in equilibrium. That systems will reach such an unique equilibrium state has been dubbed the 'minus first law' of thermodynamics (Brown and Uffink, 2001) — systems will spontaneously reach an equilibrium state, which then, by definition, will not change.

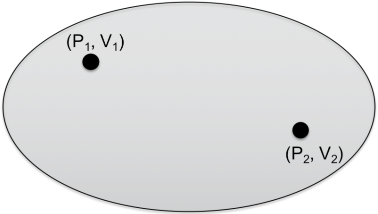

Figure : The equilibrium state-space Ξ appropriate for an ideal gas. The co-ordinates (P_1, V_1) label point x_1 and (P_2, V_2) label point x_2.

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- The curve delimits the set of processes between two equilibrium states.

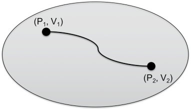

Figure : A curve through the above equilibrium state-space Ξ.

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Three types of irreversibility: quasi-static

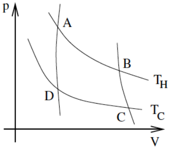

Figure : Quasi-static processes represented in the p-V plane of equilibrium states.

These 'quasi-static processes' are 'reversible': the arrows can be drawn in either direction on the curves.

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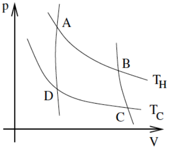

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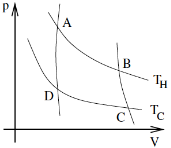

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These 'quasi-static processes' are 'reversible': the arrows can be drawn in either direction on the curves. But travelling in one direction is not straightforwardly the 'time reverse' in the TRI $t \to -t$ sense: you are performing different interventions. Furthermore, 'quasi-static reversibility' is a property of a sequence of processes, rather than of a single process.

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- **Recoverability**: the process in question can be 'fully undone'. The system can be returned to its initial state with no effect in the environment.
- But the system need not retrace its steps — it can take a different path to its destination.
- So process P is recoverable if: writing $\langle S_i, E_i \rangle \xrightarrow{P} \langle S_f, E_f \rangle$ there is a process $P*$ such that $\langle S_f, E_f \rangle \xrightarrow{P*} \langle S_i, E_i \rangle$.

The second law introduced

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The Clausius Statement: "It is impossible to perform a cyclic process which has no other result than that heat is absorbed from a reservoir with a low temperature and emitted into a reservoir with a higher temperature." (Clausius (1864) as cited in Uffink, 2001. p. 328).

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The Kelvin Statement: "It is impossible to perform a cyclic process with no other result than that heat is absorbed from a reservoir, and work is performed" (Kelvin et al. (1882) as cited in (Uffink, 2001, p.328)).

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*For a wonderful introduction to the historical subtleties about the second law, see Uffink (2001).

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$$\int_0^B \frac{đQ}{T} = S_{TD}(B) \qquad (1)$$

For an adiabatic process (i.e. a thermally isolated system), $\Delta S \geq 0$, where the equality holds if the process is quasi-static.

Three key features

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- Uffink emphasises their importance: "if such processes did not exist then the entropy difference between these two states would not be defined" (Uffink, 2006, p. 19)[1], adding that "this warning that the increase of entropy is thus conditional on the existence of quasi-static transitions has been pointed out already by Kirchhoff (1894, p. 69)", as cited in (Uffink, 2006, p. 19).

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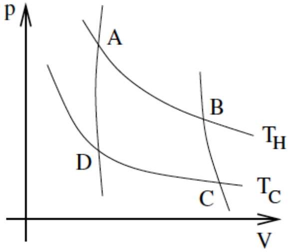

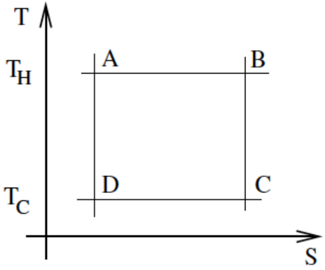

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Irrecoverability and the ravages of time

The Minus First law vs. Second law

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- Finding the microphysical ‘underpinning’ for these two Laws are distinct projects (cf. Luczak (2018)).
- The H-theorem and coarse-graining approaches in SM are concerned with quantitatively describing the approach to equilibrium (minus first law).

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- Having outlined the role in TD, we now need to search for the realiser in SM.
- But first, note that this role differs from the one discussed in much of the literature: what Callender (1999) calls ‘The Holy Grail’.

The traditional holy grail

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- Finding the distinction between heat and work in SM is at best *complicated* (cf. Maroney (2007); Prunkl (2018)) and at worst *'unnatural'* (Knox, 2016, p. 56) or *'anthropocentric'* (Myrvold, 2011).

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- Finding the distinction between heat and work in SM is at best *complicated* (cf. Maroney (2007); Prunkl (2018)) and at worst *'unnatural'* (Knox, 2016, p. 56) or *'anthropocentric'* (Myrvold, 2011).
- Maxwell claimed the distinction between heat and work is one of disordered and ordered motion, which *"is not a property of material things in themselves, but only in relation to the mind which perceives them"* (Maxwell, 1878, p. 221); (Niven, 1965, p. 646) as quoted in Myrvold (2011).

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- Finding the realiser of the TD entropy in SM seems key to finding the 'image' of the TDSL in SM.
- Callender (1999) calls this the search for 'The Holy Grail': find a SM function to call 'entropy' and establish that it is non-decreasing.

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- **The new grail:** find a SM realiser which is increasing in non-quasi-static adiabatic processes, but non-increasing in quasi-static adiabatic processes.

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- Then I will connect my claims about S_G back to heat.

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where

$$w_i = \frac{e^{-\beta E_i}}{Z}, \tag{3}$$

where Z is the partition function.

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which is the quantum analogue of the classical Gibbs entropy:

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- ...but why think that $\rho(t)$ will still be canonical?

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If the energy eigenstates of $H(t)$ are non degenerate for times $t > t_0$, if $|E_i(t_0)\rangle$ is an energy eigenstate of $H(t_0)$, if $|E_i(t)\rangle$ is the state evolved from $|E_i(t_0)\rangle$ according to the Schrödinger equation, and if the external parameter changes very slowly, then $|E_i(t)\rangle$, for each time $t > t_0$, is very nearly an energy eigenstate of $H(t)$ at the corresponding time. In the mathematical limit of a finite change in the external parameter occurring over an infinite time interval, "is very nearly" becomes "is" (Baierlein, 1971, p. 380).

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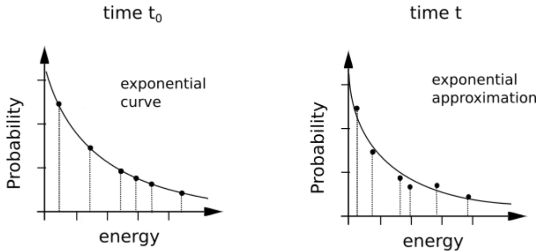
- But, just like in the thermodynamic situation, an intervention is 'slow enough' if $t_1 - t_0$ is large than characteristic timescale.



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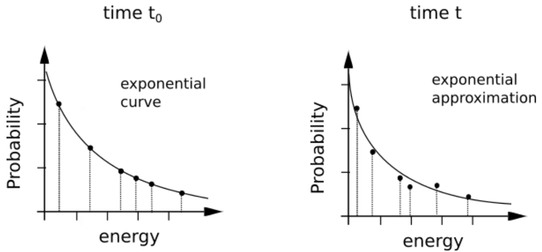

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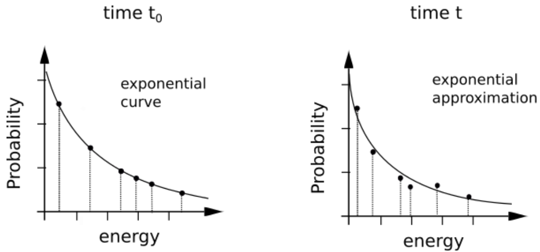

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- Thus, if the change to the external parameter is slow (i.e. qs) and $\star$ holds, then the system will remain (close to) the canonical ensemble, with a varying temperature.
- The one hitch: there's no general proof of $\star$ (Baierlein, 1971, p. 380), but it does hold for a realistic gas (Katz, 1967, p. 84-90).

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- This is wholly unsurprising: the problem with S_G is working out to make it *increase*.

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where we assume that the off-diagonal terms $w_{ij}, i \neq j$ are small so $\Sigma_{ij}\omega_{ij} \left| E_i(t) \right\rangle \left\langle E_j(t) \right| \approx \Sigma_i \omega_{ii} \left| E_i(t) \right\rangle \left\langle E_i(t) \right|$, where t is a long time after the external parameter has stopped changing.

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where we assume that the off-diagonal terms $w_{ij}, i \neq j$ are small so $\Sigma_{ij}\omega_{ij} |E_i(t)\rangle \langle E_j(t)| \approx \Sigma_i \omega_{ii} |E_i(t)\rangle \langle E_i(t)|$, where t is a long time after the external parameter has stopped changing.

- $S_G(\rho)$ increases as ρ is coarse-grained.

Rapid change

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- I conclude (in agreement with Maroney (2007)): S_G is the realiser of S_{TD} since it plays the right role — and so the TDSL is reduced to SM.

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If the external parameter V is changed slowly enough that the system remains in the canonical distribution, then the differential form is:

$$dS_G = k(d\beta\langle E\rangle + \beta d\langle E\rangle + \frac{\partial lnZ}{\partial\beta}\partial\beta + \frac{\partial lnZ}{\partial V}dV) \qquad (13)$$

$$= \frac{1}{T}(d\langle E\rangle + \langle p\rangle dV) \qquad (14)$$

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- There is one obvious difference between equation 14 and 11: in QSM, we are dealing with expectation values.
- But this is a feature, not a bug! The variance gives us useful information about fluctuation phenomena (Wallace, 2015).

Expectation values, and limiting the TDSL

- A successor theory often limits the domain — or scope — of the older theory, and this is the case with TD.
- Since Maxwell (1891), all hands admit that the TDSL can be violated. The idea that the TDSL is not a strict law was suggested by Maxwell: "Hence the TDSL is continually being violated, and that to a considerable extent, in any sufficiently small group of molecules belonging to a real body." Maxwell (1891) as quoted by Cercignani (1998).

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- Thus, the key issue is to establish under what circumstances the TDSL can be violated, and then restrict the scope of TDSL to exclude those circumstances. Here the orthodoxy is that the TDSL must be weaken to a probabilistic statement, at the very least...
- Fluctuation phenomena imply that heat can spontaneously flow from colder to hotter bodies (with no other effect), but *on average* there will be no net such flow. Thus, a weakening the TDSL to a probabilistic version, as reflected in the use of expectation values in SM, is appropriate.

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  1. Discussing the ensemble is just a vivid way to give SM probabilities a frequency interpretation.
  2. Admittedly, there are many puzzles over understanding SM probabilities (e.g. Gibbs phase averaging)...
  3. But ρ needn't be given a subjective interpretation following Jaynes (1957), instead SM probabilities can be considered to have an objective origin (cf. Myrvold (2012); Popescu et al. (2005))

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- As Callender (2001) emphasises, S_{TD} is a feature of the individual system, and so S_G does not match S_{TD}.
- In contrast, the Boltzmann entropy $S_B = k_B ln\Omega$ *is* a property of the individual system. Thus, Boltzmannians (cf. Callender (1999, 2001); Goldstein and Lebowitz (2004); Frigg (2010)) claim that S_B is superior, since it is a function of the microstate of the system.

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- According to functionalism, provided S_G plays the role of S_{TD}, then other differences are tolerated.
- S_G is not bad merely in virtue of not matching S_{TD} exactly. Such as, if 'being a property of the individual system' or 'being non-probabilistic' is not part of the essential role of S_{TD}, then the ensemble nature of the Gibbs entropy is not worrying.

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- A probability distribution over these 'fundamental microstates' of QM, density matrices, just gives...another density matrix!
- As such, there is no difference in the mathematical object that represents the state of the individual system, and a probability distribution over it.
- Thus, in QSM, the dichotomy between 'being a property of a probability distribution' and 'being a property of the individual system' never arises.

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- BUT...
- Insofar as this topic stemmed from the mystery mongering about probability in SM, there is bad news.
- Understanding, and giving an account of, probability in QSM involves tangling with the quantum measurement problem, and so in this way, we are out of the frying pan but into the fire.

Conclusions

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Thank you!

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Functionalism fit for physics

- Causal roles used in philosophy of mind not appropriate/uncontroversial in physics.
- Lewis' analytic functionalism: taking the Ramsey sentence implicates the whole web of the theory, and we might want a more narrowly circumscribed role.
- Instead 'functional' or 'nomological' roles - but spelling out the roles in particular case studies is the hard work.
- In other words, functionalism illuminates certain debates but doesn't itself resolve them.

Functionalism fit for physics

- In the philosophy of mind, *causal* roles are key — but perhaps inappropriate in physics (cf. Russell, Norton, Frisch).
- I think that there is no global, or blanket way to define the roles, instead: a case-by-case basis.
- Are some theories amenable to a functionalist treatment, and others not?
- According to Lewis' strategy (Lewis 1970) for defining theoretical terms, we can define *any* theoretical term by the web of relation it enters into.
- "Functionalism is the idea enshrined in the old proverb: handsome is as handsome does. Matter matters only because of what matter can do. Functionalism in this broadest sense is so ubiquitous in science that it is tantamount to a reigning presumption of all science" (Dennett, 2001, p.233).

Functionalism in thermal physics

Functionalism in thermal physics

p. 350 Sklar, p. 161 Batterman

It should not surprise us that Gibbs, when he came to associate ensemble quantities with thermodynamic quantities in Ch XIV of his book, spoke of the "thermodynamic analogies" when he outlined how thermodynamic functional interrelations among quantities were reflected in structurally similar functional relations among ensemble quantities. He carefully avoided making any direct claim to have found what the thermodynamic quantities "were" at the molecular dynamic level."

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According to my view — there is nothing more to the reduction.

Functionalism: the TD-SM reduction

A sketch of how functionalism helps with the TD-SM reduction: spell out the roles of various quantities in TD, and then find the realisers in SM.

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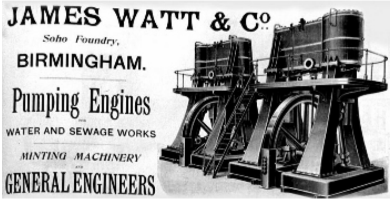
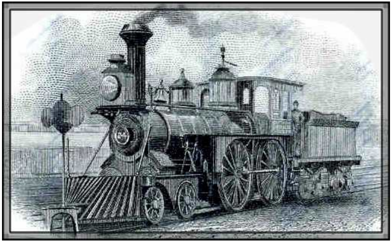
- The First law implicitly defines E
- The Second law implicitly defines S

Doubting the second law





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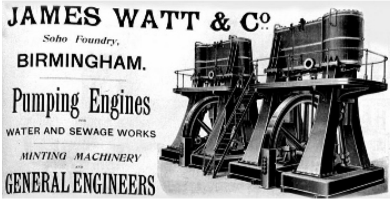

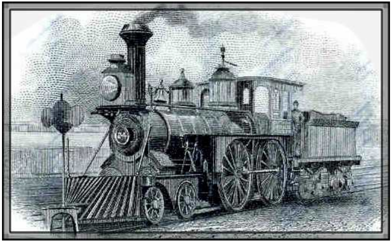

Ignorance about the nature of matter, cf. Mach's scepticism about the atomic hypothesis. In 1882, Planck said "the atomic hypothesis, despite its successes... will ultimately have to be abandoned".

Doubting the second law

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Doubting the second law

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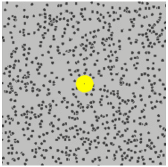
- Thermodynamics is an old theory: does the TDSL have exceptions?

Brownian motion



- Poincaré - Brownian motion violates the TDSL (Cercignani, 1998, p. 215)
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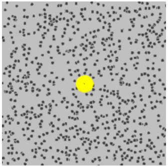
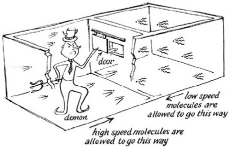
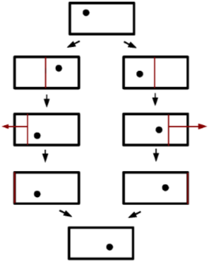


- Poincaré - Brownian motion violates the TDSL (Cercignani, 1998, p. 215)
- "the entropy law, in Planck's formulation, is simply falsified by the Brownian movement, as interpreted by Einstein" (Popper, 1957, p. 152).
- But is this really a violation? Only a microscopic violation...? We certainly can't use Brownian motion to make an engine more efficient than a Carnot engine... for that we need Maxwell's demon.

A MENAGERIE OF MAXWELLIAN DEMONS





The Intelligent Demon The miniature demon The lucky demon

Shrinking the scope of the Second Law

- Do the doubts and demons suggest that the TDSL is false?

Shrinking the scope of the Second Law

- Do the doubts and demons suggest that the TDSL is false?
- But the TDSL captures something: engines more efficient than a Carnot engine are hardly common...
- Instead of out-and-out falsity: reduce the scope of the TDSL?

Different views of the scope

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3. *(The Statistical view)*: the TDSL only applies to large numbers of DOF. (Brownian motion motivates this view).
4. *(The Maxwellian view)*: the TDSL only applies to large numbers of DOF and is contingent on our current, but perhaps temporary, technological inability to manipulate individual molecules. (Maxwell's demon motivates this view).

Against the Maxwellian view

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Against the Maxwellian view

- Loschmidt's demon meets Maxwell's demon, Maroney (2009).
- If we were able to manipulate individual molecules, would we expect to see violations of the Second Law?
- Maxwell thought so: "For Maxwell, no matter of *physical principle* precludes the operation of a Maxwell demon; it is only our current, but perhaps temporary inability to manipulate molecules individually that prevents us from doing what the demon would be able to do" (Myrvold, 2011, p. 2).

Against the Maxwellian view

- The TDSL says there exists some process I that takes the $\langle S_i, E_i \rangle \xrightarrow{I} \langle S_f, E_f \rangle$, where S_{TD} associated to $\langle S_f, E_f \rangle > S_{TD}$ associated to $\langle S_i, E_i \rangle$. Because I is irrecoverable there is no process $I*$ which takes the system and environment back to its initial state.

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- The Maxwellian view suggests that $I*$ is only unavailable to *us* — the demon can implement $I*$, and perhaps one day we can too...

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- This is unsurprising: were it possible to use microscopic manipulations to have a greater-than-Carnot engine, then it would be a hive of research.
- Contra Maxwell, and unlike the Loschmidt demon, there *is* a physical principle that precludes the operation of a Maxwellian demon.

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- Considering how the demon works is crucial, because demon only succeeds in violating the TDSL if there's no compensating S_{TD} increase in the environment.
- But SM supplies a principle that prevents the demon: Landauer's principle.

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- Landauer's principle: there is an increase of $S_G = kln2$ associated with resetting one bit of information.

Thermodynamics

Statistical mechanics

CM/QM

Dissecting the demon: how does it work?

- The demon uses 'controlled operations': which action the demon takes depends on the state of the system.
- Within SM, the system is described by a probability distribution $\rho(V_1)$, and the Gibbs entropy S_G.
- Isothermal and adiabatic interventions can be performed on the system, transforming the system into any another state $\rho(V_2)$, provided that ΔS_G.
- If the toolbox of interventions is expanded to include 'controlled operations', also known as feedback processes, then there is no constraint to which states the system can be transitioned into — and violations of the TDSL can be created.

Dissecting the demon: how does it work?

- The automaton constraint (Wallace, 2014) — the demon can be treated as an automaton.
- The total collection: controlled system plus automaton is describable by unitary dynamics, which are ‘phase space volume preserving’.
- In other words, S_G of the total collection is constant.
- Thus, if the S_G of the controlled system decreases, there must be an increase in S_G associated to the demon.
- But how does this increase come about?
- Landauer’s principle: there is an increase of $S_G = kln2$ associated with resetting one bit.

Landauer's principle: a sketch

- To implement a controlled operation, you need a memory.
- Why do you need to reset this memory?
- So that the operation of the demon is cyclic. If it not cyclic, then it is not reliable, and so no more interesting than the 'lucky demon'.
- Then Landauer's principle quantifies the entropy increase associated with resetting.

Landauer's principle: its status

- In Earman and Norton's terminology: sound or profound? Is LP a new physical principle?
- 'New physical principle' is ambiguous between 'never before seen' and 'external to TD'.
- The latter is appropriate here: Maxwell demon is a probe used for understanding TD, not a request for new fundamental physics.
- Hence Wallace's claim: LP is sound wrt to SM, but profound wrt to TD.
- The dynamical assumption S_G is non-decreasing $\neq$ to the TDSL.

Conclusions about the scope

1. *(The Strict view)*: there are never violations.
2. *(The Probabilistic view)*: it is very unlikely that there will be large violations.
3. *(The Statistical view)*: the TDSL only applies to large numbers of degrees of freedom (here after DOF).
4. *(The Maxwellian view)*: the TDSL only applies to large numbers of DOF and is contingent on our current, but perhaps temporary, technological inability to manipulate individual molecules.

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Conclusions about the scope

2. *(The Probabilistic view)*: it is very unlikely that there will be large violations — we can't rule this out — there could be a 'lucky demon'.

- However, the lucky demon is not *reliable.*
- Add a 'reliability caveat' to the scope of the TDSL?
- But notice similar this is to:
  1. *(The Strict view)*: there are never violations.
- One way to ensure that a process can be implemented reliably is if the final state is the initial input state — i.e. if the process is *cyclic*, as is familiar from the original TDSL.

Defining Entropy

The Second Law allows us to define a new state function, entropy S_{TD}. From considering the efficiency of a Carnot engine, we find $\frac{Q_h}{Q_c} = \frac{T_h}{T_c}$.

We now change notation so that Q represents the heat absorbed by the system: in the isothermal compression the heat absorbed by the system is $-Q_c$. We can also relabel as follows $Q_1 = Q_h$, $Q_2 = -Q_C$. In a Carnot cycle:

$$\Sigma_{i=1}^{2} \frac{Q_i}{T_i} = 0. \tag{15}$$

In a reversible cycle (like Carnot),

$$\oint \frac{đQ}{T} = 0. \tag{16}$$

Defining Entropy

Now consider the reversible cycle AEFGCDA in Figure **??**. This is the original Carnot cycle with a corner chopped out of it: the cycle EBGFE is also a Carnot cycle. We know that $Q_{AB}/T_h + Q_{CD}/T_c = 0$. Likewise in the mini Carnot cycle, $Q_{EB}/T_h + Q_{GF}/T_{FG} = 0$.

Now we can write out the heat flow in the cycle AEFGCDA:

- The heat flow in the segment FG is the reverse of GF: $Q_{FG} = -Q_{GF}$.
- Thus, the heat flow in the (non-Carnot) cycle AEFGCDA is: $Q_{AE}/T_h + Q_{FG}/T_{FG} + Q_{CD}/T_c = 0$.

By cutting more corners, i.e. by having many infinitesimal adiabats and isotherms, any reversible$_Q$ cycle in the plane can be considered. If we sum up all the contributions Q/T along the cycle, we find:

Defining Entropy

Clausius' inequality generalises away from the reversible cycle above to any cycle:

$$\oint \frac{đQ}{T} \leqslant 0 \tag{18}$$

$$\oint \frac{đQ}{T} = \int_1 \frac{đQ}{T} - \int_2 \frac{đQ}{T} \leqslant 0. \tag{19}$$

If path 1 is an irreversible and path 2 is reversible path from state A to B, and path 1 is adiabatic (so dQ $=$0), then we learn that the thermodynamic entropy of an *isolated* system cannot decrease:

$$S(B) - S(A) \geqslant 0. \tag{20}$$

The Role Playing Metaphor

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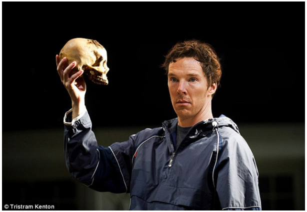

Vertical and horizontal reduction

1. Newtonian mechanics and special relativity: a case of old-to-new theory reduction. Here:
   - *t* and *b* stand for ‘tainted’ and ‘better’.
   - Call this *horizontal reduction*.
2. Statistical mechanics and underlying microdynamics: the two theories describe different phenomena, and so this is an example of reduction between different levels of description/subject matters.
   - Call this *vertical reduction*.

Vertical and horizontal reduction

- For vertical reduction, we do not want to eliminate T_t — it describes a different set of phenomena.
- In horizontal reduction, T_t and T_b describe the same phenomena, but T_b does so more successfully.
- Nonetheless, often we don't eliminate T_t but just limited its scope: it is only true within a certain domain of applicability.
- Horizontal and vertical reduction differ in degree, not kind.
- The motivation for distinguishing vertical from horizontal reduction: I want to claim that that higher-level entities are real, but emergent and the aim of reduction is not to eliminate them.

Vertical and horizontal reduction

- This is a non-eliminative reductionism, contra the reductionism of Putnam and Oppenheim who claim that a completed physics would tell us about everything, including minds and society (cf. Sober).
- This brings a certain peace between antireductionists and reductionists in philosophy of physics: anti-reductionists such as Batterman are keen on emphasising the important of the higher-level - and so do not want to eliminate it.
- But reduction need not be eliminative.