Theories of Everything:
Thermodynamics
Statistical Physics
Quantum Mechanics

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Fluctuations
and
Maxwell's Demon

Ludwig Boltzmann, who spent much of his life studying statistical mechanics, died in 1906, by his own hand. Paul Ehrenfest, carrying on the same work, died similarly in 1933. Now it is our turn to study statistical mechanics.

Perhaps it will be wise to approach the subject cautiously.

David Goodstein, *States of Matter*

Ehrenfest Dog–Flea Model

The Ehrenfest Urn Model

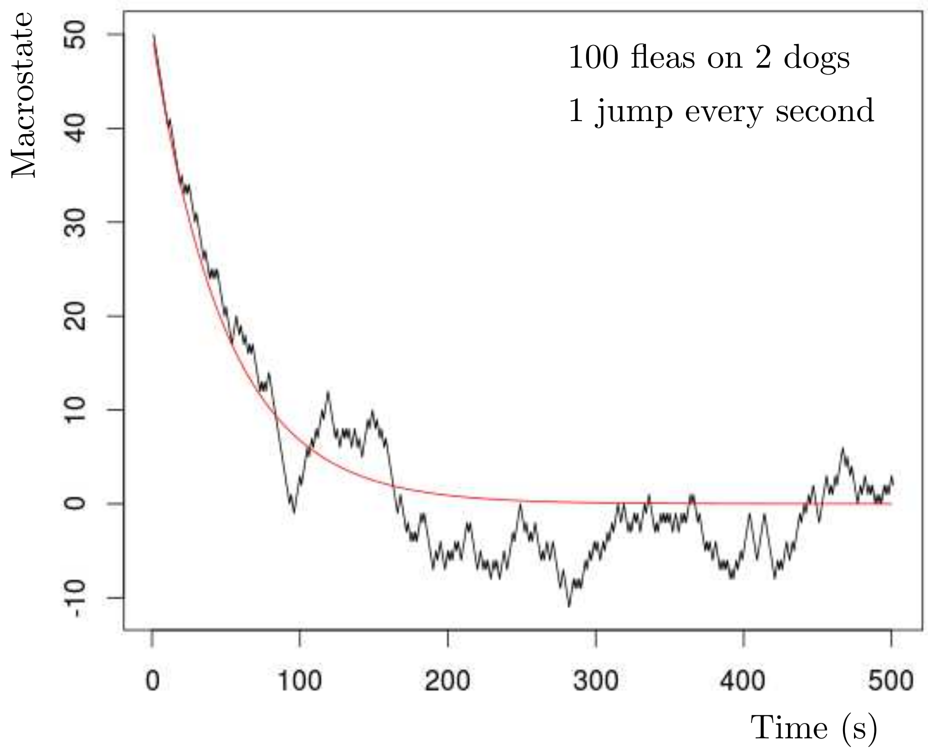
- Dog 1 (on the left) has $2N$ numbered fleas, dog 2 (on the right) is initially flea free.
- Every second we pick a random number between 1 and $2N$, look up the corresponding flea, and put it on the other dog.

P. Ehrenfest and T. Ehrenfest, Über zwei bekannte Einwande gegen das Boltzmannsche H–Theorem, *Phys. Z.*, **8** , (1907), 311.

Microstates and Macrostates

- A <u>microstate</u> is a complete specification of the positions of all fleas: fleas $n_1, n_2, n_3 \cdots n_{N+n}$ on dog 1, and fleas $n_{N+n+1}, \cdots n_{2N}$ on dog 2.
- A <u>macrostate</u> n is the number of fleas on each dog: $N + n$ on dog 1, and $N - n$ on dog 2.
- With macrostate n correspond $N_n = \frac{(2N)!}{(N+n)!(N-n)!}$ microstates.
- For 100 fleas there are in total $2^{100} \approx 1.3 \times 10^{30}$ microstates.
- Every jump brings you to another microstate. In the course of time all microstates are visited.
- The lifetime of the universe is $\sim 10^{18}$ s.

Simulations



- Black line: one realization.
- Red line: expectation for the average.

Program in R made available (Ehrenfest.R)

Master Equation and Some Elementary Results

$P(n|m;s)$: Probability of finding macrostate m after s steps if we start in macrostate n at time 0.

Master equation:

$$P(n|m,s+1) = \frac{R+m+1}{2R} P(n|m+1,s) + \frac{R-m+1}{2R} P(n|m-1,s) \tag{1}$$

Can be solved analytically (Kac*), The first moment can be derived directly from the equation

$$\langle m \rangle (s) = n\left(1 - \frac{1}{R}\right)^s \approx n e^{-s/R} \tag{2}$$

shown as the red line in the figure.

* In Wax's book.

Boltzmann and Gibbs Entropy

Boltzmann: The entropy is proportional to the number of microstates compatible with a given macrostate

$$
\begin{aligned}
S_{\mathrm{B}} = k_B \ln N_n &= k_B \ln \frac{(2N)!}{(N+n)!(N-n)!} \\
&\approx k_B \left[2N \ln 2N - (N+n)\ln(N+n) - (N-n)\ln(N-n)\right]
\end{aligned}
\tag{3}
$$

- S_{B} is a fluctuating quantity that can occasionally decrease.
- The equilibrium state is the one with maximum entropy: $n = 0$, for which

$$
S_{\mathrm{B}}^{\mathrm{eq}} = 2N k_B \ln 2 + \mathcal{O}(\ln N) \tag{4}
$$

Boltzmann and Gibbs Entropy II

Gibbs: Entropy is an ensemble property.

- $S_{\rm G} = -k_B \sum_i p_i \ln p_i$

  $p_i =$ probability for a microstate.
- $S_{\rm G}^{\rm cg} = -k_B \sum_m P_m \ln \frac{P_m}{N_m}$

  $P_m =$ probability for a macrostate.

For the dog–flea model:

- $p_i = \frac{1}{2^{2N}}$: all microstates are equal.
- $P_m = \frac{1}{2^{2N}} \binom{2N}{N+n}$: some macrostates are more equal.

The Gibbs entropy does not fluctuate, and only increases in time.

Some Further Results

1. P_m is a stationary, or equilibrium distribution.
2. Detailed Balance:
   $P_m P(m|m+1,1) = P_{m+1} P(m+1|m;1)$.
3. Decay to the stationary state.
4. Continuum limit: Smoluchowski equation for an elastically bound Brownian particle
5. Return to the initial state takes a long time.
6. How long does it take for 100 fleas?

Boltzmann Brains

How did it all start?

> There must then be in the universe, which is in thermal equilibrium as a whole and therefore dead, here and there relatively small regions of the size of our galaxy (which we call worlds), which during the relatively short time of eons deviate significantly from thermal equilibrium. Among these worlds the state probability increases as often as it decreases.
>
> Ludwig Boltzmann, 1897.

This idea is rather old:

> For surely the atoms did not hold council, assigning order to each, flexing their keen minds with questions of place and motion and who goes where. But shuffled and jumbled in many ways, in the course of endless time they are buffeted, driven along, chancing upon all motions, combinations. At last they fall into such an arrangement as would create this universe.
>
> Lucretius, *De Rerum Natura*, 50 BC

http://www.preposterousuniverse.com/blog/2013/08/22/the-higgs-boson-vs-boltzmann-brains/

Penrose estimates the total number of microstates of the visible universe to be of the order of $10^{10^{123}}$.

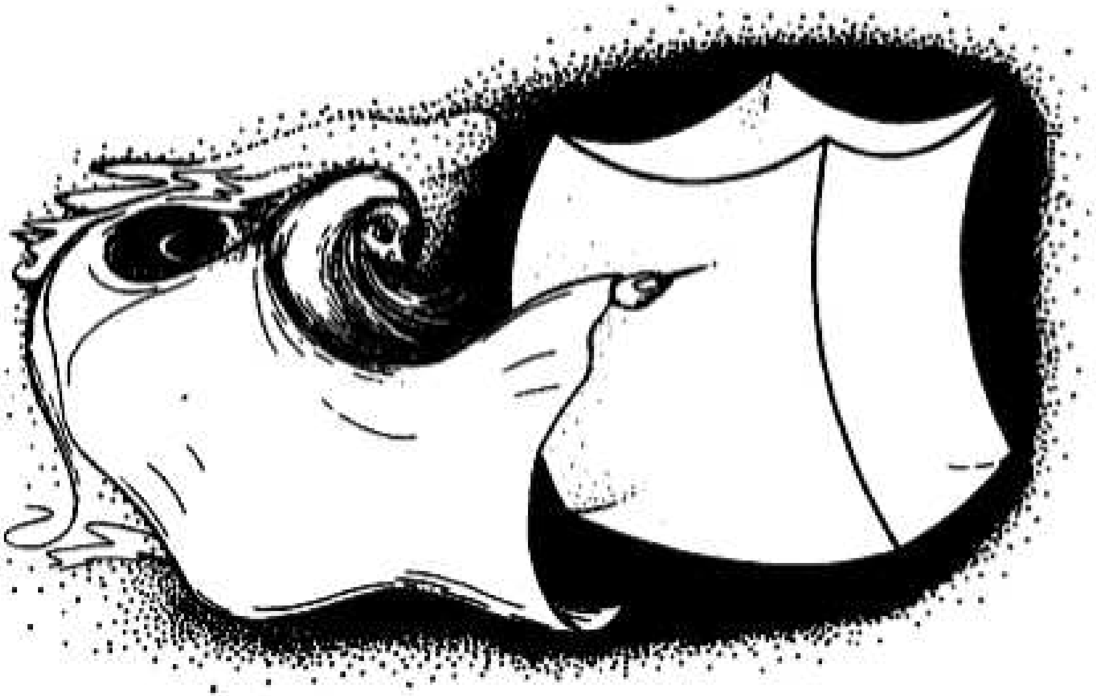
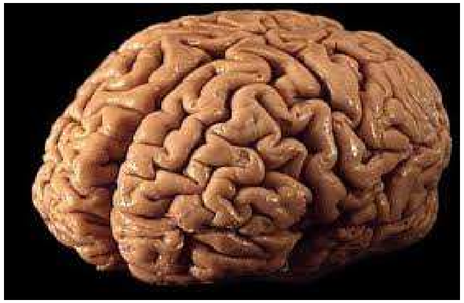
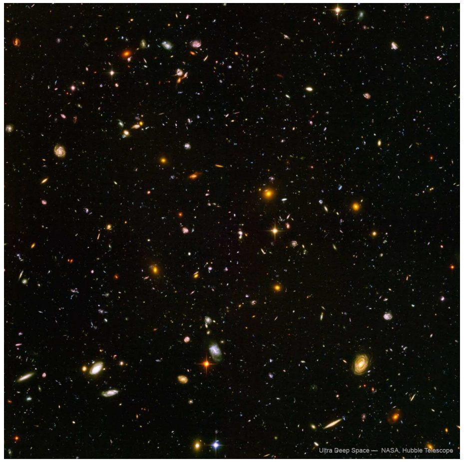


FIGURE 30. In order to produce a universe resembling the one in which we live, the Creator would have to aim for an absurdly tiny volume of the phase space of possible universes —about $1/10^{10^{123}}$ of the entire volume, for the situation under consideration. (The pin and the spot aimed for are not drawn to scale!)

Universe or just one brain?





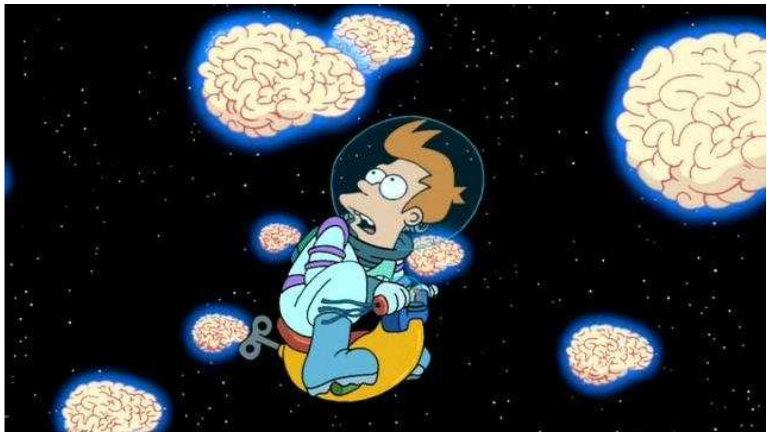
Spontaneous formation of a single brain...

has a much higher probability than of a galaxy...

and a much, much, much, much, much... higher probability than a universe.

In fact the probability of formation of the universe one second ago with all memories and history is much cheaper (entropywise) than a Big Bang 15 billion years ago.

Attack of the Boltzmann Brains



If the universe expands exponentially without end, 'ordinary observers' like ourselves may be vastly outnumbered by 'Boltzmann's brains,' transient observers who briefly flicker into existence as a result of quantum or thermal fluctuations. One might then wonder why we are so atypical. I show that tiny changes in physics–for instance, extremely slow variations of fundamental constantscan drastically change this result, and argue that one should be wary of conclusions that rely on exact knowledge of the laws of physics in the very distant future.

S. Carlip, *J. Cosmol. Astropart. P.*, 001, (2007)

Other Infinite Universes

1. Boltzmann: the (infinite) universe is in thermal equilibrium. Fluctuations bring small parts out of equilibrium, leading to a local low entropy state. We are now in a period where the universe is decaying back to equilibrium. Since the universe is infinite in time and space, this will happen an infinite number of times, in all possible variations.

2. Hugh Everett III: Many Worlds Interpretation of quantum mechanics. Every time the wavefunction seems to collapse in our universe, it is not really collapsing, but a new universe splits off for the other possible choices. Actually believed by about 20% of physicists.

3. Andrei Linde: Every now and then a quantum fluctuation produces a big bang. The universe that comes into existence has arbitrary properties of the constants, so most of them amount to nothing, but in some of them, like our own, the constants are just right (This is the *Goldilocks Principle*) and life as we know it can evolve.

Universes Thicker than Blackberries

4. David Lewis: Every logically possible universe is out there, somewhere.

5. Lee Smolin: Spawning of universes is governed by Darwinian principles: if universes do better (whatever that may be, building intelligent structures?) the chance that they become more prevalent becomes larger. Universes with the good constants start to prevail.

6. Roger Penrose: Cycles of Time. The universe starts with a Big Bang, and then proceeds to the Big Crunch. A conformal transformation turns this into a new Big Bang. Traces of black hole collisions in the previous universe may still be visible in the cosmic background radiation.

M. Gardner, *Are Universes Thicker Than Blackberries*, Ch. 1, (2003)

Maxwell's Demon

Maxwell’s Demon

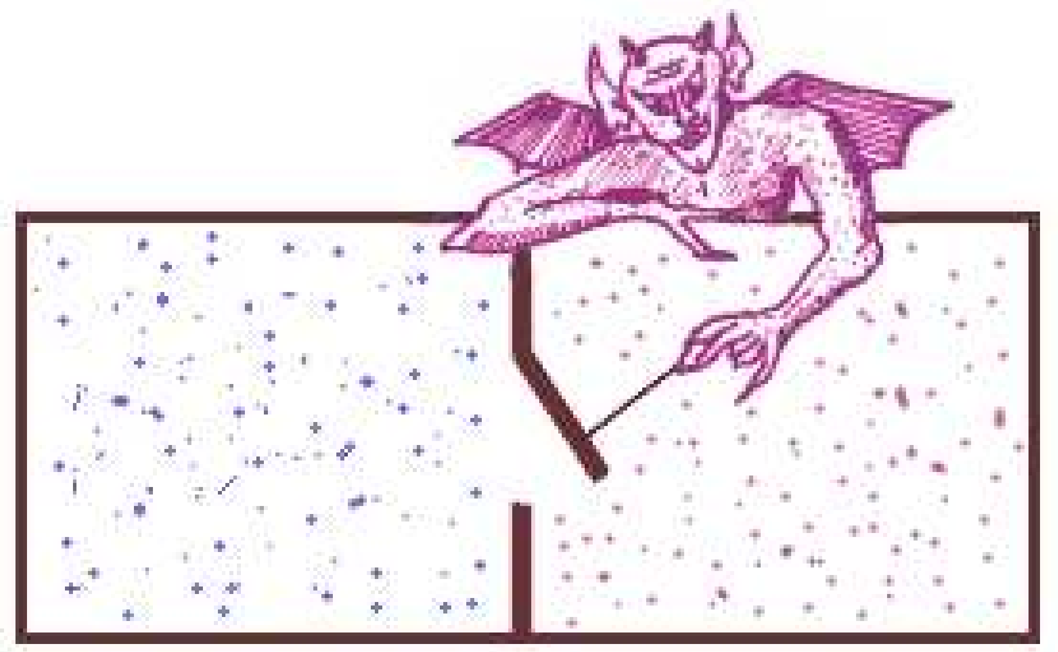
Now let us suppose that such a vessel is divided into two portions, A and B, and that a being, who can see the individual molecules, opens and closes a hole, so as to allow only the swifter molecules to pass into A, and only the slower ones to pass into B. He will thus, without expenditure of work, raise the temperature of B and lower that of A, in contradiction with the second law of thermodynamics

J.C. Maxwell, 1871.

In his paper Szillárd constructs a perpetuum mobile of the second kind by trading in entropy with knowledge. This seemingly crazy idea of equating something material with something purely spiritual turned out to be very fruitful and led in the 1930’s to Shannon’s information theory

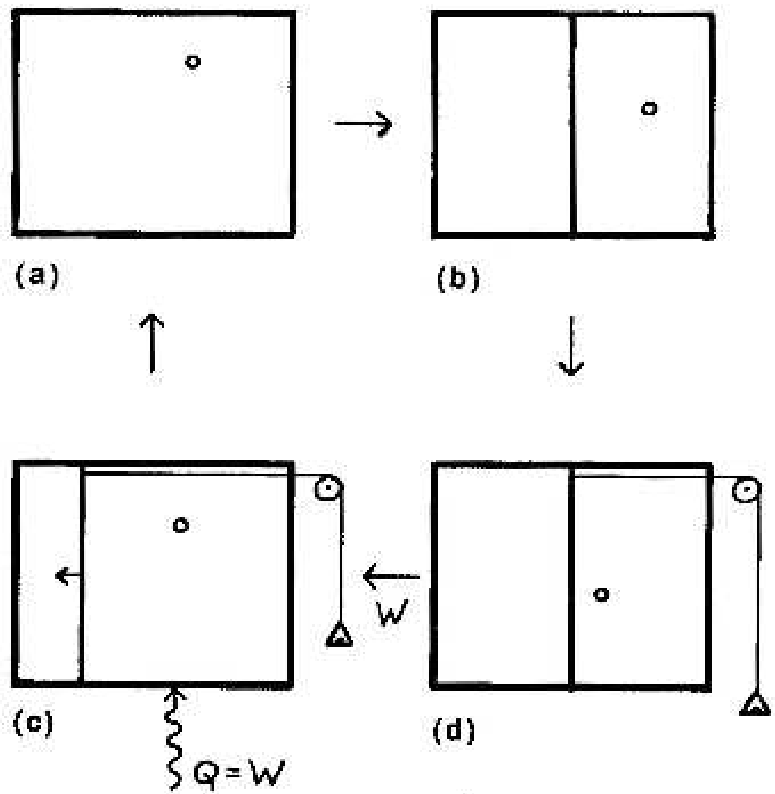
Walther Thirring in *Leo Szilárd Centenary Volume.*

Sorting Molecules



If the "neat–fingered being" opens the door for the hot molecules coming from the left, it separates hot from cold. This can be done with no expendure of energy, and hence appears to violate the second law.

Szilards One–Molecule Gas



Look where the atom is, and on the basis of that decide how to attach the weight. The work performed is equal to the heat to keep the atom at the same temperature.

L. Szilard, Über die Entropieverminderung in einem thermodynamischen System bei Eingriffen intelligenter Wesen, *Z. Physik*, **38**, (1928), 340.

Landauer's 'Solution'

- To decide if the molecule is on the left or the right we need 1 bit of information.
- For a cyclic process, the information needs to be erased.
- When information is erased, heat is generated.
- Heat dissipated in the environment increases entropy.
- The amount of entropy generated is $R \ln 2$.

R. Landauer, Irreversibility and heat generation in the computing process, *IBM J. Res. Dev.*, **5**, (1961), 183.

Entropy and Information.

> The second law is a law about information — it operates at the level of information, not energy, and hence requires a separate bookkeeping system for information in order to impose the law. An implication of this line of thinking is that a description of physics based only on energy bookkeeping (i.e. a Hamiltonian/Lagrangian mechanics with energy as the generator of time evolution for the system) is incomplete. Of course the energy and information bookkeeping systems must be consistent with each other, but the dynamics of information is independent and equally necessary to describe the world.

T.L. Duncan and J.S. Semura, p. 22–23.

T.L. Duncan and J.S. Semura, *Entropy*, **6**, (2004), 21–29.

Not Everyone Agrees

> The relationship between entropy and lack of information has led many authors, notably Shannon, to introduce "entropy" as a measure for the information transmitted by cables and so on.[...] It must be stressed here that the entropy introduced in information theory is *not* a thermodynamic quantity and that the use of the same term is rather misleading.

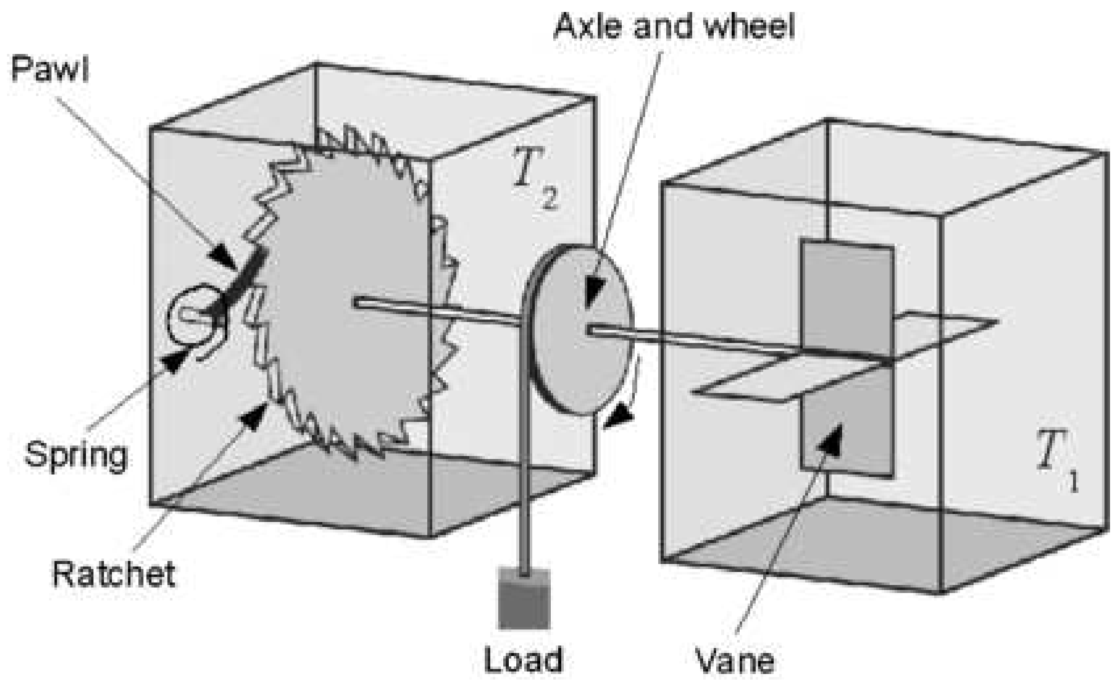
D. ter Haar, *Elements of Statistical Mechanics*, p. 161.

Feynman's Brownian Ratchet

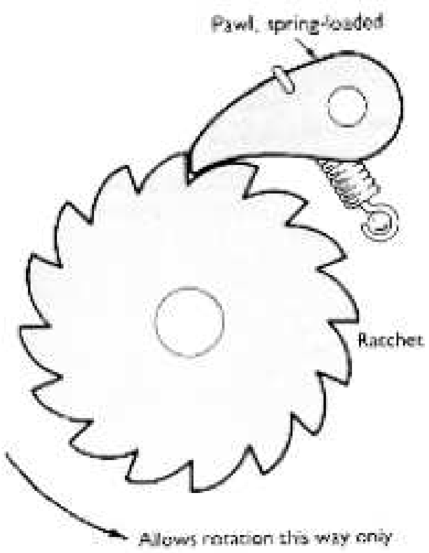
The Neverending Quest for a Free Lunch

S.T. Preston, On a means for converting the heat motion possessed by matter at normal temperature into work, *Nature*,**17**, (1878), 202–204.

G. D'Abramo, On the exploitability of thermo–charged capacitors, *Physica A*, **390**, (2011), 482–491.



The Ratchet



- The spring must be dissipative.
- It takes energy ϵ to lift the pawl to sufficient height.
- The probability for the vane to give this energy, or for the spring are the same at the same temperature.

> So, this is the reason this device does not work in perpetual motion. When the vanes get kicked, sometimes the pawl lifts up and goes over the end. But sometimes, when it tries to turn the other way, the pawl has already lifted due tot the fluctuations of the motions on the wheel side, and the wheel goes back the other way. The net result is nothing.

R.P. Feynman, p. 46.2

The Brownian Engine

If there is a temperature difference $T_1 > T_2$ the system can work as an engine.

- Probability of having a fluctuation with energy ϵ: $e^{-\epsilon/k_B T}$
- Rate for turning the ratchet counterclockwise and performing work w:

$$k_f = \frac{1}{\tau} e^{-(\epsilon+w)/k_B T_h} \tag{5}$$

- Rate for lifting the pawl to height ϵ:

$$k_r = \frac{1}{\tau} e^{-\epsilon/k_B T_l} \tag{6}$$

The Brownian Engine II

- In the reversible* case these rates are equal:

$$e^{-(\epsilon+w)/k_B T_h} = e^{-\epsilon/k_B T_l} \tag{7}$$

- Since $Q_h = \epsilon + w$ and $Q_l = \epsilon$:

$$\frac{Q_h}{T_h} = \frac{Q_l}{T_l} \quad \text{and} \quad \frac{w}{Q_h} = 1 - \frac{T_l}{T_h} \tag{8}$$

- Which is exactly Carnot's result:

$$\eta = 1 - \frac{T_l}{T_h} \tag{9}$$

* This statement was criticized by Parrondo (see Exercises, and Literature).

Exercises and Problems

Exercises and Problems

1. Derive Equations (1) and (2).
2. Derive an expression for $\langle m^2 \rangle - \langle m \rangle^2$ as a function of s.
3. Prove, or investigate the statements on slide 11.
4. Feynman more or less claims that his derivation of the amount of work that can be obtained from the heat flow is a mechanical one, based on Newton's equations of motion. Why is that claim incorrect?
5. One thing I find lacking in all discussions about information is that this concept only makes sense if there is a processor of information. Is the entropy of a stretch of DNA which codes for a peptide different from a random set of DNA bases of the same length? Give your opinion.
6. Write a short computer program to simulate the Dog–Flea model. Using this program, determine both the Gibbs and the Boltzmann entropy. Take 10 fleas and run the simulation until all fleas are on one dog. How long did that take?

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