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Energy Management at the Nanoscale

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1. Introduction

Energy management is considered a task of strategic importance in contemporary society. It is a common fact that the most successful economies of the planet are the economies that can transform and use large quantities of energy. In this chapter we will discuss the role of energy with specific attention to the processes that happens at micro and nanoscale, that are the scales where the modern ICT devices are built and operated.

2. Energy and its transformation

We start our journey toward the role of energy in ICT devices by addressing the most fundamental question of what energy is. According to Richard Feynman¹ we do not know much about energy apart from the fact that “energy is conserved”. We usually define energy as the “capability of performing work” and define work as the activity performed by a force applied to some mass that, as a consequence of this application, changes its position. Energy, in the International System of Units, is measured in Joule (symbol J). 1 J is equal to the work done by applying a force of one Newton through a distance of one metre. 1 J is the energy that it takes to raise an apple (100 g) for 1 m above the ground. It is also relevant how much time it takes to do some work. This is taken into account by the concept of *power*. Given a certain amount of work done, the power is equal to the work divided by the time that it takes to do it. Physical unit of power is Watt (symbol W; $1W = 1J / 1s$). Multiples or sub multiples of J or W are what we are used to deal with in our everyday life: one kilowatt or kW is equal to 1000 W and it is the power required to cook a cake in a microwave oven. Given that the cake takes about one

¹ “It is important to realize that in Physics today, we have no knowledge of what energy is”. The Feynman Lectures on Physics Volume I, 4-1.

hour to be properly cooked, the amount of energy used at this aim is approximately $3600 \times 1000 = 3.6$ million J or 1 kWh (*kilowatt-hour*).

In the following table we list few examples of how much power is required to perform some common tasks.

Task	Power (W)
Average power of a Boeing 747 airplane	10^8
Full power aircraft fighter	10^6
Full power car engine	10^5
Operate a microwave oven	10^3
Being alive for an average adult human	10^2
Brain functioning for an average human	10
mobile phone calling	1
Emission of a standard WI-FI router	10^{-1}
Functioning of a LED light	10^{-2}
Functioning of a miniature FM receiver	10^{-3}
Functioning of a wireless sensor node	10^{-4}
Low power radio module	10^{-5}
Functioning of a quartz wristwatch	10^{-6}
Operation of a quartz oscillator	10^{-7}
Sleep mode of a microcontroller	10^{-8}
1 bit information erasure at room T (min)	10^{-21}

Table 1. Order of magnitude of the power required to perform some common activities.

From our everyday experience we know that energy is used for many different tasks and comes in many different forms. We know that it is energy because we can use it to perform work, like moving a car or a train. Thus energy is a property of physical systems that can be used to perform work and usually comes inside physical objects like a hot gas or a gasoline tank. Thinking about it we can ask questions like: how can we make the energy contained in a litre of gasoline to push forward a car or how can we use the heat produced by burning coal to make the train run?

Questions like these were at the very base of the activities performed in the early seventeen hundreds by the first inventors of the so-called thermal machines. People like Thomas Newcomen (1664-1729) who built the first practical steam engine for pumping water and James Watt (1736-1819) who few decades after proposed an improved version of the same machine. It is thanks to the work of scientists like Sadi Carnot (1796-1832) and subsequently of Émile

Clapeyron (1799 - 1864), Rudolf Clausius (1822 - 1888) and William Thomson (Lord Kelvin) (1824 - 1907) that studies on the efficiency of these machines aimed at transforming heat (just a form of energy) into work brought us the notion of entropy and the laws of thermodynamics.

These laws do not tell us much about what energy is but they are very good in ruling what can we do and what we cannot do with energy. Let's briefly review them.

The first law of thermodynamics states that the total energy of an isolated physical system is conserved during any transformation the system can go through.

It was initially formulated by Julius Robert von Mayer (1814 - 1878) and subsequently reviewed by James Prescott Joule (1818-1889) and Hermann Ludwig Ferdinand von Helmholtz² (1821-1894). It is strongly believed to be true but, to some extent is a self-supporting law: as a matter of fact it is so strongly believed that in every instance we observe a possible violation we think harder to discover some way in which energy can be hidden and overlooked. Last time in history this happened was at the beginning of 1900 when Albert Einstein proposed the mass-energy equivalence to account for the "missing mass" during a nuclear transformation.

The second law states that there are limitations to how much work we can get from a given amount of energy present in the form of heat. There exist different formulations that are all equivalent. The two most popular are ascribed to Clausius and Kelvin:

Clausius formulation: "No process is possible whose sole result is the transfer of heat from a body of lower temperature to a body of higher temperature".

Kelvin formulation: "No process is possible in which the sole result is the absorption of heat from a reservoir and its complete conversion into work".

An important consequence of the second law is that there is a limit to the efficiency of a thermal machine. This limit was discovered by Sadi Carnot in 1824 when he was only 28. In the publication entitled *Réflexions sur la Puissance Motrice du Feu* ("Reflections on the Motive Power of Fire") he introduced the concept of thermal machine, generalizing the concept popular at that time of "steam engine", and showing that the efficiency of any thermal machine operating between two temperatures is bounded by a quantity that is a function of the two temperatures only.

Few years after the work of Carnot, Clausius used this result to introduce a quantity that is useful in describing how much heat can be changed into work during a transformation. He proposed the name "entropy" for his quantity. The idea is the following: if you want to operate a thermal machine you have to find a cyclic transformation during which heat is changed into work. The cycle is necessary because you want to operate the machine continuously and not just once. Clausius proved a theorem that states that during a cyclic transformation, if you do the transformation carefully enough not to lose any energy in other ways (like friction), then

² Feynman assertion that the notion of energy has never been very clear is testified by the fact that the key publication of Helmholtz, considered the father of the conservation of energy, is entitled "Über die Erhaltung der Kraft", "On the conservation of the strength". On the other hand the kinetic energy has been called for a long time "vis viva", Latin expression for "living strength".

the sum of the heat exchanged with the external divided by the temperature at which the exchange occurs is zero:

$$\oint \frac{dQ}{T} = 0 \quad (1)$$

The cycle does not depend on the path that you take and, clearly you start and end at the same state. This is equivalent to say that it exists a state function S defined as

$$S_B - S_A = \int_A^B \frac{dQ}{T} \quad (2)$$

(or in differential form $dS = dQ/T$) that satisfies the previous equation. If you are not careful enough and you loose energy during the transformation than the inequality holds instead:

$$\oint \frac{dQ}{T} \leq 0 \quad (3)$$

A transformation like this is also called an *irreversible transformation*. It is easy to show that if we take an irreversible transformation to compute the entropy we end up with underestimating the change:

$$S_B - S_A \geq \int_A^B \frac{dQ}{T} \quad (4)$$

In the particular case in which we are considering a transformation without any heat exchanged then the second term is zero and the final entropy is always larger than the initial one. A typical example is the so-called adiabatic expansion of a gas. If we consider an infinitesimal transformation we have:

$$dS \geq \frac{dQ}{T} \quad \text{or} \quad TdS \geq dQ \quad (5)$$

where the equal sign hold during a reversible transformation only. The previous equation is sometimes considered a concise formulation of the second principle of thermodynamics. If I put in contact a physical system that is at temperature T_1 with a heat reservoir that is at temperature $T_2 > T_1$ then some heat is transferred from the reservoir to the system. Accordingly the integral is positive and the entropy of the system increases. The other way around phenomenon by which heat is transferred from the system to the reservoir does not happen (second principle) and thus we conclude that during a spontaneous transformation (i.e. without external work) the entropy always increases. We can make the entropy of our system decrease (like in a refrigerator) but we have to add work from outside.

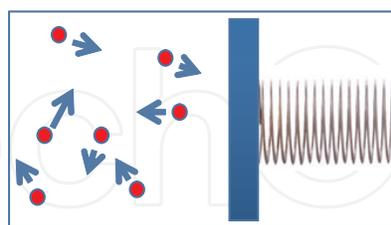
Back to the Clausius inequality, it is useful to interpret the quantity TdS as the amount of heat (meaning thermal energy) that cannot be used to produce work. In other words during a transformation, even if we are carefully enough not to waste energy in other ways, we cannot

use all the energy we have to do useful work. Part of this energy will go into producing an increase of the system entropy. If we are not careful enough the situation is even worse and we get even less work. This is sometimes accounted for by the introduction of the so-called *Free energy*. The concept of Free energy was proposed by Helmholtz in the form: $F = U - TS$. The free energy F measures the maximum amount of energy that we can use when we have available the internal energy U of a system.

In summary we can state that change in entropy is a measure of a system's thermal energy per unit temperature that is unavailable for doing useful work.

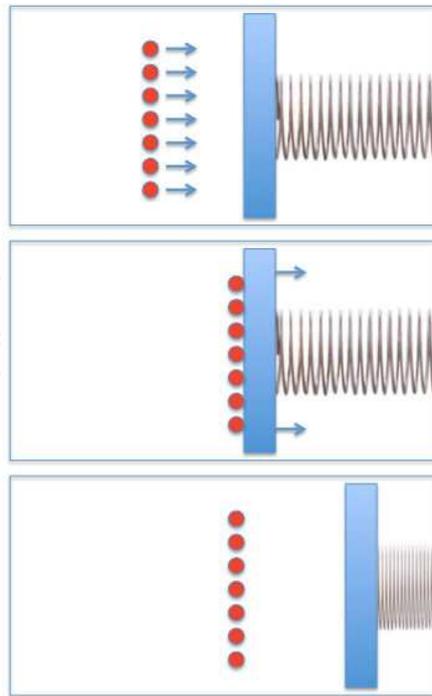
3. The microscopic perspective

Notwithstanding the above explanation, available since the late 1800, in general the entropy remained an obscure quantity whose physical sense was (and somehow still is) difficult to grasp. It was the work of Ludwig Boltzmann (1844 – 1906) that shed some light on the microscopic interpretation of the second law (and thus the entropy) as a consequence of the tendency of a physical system to attain the equilibrium condition identified with the most probable state among all the possible states it can be in. The ideal world of Boltzmann is made by physical systems constituted by many small parts represented by colliding small spheres³. To better grasp the meaning of entropy let's consider an ideal gas made by N particles in the form of tiny hard spheres of mass m that can collide elastically, i.e. conserving the kinetic energy in addition to their momentum. Let's suppose that these particles are contained in a box that has a moving set of mass $M = Nm$. The set is connected to a spring of elastic constant k , as in the figure, and is at rest.



If all the particles have the same velocity v and collide perpendicularly with the moving set at the same time (see following figure), they will exchange velocity with the set.

³ L. Boltzmann was a strong supporter of the atomistic view of the matter. An idea that was not given for granted (nor so popular) at his time. This did not help an often depressed Boltzmann that in 1906, during one of his bad mood crises decided to kill himself.



This will compress the spring up to an extent x_1 such that:

$$\frac{1}{2}M v^2 = \frac{1}{2}k x_1^2 = U \tag{6}$$

This is a simple transformation of kinetic energy into potential energy. We can always recover the potential energy U when we desire and use it to perform work. The work will be exactly U . In this case we can completely transform the energy of the gas particle into work. How comes? Well, in this case we are clearly considering a very special configuration of our gas. Unique indeed. What is on the contrary the most probable configuration for the particle in the gas? Based on our experience (and on some common sense as well) it is the configuration in which all the particles, although each with the same velocity v , are moving with random direction in the box (as in our first figure). The energy of the gas is still the same (so is its temperature T) but in this case the set will be subjected at random motion with an average compression of the spring such that its average energy is U/N . This is also the maximum work that we can recover from the potential energy of the movable set. Thus it appears clear that, although the total energy U is the same in the two cases, in the second case we have no hope of using the greatest part of this energy to perform useful work. As we have learned above, when we introduced the definition of Free energy, the quantity that limits our capability of performing work is the entropy. Thus the systems that have the smaller entropy have the larger capability of performing work. Accordingly we can use the entropy to put a label on the energetic content of a system. Two systems may have the same energy but the system that has the lower entropy will have the “most useful” energy.

This example helped us to understand how energy and entropy are connected to the microscopic properties of the physical systems. In the simple case of an ideal gas, the system energy is nothing else than the sum of all the kinetic energies of the single particles. We can say that the energy is associated with “how much” the particles move. On the other hand we have seen that there is also a “quality” of the motion of the particles that is relevant for the entropy. We can say that the entropy is associated with “the way” the particles moves. This concept of “way of moving” was made clear by Boltzmann at the end of 1800, who proposed for the entropy the following definition:

$$S = K_B \log W \quad (7)$$

where K_B is the famous Boltzmann constant and W is the number of microstates associated with a given state of the physical system. Sometimes W is also called the “number of configurations” and represents the number of ways we can arrange all the particles in the system without changing its macroscopic properties⁴. In the previous example we have only one way to arrange the N particles so that they are all parallel, aligned and with the same velocity while we have a very large number of ways of arranging the N particles to be a randomly oriented set of particles with velocity v . Thus it is clear that in the second case the value of the entropy is much larger than in the first case (where it is indeed zero).

We have seen above that during a spontaneous transformation the entropy of the system increases. This can happen without any change in the energy of the system itself⁵. In our example with the bouncing particles this is represented by the situation in which the particles trajectories are not perfectly aligned as a consequence collision between the particles can happen before hitting the movable set and soon, collision after collision the entire group of particles evolves into a randomly moving group. This is clearly a spontaneous transformation. By the moment that the collision are elastic the energy of the system has not changed but the system entropy has rapidly increased up to its maximum value. Conversely the free energy has reached its minimum value. This is what we call a “spontaneous transformation toward the equilibrium condition”. Now: can we bring the system back to its initial condition? The answer is yes but... in order to do it we need to spend some energy as required by the second principle. How much? Clearly we need to spend $T\Delta S$ of energy, where ΔS represents the difference in entropy between the final and the initial state. The bad news is that if we spend this energy and decrease the entropy back to its original condition... the energy is lost and we cannot recover it any more, meaning that the energy that we spend does not change the total kinetic energy of the system that remains the same. In other words there is no way to store energy into decreasing entropy. This last conclusion has some consequences that we will explore soon below when we will consider the energy processes in ICT devices. Before moving

⁴ Here we assume that all the microstate are equiprobable. The extension to the more general case with microstates with different probabilities has been proposed by Josiah Willard Gibbs (1839 – 1903).

⁵ There is a famous experiment performed by Joule that shows that the free expansion of a gas is a process that can happen without exchange of energy.

into that subject however we need to dig some more into the consequences of thermodynamics in the small scale⁶.

4. What does irreversible mean?

When we introduced the entropy change we specified that this is defined in terms of heat transfer, once we perform a *reversible transformation*. What does it exactly mean reversible? Well, reversible literally means that “it can be done the other way around” but in my opinion it is not a very clear definition. What is usually meant is that if we want to go from a state A toward a state B, we do need to do a transformation that it is so slow that it goes through an infinite number of equilibrium states so that at any instant all the macroscopic quantities like temperature, pressure, volume, ... are well defined. By the moment that these quantities are defined only in equilibrium condition we need to be as close to equilibrium as possible. For a number of comprehensible reasons that we will address more in detail in another chapter, this requires that we go quite slow⁷ when we change anything in the system.

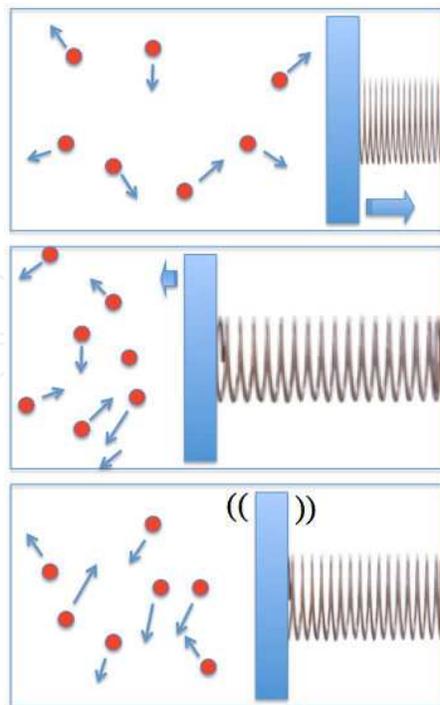
What happens if we do not go “slow”? Well, as we have seen before, in this case we are performing an *irreversible transformation*. During an irreversible transformation the entropy always increases. Moreover, due to the Clausius **inequality** it always increases some more compared to what it would be required by the second law. Why is that? The answer is that in addition to the *physiological* increase there is an extra contribution due to the *dissipative effect* of the non-equilibrium processes. With *dissipative effect* we intend a way in which some low-entropy energy is changed into high-entropy energy. A typical example of dissipative process is friction. If during any transformation there is friction then the transformation is irreversible and the increase in entropy *benefits* from the additional contribution of this process.

In this regards it is interesting to inspect more in detail the example of the movable set in contact with the gas, we introduced before. When the system represented by the particle gas + the movable set is at equilibrium the movable set is not only acted on by the collision of the particles but is also damped by the very same source. To see this effect we can consider two simple cases.

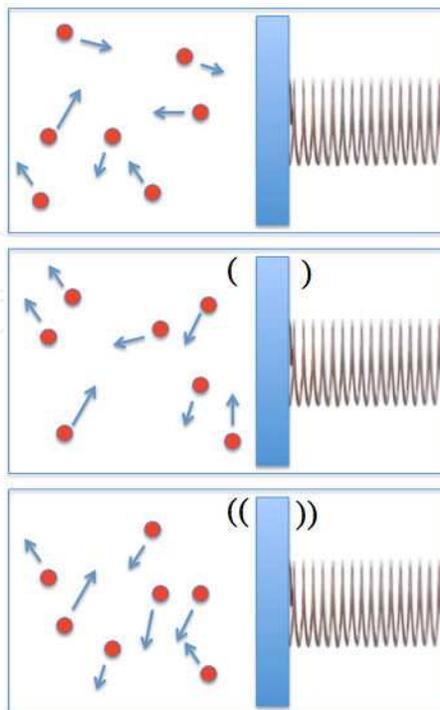
1. We compress the spring to some extent and then we release the compression leaving it free to oscillate. After few oscillations we observe that the oscillation amplitude decreases as a consequence of what we call the friction (viscous damping force) action due to the presence of the gas. The decrease ceases when the oscillation amplitude reaches a certain equilibrium value and after that it remains constant (on average, see following figure). Some energy has been dissipated into heat.

⁶ Thermodynamics in the small scale is a kind of oxymoron. According to J. P. Sethna, thermodynamics is the theory that emerges from statistical mechanics in the limit of large systems (J.P. Sethna, *Statistical Mechanics: Entropy, Order Parameters and Complexity*, 6.4, Oxford Univ. Press. 2008).

⁷ Here slow means slow compared to the time it take for the system to relax to equilibrium.



2. We now start with the movable set at rest and leave it free. After few seconds we will see that the set starts to move with increasing oscillation amplitude that soon reaches an equilibrium condition at the very same value (on average) of the first case (see following figure).



In both cases the two different roles of damping-force and pushing-force has been played by the gas. This fact led to think that there must be a connection between the process of dissipating energy (a typical irreversible, i.e. non-equilibrium process) and the process of fluctuating at equilibrium with the gas.

5. A bridge toward non-equilibrium: fluctuation-dissipation relation

In order to unveil such a link we need to introduce a more formal description of the dynamics of the movable set. This problem has been addressed and solved by Albert Einstein (1879 - 1955) in his 1905 discussion of the Brownian motion and subsequently by Paul Langevin (1872 - 1946) who proposed the following equation:

$$m\ddot{x} = -m\gamma\dot{x} - \frac{dU}{dx} + \xi(t) \quad (8)$$

As before x represents the movable set position. Here γ represents the viscous damping constant, U is the elastic potential energy due to the spring and $\xi(t)$ is the random force that accounts for the incessant impact of the gas particles on the set, assumed with zero mean, Gaussian distributed and with a flat spectrum or, delta-correlated in time (white noise assumption):

$$\langle \xi(t_1)\xi(t_2) \rangle = 2\pi G_R \delta(t_1 - t_2) \quad (9)$$

where the $\langle \rangle$ indicates average over the statistical ensemble.

Now, as we noticed before, by the moment that the gas is responsible at the same time for the fluctuating part of the dynamics (i.e. the random force $\xi(t)$) and the dissipative part (i.e. the damping constant γ) there must be a relation between these two. This relation has been established within the linear response theory (that satisfies the equipartition of the energy among all the degrees of freedom) initially by Harry Theodor Nyquist (1889 - 1976) in 1928⁸, and demonstrated by Callen and Welton in 1951. This relation is:

$$G_R = \frac{mK_B T}{\pi} \gamma \quad (10)$$

and represents a formulation of the so-called Fluctuation-Dissipation Theorem (FDT)[1,2]. There exist different formulations of the FDT. As an example we mention that it can be generalized to account for a different kind of dissipative force, i.e. internal friction type where γ is not a simple constant but shows time dependence (work done in the sixties by Mori and Kubo). In that case the random force shows a spectrum that is not flat anymore (non-white noise assumption).

⁸Nyquist established this relation while he was studying the voltage fluctuations across an electrical resistor. The random electromagnetic force arising across a resistance at finite temperature is a function of the value of the resistance itself.

Why is FDT important? It is important because it represents an ideal bridge that connects the equilibrium properties of our thermodynamic system (represented by the amplitude and character of the fluctuations) with the non-equilibrium properties (represented here by the dissipative phenomena due to the presence of the friction). Thus there are basically two ways of using the FDT: it can be used to predict the characteristics of the fluctuation or the noise intrinsic to the system from the known characteristics of the dissipative properties or it can be used to predict what kind of dissipation we should expect if we know the equilibrium fluctuation properties. Its importance however goes beyond the practical utility. Indeed it shows like dissipative properties, meaning the capacity to produce entropy, are intrinsically connected to the equilibrium fluctuations.

6. Energy transformations for small systems

How does the description of the energy transformation processes presented so far change when we deal with small systems? To answer this question we start considering an important aspect when we deal with physical systems: the condition of being an *isolated system*. If we say that a system is not isolated, we intend that it has interactions of some kind with something that we consider external to the system itself. If this is not the case (isolated system) all the dynamics is self-determined by the system itself and we can deal with it by addressing the equations of motion for each particle coupled to each other particle in the system. At this aim we may use the standard Newton laws (or in the quantum case the Schrodinger equation). If the system is *not isolated* the situation is generally more complex and we need to take into account the interaction of our system with the "external world". In principle however any system can be considered isolated provided that we include in the system all the sources of interactions. In the extreme case we can consider the universe itself as an isolated system. For this reason we will limit our consideration to systems that are isolated.

Before answering the question about the energy transformations in small systems we should be more precise in defining what a *small system* is. When we deal with real physical systems we cannot ignore that all the matter, as we know it, is composed by atoms. These are more or less individual particles whose interactions determine most of the properties that characterize the matter. The ordinary devices that we are used to deal with are composed by very a large assembly of atoms, numbers are of the order of the Avogadro number, i.e. $N_A = 6.022 \times 10^{23}$. Thus when we are dealing with small systems, in general we intend systems composed by a number of atoms N that is small compare to N_A . Clearly, due to the extremely large value of N_A , a system composed by few thousands of atoms (or molecules or "particles") can still be considered small. This is the case for example of the nanodevices like last generation transistors. Unfortunately in this case the small systems are not isolated because they exchange energy and information with the outside. On the other hand small isolated systems are quite rare. An example of the *small isolated system* can be found in the realm of what is generally called "high energy physics": here the particles are most of the time just few (small system) and isolated from the external. Back to the realm of the physics of matter we have frequently to deal with

systems that are usually not small but can be considered in good approximation isolated. What do we do in these cases?

One possibility is to do what we did just before, when we dealt with the movable set in contact with the gas of N particles. Here N is of the order of N_A . Overall our system is composed by $3N+1$ degrees of freedom (dof): 3 for each of the N particles and 1 for the movable set position coordinate x . This is clearly not a small system, although isolated, because all the interactions are inside the $3N+1$ dof. In this case we played a trick: we focused our attention on the single degree x and summarized the role of the remaining $3N$ dof by introducing the dissipative and the fluctuating force like external forces. By the moment that both these forces are necessary to account for the observed dynamics and by the moment that both are born out of the neglected $3N$ dof, it comes out that they are connected to each other and the connection is nothing else than the FDT that we discussed. Our equation of motion is not anymore the deterministic Newton (Schrodinger) equation, instead it is the novel stochastic Langevin equation where there is a both friction and fluctuation caused by the added forces due to the neglected dof. Thus the trick we played was to exchange the dynamics of a *not small isolated system* with *small not isolated system*. Such an approach has different names (adiabatic elimination, coarse graining, ...) and it is considered a very useful tool in describing the properties of dynamical systems composed by many dof.

To summarize our approach: we have transformed a *non small isolated system* into a *small non isolated system*. What is the advantage? Easy to say: the dynamics of a non small isolated system can be described in terms of $3N+1$ dof by $3N+1$ coupled motion equations and when N is of the order of N_A this is a practically impossible approach. Thus the advantage was to drastically reduce the number of equations of motion (in this case to just 1) but the price we had to pay is the introduction of dissipation and fluctuation. What we have found is that dissipative and fluctuating effects appear only if we neglect some (usually many) dof through some coarse graining approximation to the system dynamics. In this perspective the dissipation of energy appears to be only an illusion due to our choice of dynamical description.

On the other hand we know that if we perform a real experiment with our movable set, indeed we observe a decrease in the oscillation amplitude of the set until it reaches the stop and then it does start to fluctuate around the equilibrium position. This is not an illusion. The potential energy initially stored in the spring is now dissipated due to the presence of the gas particles. How does this fit with what we just said about the dissipation being an illusion? The answer is that the total energy (the kinetic energy of the gas particles + the potential energy initially stored in the spring) is conserved because the (not small) system is isolated. What happened is that the potential energy of the movable set has been progressively transformed into additional kinetic energy of the N particles that now have a slightly larger average velocity (the temperature of our gas slightly increased). Thus during the dynamics the energy is transferred from some (few) dof to others (many) dof. This is what we called before energy dissipation and now it appears to be nothing more than energy re-distribution. Before we have seen that dissipative effects during a transformation are associated with an increase of entropy. Indeed this energy distribution process is an aspect of the tendency of the system to reach the maximum entropy (while conserving the energy). This is what we have called a spontaneous

transformation: the increase of the entropy up to the point where no more energy distribution process takes place, i.e. the thermal equilibrium.

Is this the end of the story? Actually it is not. There is a quite subtle aspect that is associated with the conservation of energy. It is known as Poincaré recurrence theorem. It states that in a system that conserves energy the dynamics evolve in such a way that, after a sufficiently long time, it returns to a state arbitrarily close to the initial state. The time that we have to wait in order to have this recurrence is called the Poincaré recurrence time. In simple words this means that not only the dissipation of energy is an illusion because the energy is simply redistributed among all the dof but also that this redistribution is not final (i.e. on the long term the equilibrium does not exist). If we wait long enough we will see that after some time the energy will flow back to its initial distribution and our movable set will get its potential energy back (with the gas particle becoming slightly colder). This is quite surprising indeed because it implies that in this way we can reverse the entropy increase typical of processes with friction and thus fail the second principle. Although this may appear a paradox this answer was already included in the description of entropy proposed by Boltzmann and specifically in its intrinsic probabilistic character. The decrease of entropy for a system composed by many dof is not impossible: it is simply extremely improbable. It goes like this: for any finite observation time the dynamic system evolves most probably in a direction where the entropy increases because according to Boltzmann this is the most probable evolution. However if we wait long enough also the less probable outcome will be realized and thus the second principle *violated*. How much time should we wait? The answer depends on the dof of our isolated (energy conserving) system. The larger the number of dof the longer the time to wait... exponentially longer.

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