The enigma of irreversibility and the interplay between Physics, Mathematics and Philosophy

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Abstract

The problem of reconciling a reversible micro-dynamics with the second law of thermodynamics has been a scientific and conceptual challenge for centuries and it continues to animate heated debate even today. In my opinion, one key point lays in the interrelation between the physical, the mathematical and the philosophical aspects of the problem. In many treatments those domains of knowledge dangerously mix, generating confusion and misunderstanding. In this short work I will show how disentangling these three domains for the problem at hand will give a better understanding of the enigma of irreversibility and opens up possibility for future research.

Keywords: Irreversibility, Boltzmann, Statistical Mechanics, Lanford's Theorem

1. Prelude: the gas in the box

There is an archetypal image through which the so called *problem* or *paradox* of irreversibility is usually introduced in the literature. This image is the classical gas of particles at some temperature T expanding in a completely isolated vessel. A container of total volume V is divided by a partition into two parts. At the start of the experiment, a dilute gas, confined to the left-hand side of this container; the partition is suddenly removed and the gas is allowed to expand into the vacuum of the right-hand side of the container. The removal of the partition turns the equilibrium state of the gas into a non-equilibrium state. The gas will thus evolve from this non-equilibrium state into a new equilibrium where the molecules of the gas are spread all around in the total new volume available. At the equilibrium, all the gradients of velocities and density inside the box are zero. This is the classical "textbook"

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case in which it is possible to talk about the emergence of thermodynamic irreversibility.

The endeavor of understanding the origin of observed macroscopic irreversibility given a reversible micro-dynamics is a problem with a long history [46, 47]. This has been a major issue in statistical mechanics since its beginning [19]. Kinetic Theory of gases, the highly mathematical study of transport equations, is the arena where the problem is commonly introduced and discussed [57]. Judging by the number of the journal papers appeared recently, philosophers too continue to find the topic very attractive [7, 15, 38, 44]. In this work I intend to offer my personal view on (one possible) reason for this never-ending disagreement about the solution of this scientific *vexata quaestio*. I found that in the vast literature related to this topic the physical, the mathematical and the foundational (I can call the philosophical) aspect of the problem mix together to form a complicated *blob* that conspires against a clear understanding and sustain an enduring confusion. My aim is to disentangle these different levels of the problem and to show how this can be beneficial also for future research.

2. Philosophy, Physics, Mathematics

The relationship between physics, mathematics and philosophy is extremely complex and it has changed profoundly over the centuries. Even if the border between these three domains of knowledge sometimes is very blurred, by and large we know how to distinguish them. In the following discussion, I invite the reader to keep in mind the following distinction:

Philosophical domain. It has to do with scrutinizing the fundamental assumption and the internal logic of the reasoning used in any discourse.

Physical domain. It concerns how the empirical world (matter, energy and interactions between these entities) works and how we can predict it.

Mathematical domain. It is about formal deduction starting from a set of axioms, irrespective to the “meaning” or “range of validity” of those axioms.

Of course there can be different opinions on this matter. A purist can say that physics begins and ends with the experiment. On the other extreme it has been asserted that mathematics can be considered a branch of physics too [33]. Even if physicists usually dislike vague philosophical disputations, it is uncontroversial that every approach to empirical investigation requires (willing it or not) the use of some pre-existing assumptions about what Reality is. Metaphysics enters here. Mathematicians by themselves often blame physicists of lacking mathematical rigor in their derivations [13]. These are just some anecdotal *vignettes* that anyway capture something about the deep relation between these three domains.

The interaction between these three levels plays a role in every scientific investigation, but for the problem of the origin of irreversibility this tension appears particularly acute. The aim of this paper is to try to disentangle those three levels for the problem at hand. At the outset a disclaimer is in order. What follows does not aspire to be a complete account of the immense literature related to the topic but only a critical refection on a selected part of it. Furthermore, there is a fourth domain of knowledge that is not strictly included in the three described above that is the *computational* one. Computer experiments modeling irreversibility behavior for theoretical and practical purposes have been relevant in the past and are now growing in importance due to the development of hardware technology. I will not enter in the details of this here (the interested reader can refer to [14]).

3. Philosophy: language and logic

Philosophy starts with an hygiene of language. Philosophers tried to frame the problem in an unambiguous and clear way [7]. When the aim is to account for thermodynamic irreversibility, a usual research project is to provide a *mechanical explanation* of the second law of thermodynamics. But is this correct? One first remark is in order. Discussions about irreversibility are often conflated with those about the emergence of alleged arrows of time. I claim that for a better understanding those two issues must not be confused together. As philosopher Huw Price clearly recognized, it is important to distinguish between symmetry **in** time *versus* asymmetry **of** time [39]. As far as the expansion of the gas in the box is concerned, it must be clear that we are not interested here in any "arrow of time" but in the asymmetry of events in time. So, what is the problem? Phenomenology shows that for isolated thermodynamical systems, there exists a very special state that we call *equilibrium* ($M_{equilibrium}$). This special state describes when the gas is spread around the available volume and all spatial gradients are zero. Given any other macroscopic state M, it is always observed the following sequence in time:

$$M \longrightarrow M_{equilibrium} \tag{1}$$

Once the system is in $M_{equilibrium}$, it will never leave it. It is now clear that the characterization of this special state $M_{equilibrium}$ lays at the very heart of the problem of irreversibility. This sequences of macroscopic states can be ordered in time only in the way expressed in (1) for isolated systems. According to Brown and Uffink [5], what the "problem" of irreversibility - as it has developed historically - is not to explain the *second law* of thermodynamics but something more fundamental that they refer to as the **Minus First Law**. Starting from the Minus Firs Law, I clarify the main problem *à la* Brown and Uffink as follows:

Fundamental problem of irreversibility. *Given an isolated thermodynamical system, and given that microscopic constituents of matter obey reversible dynamical laws, explain why an equilibrium state* $M_{equilibrium}$ *: a) exists; b) it is unique; c) it is an attractor state i. e. the system converges to it and remains there, and d) the characterization of this state* $M_{equilibrium}$ *is consistent with the empirical observation.*

So if we set the problem in this form, what is the solution? Philosophers have scrutinized in deep the logical steps of the Boltzmann attempt to solve the fundamental problem in terms of the underlying mechanics working on the model of the gas in the box. Boltzmann's arguments are nowadays usually referred to as *statistical argument* or *typicality* [52, 23]. All revolves around the following formula:

$$S = k \log W \tag{2}$$

This formula represents the *Standard Model* of statistical mechanics and it is so well known that it can be considered offensive for the reader if I embark again on an explanation of the symbols involved. What is important at this point is that this formula relates micro (on the right) with the macro level (on the left). Succinctly, philosophers of science try to explain why statistical mechanics works so well and the problems of irreversibility is at the intersection of many critical issue at the foundation of the discipline like the role of ergodicity and the exact meaning to assign to probability statements

[48, 20]. Formula (2) represents a spectacular example of *dialectical thinking*. Through a process of synthesis, two apparently irreconcilable domains, thesis and antithesis (in this case mechanics and thermodynamics) are resolved in a middle ground theory that is statistical mechanics. As such, this framework is very captivating for philosophers interested in scrutinizing its internal consistency. The whole construction relies on the distinction between *detailed description* (position and velocity of each component) and *reduced description* (through averaging) of a given system. Here I summarize the main points of what I will henceforth call the **Boltzmannian synthesis**:

1. A big number of particles in the box are allowed to move independently and isotropically (i. e. no restriction to the direction of motion). This implies that equal *a priori* probability of micro-states in the phase space is assumed.
2. Macro-states supervene on micro-states.
3. The previous assumption introduce an equivalence relation over the phase space: micro-state belongs to the same equivalence class if they give rise to the same macro-state. The phase space is partitioned in a set of disjoint equivalent classes that correspond to each observable macro-state. The *quotient space* represents the system of interest in thermodynamical terms.
4. Describing the system at a macroscopic level with a set of few relevant thermodynamic variables means to operate a *canonical projection* over the quotient space. It means that what is required is just to consider equivalence classless and not the details of each micro-state. This is the most extreme form of *coarse-graining* whereas the dimensionality of the system is drastically reduced in passing from one level of description to the other.
5. The projection step introduce irreversibility in passing from a detailed description to a reduced one because, from simple combinatorial considerations: a) equivalence classes have different probability and b) there exist an equivalence class whose probability is astronomically higher then the others as the number of particles N becomes big: this is the equilibrium state $M_{equilibrium}$ i.e. the state where we *expect* to observe the system macroscopically. Of course the meaning of equilibrium must be intended in the "dynamical" sense.
6. At $M_{equilibrium}$ Boltzmann entropy given by (2) reaches its maximum.

Setting aside many technical and subtle details about the above construction that have been extensively discussed in the literature [48, 21], points 1-6 represent the standard recipe needed for solving *conceptually* the *fundamental problem* for the isolated gas: existence, uniqueness and convergence to $M_{equilibrium}$. The focus is, by definition, on sets of non-interacting particles but the consideration above can be applied to weakly interacting particles provided that interaction does not affect the validity of assumption (1) and (2). Those are the most fundamental assumptions on which the main logic is built. The term "big number" used in point (1) sounds not well defined but at the same time this is an essential element. For ordinary thermodynamics, the order of magnitude of the chemical *mole* makes the probability that a micro-state is in $M_{equilibrium}$ close to 1. In this sense it is *typical* for a micro-state to be in $M_{equilibrium}$. It is worth noting that probability does not enter in the projection step (4) but it is already present from scratch at the microscopic level in step (1) whereas we ignore (or we are not interested in) the details of the history of the evolution of the components of the system. Furthermore, provided that all the conditions are satisfied, these arguments do not require the component of the system to be "microscopic" in the common sense. Actually, the micro-macro distinction is never strictly defined and it embodies an anthropocentric bias. Indeed, statistical mechanics reasoning can be, *mutatis mutandis*, applied to molecules inside a test tube in a lab or to a cluster of stars in a galaxy. Conclusions depend on the validity of the initial assumptions and not on the size of the components.

One critical issue related to the *Boltzmannian synthesis* runs as follows: since equilibrium is the expected state, how can system out of equilibrium like a compressed gas-in-the-box exist in the first place? In thermodynamics the possibility that an experimenter can observe gasses in a box out of equilibrium requires an history where the experimental arrangement were more out of equilibrium than now. This requires a conceptual leap in the reasoning: to complete the discussion about a gas in a box we are force to consider a *super-system* that includes it and make an additional assumption about the initial entropy of this super-system (*gas+box+surroundings+experimenter*). But at a given point we will need to consider a super-super-system of the super-system and so on. Ultimately we need to consider the state of the whole universe. The statistical argument is subtle on this issue since it implies that it is more likely that the system of interest arose out in the past from a the state of equilibrium through fluctuation that are no longer prevented in the mechanical interpretation. But this openly runs against what we think to know about the past. The imposition of a low-entropy state in the past to complement Boltzmann's arguments is usually refereed to as the *past hypothesis* [55]. For some scholars the very enigma of irreversibility collapses to the problem of how we can justify the low-entropy state of the early universe and a range of opinions can be found in the literature [17, 24]. For other authors, failing to justify the *past hypothesis* invalidates the whole Boltzmannian castle [36]. This point deserves a clarification. The *Boltzmannian synthesis* is a logical reasoning that can be justified *ex-ante* (internal coherence) and *ex-post* (empirical confirmation). It works as long as condition on which is based are satisfied. For gases in boxes or drops of ink in the water, it works because conditions are (with the due approximation) satisfied. The problem of justifying the initial conditions relates to a different conceptual issue and not to the internal sustainability of the Boltzmannian reasoning.

4. Physics: matter and interactions

A box filled with non-interacting particles can be be interesting on logical and theoretical grounds but it is not so interesting from the point of view of physics. Interesting phenomena unfold from *interaction* between physically relevant entities like forces or fields acting on matter and energy. The simplest interesting physical model is the isolated gas of interacting particles where the interaction occurs only through binary collisions. This was exactly the original problem tackled by Boltzmann. The main assumption adopted in the derivation of the irreversible Boltzmann equation, that describes the evolution of this kind of model, is the well known *molecular chaos hypothesis* (Stosszzahl Ansatz): colliding particles can be considered uncorrelated. If there are correlation, it means that particles tend to move in a coordinate way. An extreme example of correlation is the motion of a flock of birds floating on air. Going back to the gas in the box, this looks like a quite anti-thermodynamic behavior. Since Boltzman equation works well in describing empirical reality, how can molecular chaos be justified? One way is purely mathematical. For the dilute gas one can try to prove that if independence and isotropy of the velocities are present at the initial condition, those properties *propagate* during the evolution to equilibrium *despite* collisions; if *so* the *Boltzmannian synthesis* can be applied and there is no need of any extra physical ingredient. This is still an open mathematical problem (see discussion in section 5 below). One the other hand the physicist may wander whether there is an underlying causal mechanism responsible for the disappearance of correlations. One *leitmotif* of the literature after Boltzmann has been the quest for this physical ingredient that account for the *Stosszzahl Ansatz*: what does it *kill* the correlations? I invite the reader to be aware of this subtlety: in order to apply the *Boltzmannian syntheses* we need a justification for the dismissal of the role of correlations. This aim has been attempted historically in two ways: through a purely mathematical effort culminated in the Lanford's theorem on one side and invoking a physical ingredient on the other. *Interventionism* is the believe that no real system can be fully isolated. According to this idea, external perturbation due to interaction with the environment represent the physical element that ultimately permits relaxation to equilibrium [28, 32].

Prigogine and the Brussels-Austin School located the physical origin of irreversibility in the intrinsic *instabilities* manifested by chaotic dynamical systems not necessarily composed by many components [41, 35]. Prigogine work about irreversibility is a complicated assemblage of philosophical conceptions, physics and mathematics (for an excellent overall evaluation see [18]). A variety of formalisms arose during the years from his (highly criticized) ideas [40, 2, 4, 26]. The idea of an intrinsic irreversibility has been embraced also by Volovich [54, 53] and Castagnino [10]. Other authors stressed the need of grounding the problem at the quantum level through *collapse of the wave function* or *decoherence* (see chapter 7 of [1] or [43]). Explanation of the second law has been also relate to the physics of *information* [16]. Other quantum suggestions have been proposed here [36].

Of course the details of $M_{equilibrium}$ - and the evolution to it - will be the more and more dependent on the interaction between the components. If for example gravitational attraction becomes relevant, equilibrium state is no longer related to the maximum volume available. This is also particularly important in the understanding of the *tempo* of relaxation to equilibrium. The *Boltzmannian synthesis* is totally silent on this since it relates exquisitely on the details of the dynamical properties and interactions between the elements of the system and so of very physical interest.

5. Mathematics: propagation of chaos

It is remarkable how the connection between the mathematics and the physics of irreversibility arose historically with a conflict. There exists a mathematical result that apparently prevents from the very beginning the possibility of an equilibrium state $M_{equilibrium}$ as defined above. This is the well known recurrence result due to Poincaré and used for the first time by Ernst Zermelo to object Boltzmann's earlier ideas about the origin of irreversibility [45]. The theorem goes as follows:

Poincaré's Recurrence Theorem. *Any bounded system returns arbitrarily close its initial state after a finite amount of time, infinitely often.*

Physicists usually easily dismiss the relevance of this theorem for systems of thermodynamic interest invoking recurrence times: they grow exponentially with respect to the degrees of freedom of the system. For a mole of gas in the box to is equivalent to a number of years that is far behind the estimated age of the universe. So here an argument about the *physical relevancy* is used to overcome the theoretical *impasse* due to the mathematical result. It is interesting to note that with another important result that I will consider below, Lanford's theorem, something similar happens but in the opposite direction.

Anyway most of the discussion related to the mathematics of irreversibility are centered around the derivation of kinetic equations, in particular the Boltzmann equation:

$$\partial_t f + v \cdot \Delta_x f = Q(f, f) \tag{3}$$

This equation describes the evolution of the one-particle distribution function $f(x, v, t)$ due to diffusion and collisions with respectively the second therm on the left and the therm on the right. The usual form of $Q(f, f)$ takes into account binary collisions and the validity is restricted to dilute gases. The mathematical theory of the Boltzmann equation related to the existence and properties of solutions of (3) is an open and challenging part of Kinetic Theory. Another major theme concerns the speed of convergence to equilibrium (Maxwellian) states. The Field medalist Cédric Villani wrote some detailed and insightful surveys on the topic (see for example [50]). Some of the main landmarks in this field are due to Carleman [8, 9], Grad [25], Lanford [29]. In particular, the theorem proved by Oscar Lanford in the 70's is considered of utmost importance [51]. This result derives the equation (3) from Hamiltonian mechanics of N hard spheres of radius r, in the *Boltzmann-Grad* limit

$$Nr^2 \to constant \tag{4}$$

for $N \to \infty$ and microscopic distributions with Gaussian velocity decay. Starting from the foundamental assumption of a (properly defined) molecular chaos at initial time, it shows how this chaos propagates on a short time interval (details here [11]). Lanford's result shows that the Boltzmann equation can be rigorously derived but it requires highly idealized assumption like the Boltzmann-Grad limit also to circumvent recurrences. Unfortunately it is plagued by the same problem of Poincaré's theorem but in the opposite direction: it holds only for an insignificantly small amount of time, the order of one-fifth of a mean free path [52]. Nevertheless, this last theorem is held in high regards by the scientific community for its great conceptual impact. For example, Gallavotti wrote:

> Thus Lanford's theorem [...] has an enormous conceptual importance (apparently not yet fully appreciated by many) because it shows in a mathematically precise and rigorous fashion that there is no incompatibility between irreversible evolutions like the one described by the Boltzmann equation and the completely reversible Hamilton equations that describe the details of the microscopic motions. In fact mathematical rigor is particularly welcome here in consideration of the enormous amount of speculation on the theme and of pretended proofs of inconsistency between macroscopic irreversibility and mechanics. ([22], p. 35,)

So here mathematical relevance gain the upper hand with respect to the physical one. It has been argued that Lanford result *complements* the Boltzmann's combinatorial argument and in a sense confirms the *Boltzmannian synthesis* [49]. As I tried to elucidate in the discussion above, I believe that this way of reasoning is flawed. The *Boltzmannian synthesis* is a form of explanation whose strength depends on the internal logical consistency and the validity of its assumptions and where interaction play no role. No mathematical result can confirm it or discredit it. As far as assumptions like independence and isotropy of velocities - in presence of extremely big number of degrees of freedom - can be assumed, the framework works, Poincaré recurrences permitting. The problem is to prove that this is also the case in presence of collisions. Here is where Lanford's theorem enters into the picture but at the price of very limited physical relevance.

6. Final remarks: moving beyond mono-causality?

Let me summarize the story so far. *Typicality* is a framework in which reversible equation of classical mechanics and thermodynamic phenomenology *coexists*, albeit not without tensions [56], through a statistical argument. The idea that the *Boltzmann synthesis* can be extended to dilute gases (binary collisions only assumed) is the starting point for the mathematical efforts culminated in the Lanford's theorem. Despite elaborated endorsements [31, 30] and confirmations [27, 12], those still not convinced by Boltzmann argument even for the gas-in-the-box case have proposed a variety of underlying physical mechanism as candidates for the correlation-breaking process.

Kinetic theory is not the only terrain related to irreversibility that requires mathematicians. There are also attempts to tackle the mathematical problem at a higher level of abstraction using the mathematical language of Dynamical Systems that is measure theory [6]. In a paper of 2001 Mackey discusses in detail a mathematical result where a microscopic explanation of the second law of thermodynamics is assured *if and only if* the system exhibit a particular and strong property called *exact dynamics*. At the end of the paper, in the final comments the author says (my italics):

> Consider the following thought experiment. Put a cat in a completely sealed [...] After one month, return and open the box. What will you find? The cat will, of course, be dead. Are we seriously to believe that this death was a consequence of coarse graining? Of a noisy environment? Of taking a trace? To me this is so patently ridiculous that I reject it out of hand. Animals *do not die in such circumstances because of our ignorance of dynamics* (coarse graining or traces) or *because of noise*. ([37])

I think this quotation is interesting in showing some enduring sources of misunderstanding that affects the problem of irreversibility. For clarity, here Mackey is conflating two different domains of the discourse: a) the conceptual (irreversibility from the coarse-graining process) and b) the physical (irreversibility due to external perturbation i.e. *interventionism*). With regard to point (a), Mackey concern here is related to the fact that this irreversibility that we introduce trough a process of coarse-graining looks like like a subjective "optical illusion" [42]. It looks as if coffee becomes colder and whiter when we ad some milk just because of the perspective we look at the system and not for an intrinsic *physical property* of the system. This was one of the main attacks to the Boltzmann program propelled by Prigogine and his School and critically considered by Bricmont [4]. Well, from the above discussion it can be said that this critics is only in part appropriate. The answer to the questions that Mackey poses in the above quotation is: *yes and no*. It is true that terms like "alive", "dead", "hot", "warm", "white", "black" are applicable only to aggregates, they are *coarse-graining* concepts that depend on the level of description like the 'number of heads'" of toy models in introductory treatments of statistical mechanics. On the other hand the process of approach to thermodynamical equilibrium in the way we observe it in ordinary situations reflects also the effect of underlying physical, empirical properties due to interaction between matter. Interactions between matter are not subjective believes of the observer. If interaction are negligible and independence and isotropy holds *in presence of huge degrees of freedom*, the *Boltzmannian synthesis* explains why at a given level of description irreversibility is observed (in the sense of the *Minus First Law*). Again, independence and isotropy does not depend on the observer but it is a physical property of material entities in universe. Regarding the role played by external perturbation, it is important to stress that this is not necessarily in competition with the *Boltzmannian synthesis* form of explanation. External noise, if present with a relevant magnitude, will definitely affect the way the system reach equilibrium and the structure of $M_{equilibrium}$. Depending on the case, when we leave simple and idealized "toy models", explanation of irreversibility can imply the need of a combination of conceptual frameworks at different domains of knowledge.

This leads me to the final note. To my knowledge so far no one tried to develop a systematic *multicausal* approach to the problem of irreversibility. There is this fixation for a search of a single ultimate cause that account for irreversibility and my impression is that different kind of explanation are always considered mutually exclusive. But this may not be the case as I hope it emerges from the discussion above. For example it has been argued by some notable scholars how the image of a deterministic universe at the microscopic level have been undermined by the development of modern physics [34]. Of course there is a perennial discussion on these issues [3]. In any case, a non-determinist universe can have something non trivial to do with its observed irreversibility at different levels of physical reality in a way that conspires together with the *Boltzmannian synthesis*. On the other hand when we jump from the gas-in-the-box model to cosmological consideration in discussing irreversibility (with for example the *past hypothesis*), a lot has still to be understood. I think that a multi-causal approach to irreversibility can be a research direction that deserves to be seriously explored.

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