Entropy from Clausius to Kolmogorov: historical evolution of an open concept

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Abstract: This communication is focused on a survey of entropy definitions that highlights the multifaceted nature of this basic concept. In literature there are more than 40 definitions, corresponding to distinct formal objects sharing a common name whose physical meanings strictly dependent on the disciplinary contexts wherein they were conceived. A historical contextualization of some paradigmatic entropy definitions helped to understand the origin of such epistemological plurality: entropy stands out as an "open concept" that underwent (and undergoes) a continuous evolution under the influence of socio-economic and cultural elements.

Keywords: Entropy Classification, Clausius, Gibbs' Free Energy, H Theorem, Communication Theory

1. Introduction

Entropy has an elusive character, well expressed by von Neumann's stunning statement: "Nobody knows what entropy really is, so in a debate you will always have the advantage". (Tribus *et al.* 1971) Irony aside, this provocative statement suggests the polysemous character of the term 'entropy' as well as a variability of meanings that can be related with distinct disciplinary contexts.

Driven by von Neumann's provocation, we undertook a survey of entropy's definitions found in the literature, with the double purpose of attempting a classification and a historical contextualization of such definitions. We spotted five main categories, referring to distinct disciplinary domains.

As for as the historical analysis of the entropy concept is concerned, we focused on the timeslot ranging from 1860s to 1960s. Within that period, we identified the following steps, based on technological and scientific arguments:

I. Clausius' thermodynamics, strongly pushed by the need of improving steam engine's efficiency;
II. the "second industrial revolution", marked by the industrial chemistry birth;
III. the foundational research at the beginning of the '*nouveau siècle*';
IV. post 2nd-world war period, marked by computers diffusion and Communication Theory development.

We sustain that entropy stands as an open concept still undergoing evolution: the starting point of such progressive path may be identified with 1865 Clausius' definition of entropy, but the final point – provided that it exists – remains undetermined. In the next sections we will give a synthetic presentation of these issues.

2. Attempting a Classification

As soon as one undertakes an investigation on entropy, it comes out that entropy is not a monolithic concept – as it could appear at a first sight: this single term hides a multitude of diverse formal objects belonging to different disciplinary domains. (Čápek *et al.* 2005) In order to handle this plethora of definitions, we attempted a classification aimed at facilitating a critical analysis of the existing relationships among these many functions. We finally managed to identify five categories, conceived on disciplinary basis, and consequently run a logical classification of 'entropies' based on some paradigmatic cases, as reported in Table 1.

First we spotted a 'physical entropy' category, gathering all functions whose definition directly refers to truly physical instances. This is the case of Clausius' original definition (Clausius 1867), but it also concerns contemporary entropy functions such as Gyftopoulous' and Beretta's. (Gyftopoulous *et al.* 1991)

A second set is represented by functions conceived within the context of an axiomatic approach to the Second Law: this is the case of Carathéodory (Carathéodory 1909), Lieb-Yngvason (Lieb *et al.* 1999) and Tsallis (Tsallis 2002) entropies. We refer to these functions as 'mathematical entropies' as they stand as formal parameters, whose physical meaning is not evident.

In his 1948 paper, Shannon (1948) defined a function (that he named entropy) as foundational element of his Mathematical Theory of Communication.

We have classified as 'informational entropies' those functions (such as Shannon's, Kolmogorov's and Fisher's (Pellegrino *et al.* 2016) related to Communication Theory.

Within the frame of density matrix formalism, Von Neumann conceived a quantum entropy function. (Čápek *et al.* 2005) Following Von Neumann's idea, other authors such as Daòczy, Rènyi, Hartley and Segal (Čápek *et al.* 2005) defined similar functions that we classified as 'quantum entropies'.

Finally we named 'statistical entropies' those statistical defined inside statistical-mechanics formal systems (e.g.: Gibbs' and Boltzmann's).

CATEGORY	DEFINITION	PARADIGMATIC CASES[1]
physical entropy	Experimentally measurable macroscopic entity, including Clausius' function that represents the transformation content (Verwandlungsinhalt) of thermodynamic systems	Clausius, Gyftopoulos, Beretta
mathematical entropy	Formal instance, including all definitions referring to the axiomatic formulations of thermodynamics Second Law	Caratheodory, Lieb-Yngvason, Tsallis
informational entropy	Mathematical functions related to the Theory of Communication	Shannon, Fischer, Kolmogorov
statistical entropy	Functions defined inside the diverse Statistical Mechanics' formal systems	Boltzmann, Gibbs
quantum entropy	The original variant was outlined by von Neumann with reference to the Density Matrix formalism; it can be seen as a measure of the "purity" of an arbitrary quantum state	Von Neumann, Daoczy, Renyi, Hartley, Segal

Table 1. Classification of entropy definitions

Such a systematic approach highlights that multiple entropy definitions are definitely not a pure linguistic issue. In fact, distinct entropic functions belong to truly different disciplinary domains. This is particularly evident when considering two extreme examples, such as Clausius' physical entropy and Shannon's informational entropy. Faced to this huge disciplinary multiplicity, we have decided to address our investigation towards the use of history as a connecting platform. In the next section we show how this choice allowed us to trace back a sort of historical *fil rouge* that eases the interpretation of entropy's ontological plurality.

3. History as a cognitive vehicle

The historical perspective whereby the epistemic analysis of entropy was pursued exploits history as an effective cognitive vehicle. The Entropy concept has been followed alongside an ideal time arrow displaying from 1860s to 1960s: within this period, we identified four major milestones, pictorially represented in Fig. 1.

[1] Author's names are used to label the corresponding entropic functions

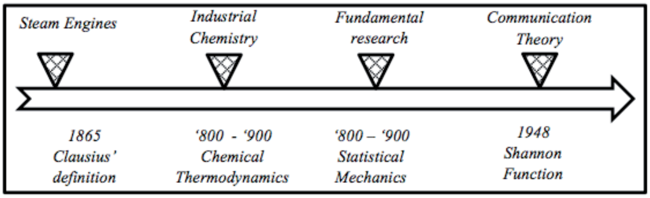

Fig. 1. Relevant Scientific and technological milestones taken into account in the timeslot ranging from 1860s to 1960s

The 'added value' of this approach is impressive. Entropy appears to be a still in-progress concept, undergoing an evolution: the starting point of such progressive path may be easily identified, whereas the final point – provided that it exists – remains undetermined. From a complementary perspective, entropy can be considered as a very "reactive" concept that absorbs features of the scientific-socio-historical context and responds to specific needs. Apart from these general insights, the results of our historical investigation are briefly reported in the following subsections.

3.1. Clausius' entropy: the beginning of the story

Clausius' definition of entropy, reported in his Ninth and last memoir (Clausius 1867), is the conclusion of a 15-year-long cognitive process that led to an exploitable mathematical expression of the Second Law. (Pellegrino *et al*. 2015) Clausius' contribution historically belongs to the tradition of 19th century thermodynamics sparked off by Carnot's famous paper (Carnot 1897), whose aim was to face the problem of improving heat engines' efficiency. Carnot figures out the economic importance of steam engines for a leading country, such as England at that time, in this hyperbolic passage:

> To take away today from England her steam engines would be to take away at the same time her coal and iron. It would be to dry up all her sources of wealth, to ruin all on which her prosperity depends, in short, to annihilate that colossal power. (Carnot 1897, p. 40)

Müller argues that the economic pressure exerted by 19th-century industrial needs – emerging from a dominant steam engine technology – actually oriented early thermodynamics research. More precisely, he points out that entropy emerged "in the context of the engineering proposition". (Müller 2007, p. 47)

It is worth reporting and briefly commenting the truly original entropy definition provided by Clausius:

$$dS = \frac{dH}{dt} + dZ \qquad (1)$$

This definition was given in terms of two pre-modern quantities – disgregation dZ and the internal heat dH – whose meaning was to be found within an archaic microscopic model of heat developed by Clausius.[2] This new quantity – the entropy – allowed Clausius to reformulate his "second fundamental theorem extended to non-cyclic process":

$$\frac{dH + dQ}{T} + dZ \qquad (2)$$

and obtain the famous inequality, that is a mathematical representation of the Second Law:

$$dS \geq \frac{dQ}{T} \qquad (3)$$

The final step of Clausius' work on entropy was to provide an exploitable way to determine this quantity by integrating the Second Law for reversible transformations:

$$S = S_0 + \int \frac{dQ}{T} \qquad (4)$$

3.2. Entropy and Industrial Chemistry

The second half of the 19th century was marked by profound socio-economical changes, as the industrial landscape saw the transition from plants fuelled by steam engines to chemical and electric industry. As far as chemical industry is concerned it is worth mentioning the paradigmatic case of indigo industrial synthesis. In 1897 the German chemical corporation "Badische Anilin und Soda Fabrik" (BASF) launched synthetic indigo on the market after a 30-year-long industrial research. As reported by Cerruti (2003), this event had at least a double relevance. First, it represented a prototype of industrial research – achieving the transition from the laboratory desk to a production plant. Second, from an economic standpoint the replacement of natural indigo by the synthetic molecule ignited the 'ideology' of Ersatz,[3] i.e. the use of synthetic chemical products instead of their natural homologues. Finally, the commercialization of synthetic indigo had dramatic consequences on the market of natural indigo. Just to fix the ideas, four years after the implementation of BASF indigo process, English planters had to reduce the surface of their plantations in Bengal by one-third. This example can efficiently evoke the historical, economic and scientific scenario of the second half of the 19th century that was clearly marked by new industrial needs and prompted scientific and technological research with new aims. In particular early industrial chemistry was in need of a formal system to handle the energetics of industrial processes involving chemical reactions. It was under the pressure of these external

[2] For a wider discussion on this matter, the reader can refer to Pellegrino *et al.* (2015).
[3] Ersatz can be translated as 'replacement'.

factors that thermodynamics – originally conceived to treat compression-expansion cycles in piston-cylinder systems – was extended to more complex systems involving chemical reactions. This cognitive extension of thermodynamics – whose foundations were mainly due to J.W Gibbs – took some decades to be accomplished and "accepted" by the worldwide chemical community. (Kragh *et al.* 1996)

Concurrently, the concept of entropy underwent an important epistemic transformation that can be traced back inside Gibbs' equilibrium theory. (Gibbs 1906) This latter is grounded on the geometrical representation of Clausius' laws for reversible systems, wherein entropy becomes a 'mere' geometric parameter (i.e. one Cartesian axis in the thermodynamic 3D-space). This new epistemic valence of entropy – along with energy and volume – allowed Gibbs to express the condition of thermodynamic stability of a system as the condition where entropy is maximized. Based on this conceptual foundation stone, Gibbs conceived a general thermodynamic theory suitable for the treatment of heterogeneous systems undergoing chemical reactions. This implied the introduction of new extensive quantities suitable to express stability conditions. It is worth mentioning Gibbs' 'free energy' that – in the conventional thermodynamic notation – corresponds to:

$$G = U + pV\text{-}TS \quad (5)$$

This function is currently used in physical chemistry to establish the direction towards which a chemical heterogeneous system can evolve spontaneously.[4] In the treatment of physical chemical systems, Gibbs' 'free energy' actually plays the same central epistemic role played by Clausius' entropy in thermo-mechanical contexts. Hence, part of Clausius' entropy epistemic content has been transferred to Gibbs' free energy, to the point that the latter is often considered as 'disguised entropy'.

3.3. Entropy and Statistical-Mechanics

Between the end of 19[th] and the beginning of 20[th] century, several disciplinary scientific domains saw a new foundation. Within a single year, 'annus mirabilis 1905', Einstein, Nernst and Planck published five fundamental papers.[5] (Müller 2007) This creative wave did not concern only physics but had a wider extension. Poincaré's fundamental works on three-body systems and the axiomatic definition of number by Giuseppe Peano are two further relevant examples.

During this 'gold period' for 'foundational research', the groundwork for modern Statistical Mechanics was also carried out. Based on Boltzmann's seminal intentions[6]

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[4] A heterogeneous system is stable at a Gibbs' free energy minimum.

[5] That is to say: I) Planck: Black Body Radiation, II-IV) Einstein: Special Relativity; Brownian motion; Photoelectric effect; V) Nernst: Heat Theorem.

[6] Boltzmann writes: "Aim of this treatise is to provide a truly analytic and general proof of the second law of mechanical theory of heat" (Translated by the author).

(Boltzmann 1866), kinetic theory original goal was to settle a cognitive justification for the Second Law at the microscopic level. Concerning Statistical Mechanics current status, Frigg clearly remarks that

> Unlike quantum mechanics and relativity theory, Statistical Mechanics has not yet found a generally accepted theoretical framework, let alone a canonical formulation. What we find in Statistical Mechanics is a plethora of different approaches and schools, each with its own program and mathematical apparatus, none of which has a legitimate claim to be more fundamental than its competitors. (Frigg 2008, p. 6)

This plurality is commonly approached by referring to "two theoretical frameworks, one of which can be associated with Boltzmann (1877) and the other with Gibbs (1902)", that can be classified as either 'Boltzmannian' or 'Gibbsian'. (Frigg 2008, p. 7)

As far as entropy is concerned, two relevant issues can be mentioned. First, entropy played a key role, in both statistical approaches, inside bridge equations relating the microscopic statistical formal system to the macroscopic thermodynamic model. Second, 'Boltzmannian' and 'Gibbsian' approaches foundationally differ for the mathematical expression of entropy (as to say H functions) and equilibrium definitions, given in terms of these latter functions. More precisely, in Boltzmann approach – for a N-particles-system – H_B is given by:

$$H_B = N \int w_1 log w_1 d\tau_1 \qquad (6)$$

and depends on a single particle probability density (w_1). Conversely, Gibbs' function H is defined in terms of a Liouville function or N-particles probability density (W_N) defined on the ensemble:

$$W_N = N \int W_N log W_N d\tau$$

Discussing the foundations of Statistical Mechanics is far from the aim of this presentation. Nevertheless we can mention the emerging centrality of H definitions in both statistical models. This mirrors the key role of entropy inside Statistical Mechanics (Jaynes 1965) and witnesses a first profound ontological transformation of the entropy concept.

3.4. Entropy and Communication Theory

The *post* 2nd-World-War period saw the development of modern Information Technology. Its origins are commonly traced back to Turing's machine and to the construction of Colossus – the analogical computer designed to decrypt Enigma, the Germans' secret code. Just after the war, computers started to be serially produced and underwent a large diffusion. Cybernetics, Semiotics and Communication Theory developed in this context under the pressure of external factors including the above-mentioned technological enhancements.

In his 1948 foundational paper (Shannon 1948), Shannon – a father of Communication Theory – defined a new function representing the number of bits exchanged through a communication channel. Shannon proposed three distinct names for such function: information, uncertainty and entropy. This latter choice – as witnessed by the author – was mainly due to its formal similarity with "the *H* in Boltzmann's famous H theorem". Nevertheless, the dimensions of Shannon's entropy correspond to the number of bits; hence it is clearly not an entropy *stricto sensu*.

Kolmogorov's contributions to Communication Theory are also worth to be mentioned. (Grünwald *et al.* 2003; Grünwald *et al.* 2004) In 1965, he defined another function to represent information. Kolmogorov function (or Kolmogorov complexity) applied to an information string is defined as its shortest binary description or alternatively as the length of the shortest computer program generating it. In this case the name entropy disappeared, highlighting that the function belonged to a new disciplinary domain, distinct from physics where entropy had started its long story.

4. Conclusions

Our analysis shows that entropy behaves as an open concept undergoing a continuous evolution. The historical survey highlights that entropy's polysemy has enriched the thermodynamics formal arsenal with a great epistemological plurality, albeit not devoid of inconsistencies. Moreover, entropy can be seen as a *still-in-progress* concept that has undergone several semantic changes under the pressure of evolutional factors such as cultural and social textures, depending on the specific historical background.

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