

## Chapter 7

# For a Fistful of Entropy

[... N]o one knows what entropy really is, so in a debate you will always have the advantage.

*J. von Neumann*

Among the thermodynamical terms that demand a statistical mechanical conceptualization, the case of entropy is an illuminating one. Originally invented by Clausius as a state function of an individual system in equilibrium which measures its energy degradedness, entropy remains one of the most elusive theoretical concepts in modern physics. The problem with TD entropy, as defined by Clausius and presented in the first section of this chapter, is not that it lacks a statistical mechanical analogue. Given that entropy is one of the most abused thermodynamical terms outside TD, it is natural that the situation in SM is quite to the contrary: SM seems to offer multiple realization of entropy, and the problem transforms into a case of a coherent choice between possibilities.

TD entropy, which is defined only in equilibrium state, has two counterparts in SM: Boltzmann's and Gibbs' entropies. In classical SM the two definitions of entropy yield similar, yet not identical, results in certain circumstances,<sup>1</sup> but rest on different conceptual foundations: the first applies to individual systems; the second to ensembles of systems. Notwithstanding instrumental arguments for preferring the latter, the aim of the second section of this chapter is to establish the conceptual superiority of the former in the classical realm.

In the third section we shall present the quantum mechanical entropy,

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<sup>1</sup>E.g., for an ideal gas in equilibrium. See Jaynes (1965).

the von Neumann entropy, and discuss some technical details necessary for evaluating the plausibility of the decoherence and the GRW approaches in the foundations of SM. Remarkably, Gibbs' old neglected fine-grained entropy becomes an attractive candidate in this regime. Finally in the fourth section we explore how the different approaches divide the above inventory of entropies between them.

## 7.1 Holy Entropy, Its Boiling! (G. Gamov)

Historically, heat was conceived as a weightless, elastic and fluid substance, or *caloric*, but at the end of the 17th century, after being the subject of much respectable scientific work, it was pronounced non-existent, and the caloric theory of heat was put on the shelf.<sup>2</sup> The concept of energy was introduced in 1847 by Helmholtz, who cited the work of Joule and used the term *Kraft* to denote the causal power of nature to act upon matter. Helmholtz contemporaries and successors believed that energy was present in bodies in two main forms only: (i) as energy of motion, or *kinetic energy*, equal to one-half the body mass times its squared velocity, and (ii) as energy of position or *potential energy*, equal to the work that must be done against ambient forces to carry the body from a position of (conventionally) zero potential energy to its present place. It was Joule's contribution that led to the recognition of the principle of conservation of energy. In this context heat was then regarded as kinetic energy.<sup>3</sup>

Already within the caloric theory of heat it was known, due to Sadi Carnot, that just as water yields mechanical work as it falls from a higher to a lower level, so does heat, then regarded as a substance, yields mechanical work as it falls from a higher to a lower temperature. Carnot showed that the efficiency of a heat engine, i. e. , the amount of work it can obtain from a unit of heat as this falls to a lower temperature, has an upper bound that depends only on the temperatures between which the engine operates.

The two principles, the first and the second laws of TD, were the building blocks of the new science of heat, founded by Clausius and Kelvin in the midst of the 19th century. Kelvin and Clausius gave two different versions of the second principle, embodying the gist of Carnot's idea without the water metaphor:<sup>4</sup>

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<sup>2</sup>For a detailed report see Fox (1971).

<sup>3</sup>Maxwell (1883).

<sup>4</sup>The citations are taken from Fermi (1936, 30).

A transformation whose only final result is to transform into work heat extracted from a source which is at the same temperature throughout is impossible (Kelvin).

A transformation whose only final result is to transfer heat from a body at a given temperature to a body at a higher temperature is impossible (Clausius).

Building on Carnot's work, Kelvin developed the absolute scale of temperature and, more relevant to us, Clausius the concept of entropy. It was defined by using the ratio between the amount of heat,  $Q$ , and the temperature,  $T$ , in a cyclic Carnot engine  $\mathcal{E}$ . Multiplied by the temperature difference in such an engine this ratio yields the amount of work that the engine can produce. Because this work has an upper bound, and because all reversible Carnot engines have the same efficiency, in this special case of *reversible thermodynamic process* entropy is a conserved quantity.

In the general continuous case of exchanging infinitesimal quantities of heat we then get:

$$\oint_{\mathcal{E}} \frac{dQ}{T} \leq 0. \quad (7.1)$$

the integral being taken over a complete cycle of  $\mathcal{E}$ . If the cycle is reversible we get,

$$\oint_{\mathcal{E}} \frac{dQ}{T} = 0. \quad (7.2)$$

and because the integral is independent of the course of the process then given a conventional reference state  $\mathcal{O}$ , we can now define a property of the thermal state  $\mathcal{A}$  by:

$$S(\mathcal{A}) \stackrel{\text{def}}{=} \int_{\mathcal{O}}^{\mathcal{A}} \frac{dQ}{T}. \quad (7.3)$$

Clausius called the quantity  $S(\mathcal{A})$  the *entropy* of  $\mathcal{A}$ . Evidently we get:

$$\int_{\mathcal{A}}^{\mathcal{B}} \frac{dQ}{T} = \int_{\mathcal{A}}^{\mathcal{O}} \frac{dQ}{T} + \int_{\mathcal{O}}^{\mathcal{B}} \frac{dQ}{T} = \int_{\mathcal{O}}^{\mathcal{B}} \frac{dQ}{T} - \int_{\mathcal{O}}^{\mathcal{A}} \frac{dQ}{T} = S(\mathcal{B}) - S(\mathcal{A}). \quad (7.4)$$

The definition of entropy as a property of state in eqn. (7.3) presupposes that the integral on the right-hand side depends only on  $\mathcal{O}$  and  $\mathcal{A}$ . The

integral must therefore be taken over a continuous succession of *reversible* or *quasi-static* heat exchanges. But once entropy was defined as a property of thermodynamic systems, one may well compare the entropy difference on the right-hand side in eqn. (7.4) taken over a continuum of *arbitrary* heat exchanges. Consider a cycle formed by an arbitrary process from  $\mathcal{A}$  to  $\mathcal{B}$  combined with a reversible one from  $\mathcal{B}$  to  $\mathcal{A}$ . We then get by eqn. (7.1),

$$0 \geq \oint_{\mathcal{A}\mathcal{B}\mathcal{A}} \frac{dQ}{T} = \int_{\mathcal{A}}^{\mathcal{B}} \frac{dQ}{T} + \int_{\mathcal{B}}^{\mathcal{A}} \frac{dQ}{T}.$$

Hence, by eqn. (7.4),

$$0 \geq \int_{\mathcal{A}}^{\mathcal{B}} \frac{dQ}{T} + S(\mathcal{A}) - S(\mathcal{B}).$$

and in the general case:

$$S(\mathcal{B}) - S(\mathcal{A}) \geq \int_{\mathcal{A}}^{\mathcal{B}} \frac{dQ}{T}. \quad (7.5)$$

If the process under consideration occurs in a completely isolated system,  $dQ = 0$ ; therefore, the entropy of the final state  $\mathcal{B}$  is always equal to or greater than that of the initial state  $\mathcal{A}$ . Thus, *in a closed thermodynamic system the entropy can never decrease.*<sup>5</sup>

Three remarks are in order. First, note that Clausius – relying as he was on the intuitive premise of the impossibility of a *perpetuum mobile* of the second kind which states that heat cannot, of itself, pass from a colder to a hotter body – introduced entropy as a primary concept. This has led many to regard irreversible phenomena as essential to the proof of the existence of entropy. Thus Sklar (1993, 21) writes:

The crucial fact needed to justify the introduction of such definite entropy value is the irreversibility of physical processes. It is the fact that heat engines cannot not only not generate mechanical work without the consumption of heat, but that they cannot be run in such a way as to produce work without degrading the

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<sup>5</sup>Note that this result applies only to *isolated* systems. Thus, it is possible with the aid of external system to decrease the entropy of a system. The entropy of both systems taken together, however, cannot decrease.

quality of heat in the world, that is crucial to the proof of the existence of entropy.<sup>6</sup>

But clearly the existence of the definite state function  $S$ , rather than being a consequence of the irreversible character of *spontaneous* heat processes is a result of nothing more than the mere fact that the integral

$$\int_A^B \frac{dQ}{T}$$

depends only on the extreme states of the transformation and not on the transformation itself.<sup>7</sup> This point is important since in many textbooks on SM misleadingly state that the second law of thermodynamics ‘drives’ systems to their equilibrium states and that entropy increases monotonically during this approach to equilibrium.

Sklar should have been more cautious to spell out exactly what he means when he says a sentence later that ‘the fundamental fact of irreversibility is summarized in the second law’. The second law simply states that *when* a process is irreversible, that is, in Clausius’ terms, non-quasi-static,<sup>8</sup> then the entropy difference between its initial and final states is positive. It is true that a simple reasoning leads to the conclusion that when a system reaches its maximum entropy state then it stays there forever unless external intervention drives it away from this state, but the fact that thermal systems *spontaneously* evolve towards equilibrium is *not* encompassed in the second law unless further conditions are satisfied.<sup>9</sup> In sum, the connection between entropy and the second law, if there is one, is quite simple and unfortunately different than what Sklar wants us to believe: the essential content of the second law of thermodynamics is the *existence* of an entropy function (and of absolute temperature) for every equilibrium state.<sup>10</sup>

Next, the classical understanding of Carnot cycles on which Clausius relies involves ‘quasi-static’ processes and these are by definition traceable by trajectories (or transformations) entirely contained in the space of possible

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<sup>6</sup>By now the attentive reader begins to appreciate the sloppy editorial mistakes Sklar’s monumental book suffers from. This is surprising since a good editor could have made the book much shorter yet no less monumental...

<sup>7</sup>Fermi (1936, 49–50).

<sup>8</sup>Uffink (2001, 318–319).

<sup>9</sup>For more on the truth and myth behind the second law see Uffink (2001) and Uffink and Brown (2002). These issues are discussed below in chapter eight.

<sup>10</sup>This result is also known as the Heat Theorem. See also Emch and Liu (2002, 78).

states of the system. But since all that is needed to construct the entropy function is that the initial and final states belong to this space, the value of the entropy function depends only on the state and not on its history. From this it is clear that TD entropy can be defined only in equilibrium, and that rather than a primary concept, entropy should be best regarded as derivative.<sup>11</sup>

Finally, Clausius' definition of entropy requires an arbitrary choice of a standard state. It can be easily shown that the difference between the entropies of a state  $\mathcal{A}$  obtained with two different standard states is a constant,<sup>12</sup> and since we are dealing with entropy *differences* this indeterminacy should not trouble us. However, it was only the third law of TD which completed the entropy definition and enabled to determine this constant.

So far we have described TD entropy as a state function of an individual system in equilibrium which never decreases in thermodynamical transformations. But as a function entropy has many more properties, of which three – additivity, extensivity, and concavity – are important to the discussion that follows.

1. **Additivity.** Assuming that the energy of a system is the sum of the energies of all its parts, and that the work performed by the system is equal to the sum of the amounts of work performed by all the parts, the entropy of a composed system is equal to the sum of the entropies of all its parts. In the axiomatic framework of Lieb and Yngvason (1999) the requirement of sum functions is subsumed under the axioms, i.e., under the definitions of adiabatic processes and states in state space. It is then possible to write

$$S(\mathcal{X}, \mathcal{Y}) = S(\mathcal{X}) + S(\mathcal{Y}). \quad (7.6)$$

for every state of any composed system.<sup>13</sup>

2. **Extensivity.** An extensive variable scales with the size of a macroscopic system. Thus, entropy, energy and volume are extensive (but temperature is intensive) and we can write for each  $t > 0$  and for each

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<sup>11</sup>A way to formulate TD in these terms was pioneered by Cartheodory in 1909 and was later consolidated by Giles (1964) and Lieb and Yngvason (1999).

<sup>12</sup>Fermi (1936, 52).

<sup>13</sup>Recall that  $\mathcal{X}$  and  $\mathcal{Y}$  are equilibrium states on the state space of the system.

state  $\mathcal{X}$  and its scaled copy  $t\mathcal{X}$ :<sup>14</sup>

$$S(t\mathcal{X}) = tS(\mathcal{X}). \quad (7.7)$$

3. **Concavity.** Assuming that the state space of a thermodynamic system is a convex set, the entropy of an isolated system is a strictly concave function of its arguments.<sup>15</sup> Why is concavity considered important? It means that for  $\lambda_1, \lambda_2 > 0; \lambda_1 + \lambda_2 = 1$ :

$$S((\mathcal{X} \oplus \mathcal{Y})) \geq \lambda_1 S(\mathcal{X}) + \lambda_2 S(\mathcal{Y}). \quad (7.8)$$

where equality holds when  $\mathcal{X} = \mathcal{Y}$  or when the  $\lambda$ s are 0 or 1. We shall see that when one moves to SM, entropy is usually regarded a measure of the lack of information, hence if two ensembles of identical systems in different states  $\mathcal{X}$  and  $\mathcal{Y}$  are fitted together,<sup>16</sup> one loses information that tells from which ensemble a specific sample stems, and therefore entropy increases.

Summarizing, entropy in TD is a well-defined state-function of an individual physical system in equilibrium. Its elusive character, however, is revealed once we move to the realm of statistical mechanics and join the quest for the ‘holy grail’ – a mechanical model for thermal phenomena.

## 7.2 Entropy in SM - Boltzmann vs. Gibbs

The gap between continental philosophy and the Anglo-American tradition has drawn much attention in many different contexts. It is thus not surprising that also in classical SM two orthodoxies – continental and American –

<sup>14</sup>A scaled state space is physically interpreted as a state space of a system whose properties are the same as in the original one, except that the amount of each chemical substance in the system has been scaled by the factor  $t$  and the range of other extensive variables, e.g., energy, volume, has been scaled accordingly.

<sup>15</sup>We say that a function  $f$  is (strictly) concave if  $-f$  is (strictly) convex. What is convexity? Let  $R^n$  denote  $n$ -dimensional Euclidean space (i.e. the set of all real-valued vectors of length  $n$ ). A subset  $D$  of  $R^n$  is said to be convex if,  $\forall(x, y) \in D$ , and  $\forall\lambda \in [0, 1]$ , we have  $\lambda x + (1 - \lambda)y \in D$ . (i.e., for any two points in  $D$ , the line segment connecting the two points lies entirely in  $D$ ). Now Let  $f$  be a function defined on a convex subset  $D$  of  $R^n$ . We say that  $f$  is convex if  $\forall(x, y) \in D$  and  $\forall\lambda \in [0, 1]$ , we have  $f(\lambda x + (1 - \lambda)y) \leq \lambda f(x) + (1 - \lambda)f(y)$ . For function  $f$  defined on  $R$ , this inequality says that the chord connecting any two points on the graph of  $f$  lies above the graph. If equality holds if and only if either  $x$  and  $y$  are identical, or  $\lambda = 0$  or  $\lambda = 1$ , then  $f$  is said to be strictly convex.

<sup>16</sup>What in the mathematical language is described by a ‘convex combination’ of  $\lambda_1\mathcal{X} + \lambda_2\mathcal{Y}$ , and is noted here with the sign  $\oplus$ .

clash. Back in the continent contemporary debates on the atomic hypothesis and the kinetic theory led Boltzmann to introduce his concept of entropy. On the other side of the ocean it was Gibbs who formulated SM in pragmatic terms of which one was his coarse-grained entropy. Both approaches and the entropies they introduce as counterparts to the thermodynamic concept presented briefly above are in many cases in perfect agreement in equilibrium states. Yet, as a matter of fact, Gibbs' approach governs the literature. It is the purpose of this section to persuade the reader that from a foundational point of view and within the context of constructing a mechanical model for thermodynamic phenomena on the basis of Hamiltonian dynamics, one should prefer Boltzmann's entropy to Gibbs'.

My strategy in achieving this goal is an old one. Rather than defending Boltzmann's entropy I am going to attack Gibbs'. The tactic, however, is novel. I am going to elaborate on a long forgotten essay of Carnap (1977) written when he was a visiting fellow in Princeton. What is interesting in this essay is that although Carnap is right on the money when he criticizes Gibbs' approach and the hastiness in identifying entropy with information-theoretic uncertainty which accompanies it, he does so on the basis of what he considers an epistemological flavour which the Gibbsian approach introduces into an otherwise strictly physical context. This, unfortunately, blunts his criticism since he can be accused of committing the fallacy of exchanging 'subjectivity' with 'contextuality'. By amending this flaw I expose the genuine and more serious problem in Gibbs' coarse-grained entropy and conclude that within the standard Hamiltonian framework Boltzmann presents a far more desired alternative to the foundations of SM.

### 7.2.1 Gibbs

In Gibbs' approach one represents the microstate of a physical system with  $N$  particles each with  $f$  degrees of freedom by a point  $X \in \Gamma$  where  $\Gamma$ , the phase space of the system, is a  $2Nf$ -dimensional space spanned by the  $Nf$  momenta and  $Nf$  configuration axes. As the system evolves this representative point will trace out a trajectory in  $\Gamma$  which obeys Hamilton's equations of motion.<sup>17</sup>

Next, one considers a fictitious ensemble of individual systems (represented by a 'cloud', or a 'fluid', of points on phase space) each in a microstate compatible with a given macrostate (say, such and such energy in such and

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<sup>17</sup>See Gibbs (1902) and Appendix B.



such pressure contained in such and such volume). The macroscopic parameters thus pick out a distribution of points in  $\Gamma$ . We then ascribe a normalized density function to the ensemble,  $\rho(p, q, t)$ , and, except for entropy and temperature, the mean value of phase function with respect to  $\rho$  describes the system's thermodynamic properties.<sup>18</sup>

For entropy Gibbs chooses the expression

$$S_{FG}(\rho(X)) = -K \int \rho(X) [\log \rho(X)] d\Gamma. \quad (7.9)$$

where the integral is over  $\Gamma$  and  $K$  is Boltzmann's constant.

For isolated systems we use the microcanonical probability distribution in (7.9),<sup>19</sup> and this will match up to an additive constant the value for TD entropy. Eqn. (7.9) also allows us to define a temperature. Remarkably, using these definitions Gibbs recovers the familiar thermodynamic relations for systems in equilibrium.

All this is so very fine, but if Gibbs' systems obey Hamilton's equations of motion then the 'cloud' representing them in phase space swarms like an incompressible fluid.<sup>20</sup> Consequently his 'fine-grained' entropy as defined in (7.9) is *invariant* under the Hamiltonian flow:

$$\frac{dS_{FG}(\rho)}{dt} = 0. \quad (7.10)$$

If there is a problem in  $S_{FG}$  it is not just the fact that it does not move. Recall that TD entropy is defined only in equilibrium, so in order to construct a mechanical counterpart one only needs to find a function whose value at a later equilibrium state is higher than at an earlier equilibrium state.<sup>21</sup> But since the macroscopic parameters change between the two equilibrium states, the Gibbs' approach has no problem in doing this just by defining a new ensemble with a new probability distribution for the new equilibrium state and this will match the thermodynamic entropy as before.

This solution, however, reminds one of a famous exchange in the Journal of Philosophy where, in commenting on a paper titled "Supervenience Is a

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<sup>18</sup>This follows from the fact that for extensive functions of macroscopic systems with large number of particles the mean value is identical with the maximum value.

<sup>19</sup>That is, we regard each microstate as equiprobable.

<sup>20</sup>This fact is also known as 'Liouville's theorem'. See Appendix B.

<sup>21</sup>Callender (1999, 358).

Two-Way Street” G. Hellman wrote “Yes, But One of the Ways is the ‘Wrong Way’!”<sup>22</sup> Indeed, as Callender (*ibid.*) who follows Sklar (1993, 54) notes, it is not fair to use the macro-parameters, which are supposed to be derived from the micro-parameters, in order to construct the latter. In other words, the ensemble at later equilibrium state should be the Hamiltonian-time-evolved ensemble of the earlier equilibrium state, otherwise the system is not governed by Hamilton’s equations as one originally presupposes. Thus, if one wants to use Gibbs’ fine-grained entropy as a mechanical counterpart to TD entropy, then one must abandon standard, Hamiltonian, dynamics since it does not connect the two fine-grained equilibrium states.

That *this* is the true problem with Gibbs’ fine-grained entropy escaped many commentators, and as a result the foundations of SM were soon piled with a lot of dead wood. Stemming from the famous Ehrenfests’ paper (1912, 43–79) where Boltzmann’s students complained on Gibbs’ treatment of irreversibility by categorizing it bluntly as “incorrect”,<sup>23</sup> the last century was consumed with attempts to find a monotonically increasing function as a counterpart for TD entropy.

One way to achieve this goal is to follow Gibbs himself, who introduces the mathematical trick of ‘coarse graining’ and devises new notions of entropy and equilibrium. In this approach one divides  $\Gamma$  into many small finite cells of volume  $\omega$  and then takes the average of  $\rho$  over these cells. The result,  $\hat{\rho}$ , is attributed to all the points in the cell  $\Omega_i$ . This allows us to write the coarse-grained probability distribution as the ensemble density in each cell:

$$\hat{\rho} = \frac{1}{\omega} \int_{\Omega_i} \rho(p, q, t) d\Gamma. \quad (7.11)$$

And although  $\rho$  is conserved by the Liouville flow, its density in each cell need not be so. Thus, equilibrium is defined as a state in which  $\rho$  has fibrillated uniformly throughout the available  $\Gamma$ , and by substituting  $\hat{\rho}$  with  $\rho$  in (7.9) one then defines the coarse-grained entropy as:

$$S_{CG} = -K \int \hat{\rho}(\log \hat{\rho}) d\Gamma. \quad (7.12)$$

But as Callender (*ibid.*, 360) notes, this cannot be the whole story, since according to Gibbs the irreversible behaviour of  $S_{CG}$  is due solely to coarse graining, that is, to our incomplete knowledge of the microstates:

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<sup>22</sup>Hellman (1992).

<sup>23</sup>Ehrenfest (*ibid.*, 71).

Thermodynamic behaviour does not depend for its existence on the precision with which we measure systems. Even if we knew the positions and the momenta of all the particles in the system, gases would still diffuse through their available volume.

Callender, however, is both right and wrong. He is right that in order to account for irreversibility coarse graining alone is not sufficient. As Ridderbos (2002, 69) tells us, to complete the Gibbsian story the dynamics of the system must also lead representative points far away from each other, that is, the dynamics should satisfy mixing conditions or any of the stronger conditions in the ergodic hierarchy.<sup>24</sup> But Callender claims further that coarse graining cannot be necessary for the explanation of irreversibility since it hinges on a kind of epistemological subjectivity which seems irrelevant to the physical course of events, and although I agree with his further claim, I beg to differ on the reason behind it.

While it is true that coarse graining introduces a kind of ‘subjectivity’ into SM which presumably not only has no counterpart in TD but also depends on an arbitrary choice of resolution on the experimenter’s side, Callender’s criticism and the line of thought it gives voice to has only limited validity. There are more serious criticisms of the coarse graining method and the concept of entropy which accompanies it. Before fleshing these out let me mention here yet another philosopher who took the claim about subjectivity to its extreme.

### 7.2.2 Carnap Against ‘Subjectivity’

Carnap’s two essays on entropy were written during his tenure fellowship at the Institute of Advanced Studies in Princeton between 1952 and 1954. Here is a passage that summarizes best his conclusion from conversations concerning entropy with mathematicians and physicists in Princeton:<sup>25</sup>

It seemed to me that the customary way which the statistical concept of entropy is defined or interpreted makes it perhaps against the intention of physicists a purely logical instead of a physical concept; If so, it can no longer be, as it was intended to be, a counterpart to the classical macro-concept of entropy

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<sup>24</sup>See Appendix B and also Krylov (1979) who constructs the entire foundations of SM on the basis of dynamical instability of trajectories in phase space.

<sup>25</sup>Carnap (*ibid.*, xii).

introduced by Clausius, which is obviously a physical and not a logical concept. The same objection holds in my opinion against the recent view that entropy may be regarded as identical with the negative amount of information.

The core of Carnap's argument is that TD entropy has the same character as temperature, pressure, heat, etc. all of which serve "for the quantitative characterization of some objective property of a state of physical system".<sup>26</sup> Gibbs' entropy, according to Carnap, cannot be regarded a counterpart to TD entropy since by definition it depends upon the specificity of the description, hence it is an epistemological rather than a physical concept.

Furthermore, by referring to an unpublished paper of his, "The concept of degree of order", Carnap (*ibid.*, 10) criticizes the view which regards entropy as a measure of disorder. If one distinguishes, as he does in his unpublished paper (and as we have done in chapter three, section 3.4), between epistemic and ontological randomness, it becomes clear that the existence of genuine randomizing procedure entails disorder, or epistemic randomness, in any chosen level of description, but the converse does not hold. It then follows that if entropy is defined in terms of genuine randomizing procedure or mechanism it would provide more information about disorder in various levels than an entropy concept defined in terms of disorder at a certain chosen level.

In order to see why this line of criticism has only limited validity, and why, if one wants to reject Gibbs' entropy on a *foundational* basis, a more serious line of criticism should be taken, consider the following three points:

1. Contrary to what Carnap (and Callender) claim, there are many thermodynamic entropies, corresponding to different degrees of experimental discrimination and different choices of parameters. As E.T. Jaynes (1965, 398) famously remarks, "[E]ven at the purely phenomenological level entropy is an anthropomorphic concept". Similarly, in SM the definition of entropy depends on what macroscopic description of the system is chosen, and in a given macroscopic description a variety of definitions are possible.<sup>27</sup> If this is so, then (a) Carnap's reasoning can be accommodated with the different entropies in TD, to each of which one can construct a physical *objective* counterpart, and (b) that

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<sup>26</sup>Carnap (*ibid.*, 35).

<sup>27</sup>Grad (1961); Penrose (1981).

human choice dictates the use of this or that family of concepts does not discredit the objectivity of each *member* of the family.

2. Even if we accept Carnap's demand for a randomizing procedure in the definition of an objective concept of entropy, Gibbs's approach is still consistent with such demand. Entropy, according to Gibbs, is a functional of the probability distribution on  $\Gamma$ . If this probability distribution were established by a random procedure then Carnap's requirement would be fulfilled. A careful reading of Gibbs' (1902, ch. 14) shows that this is indeed the case – the canonical distribution is appropriate for a system which has reached equilibrium with a heat reservoir, while the contact with the latter serves as a physical randomizing process.<sup>28</sup>
3. Finally, if entropy is defined according to a level of description, and if the latter is justified by the experimental arrangement and the physics involved, then this only means that entropy is a *contextual*, or a *relational*, concept, and not a primitive one. *Given* a specific observer with a given, fixed, measurement resolution, it is the dynamics of the system which uniquely determines whether or not a particular non-uniform probability distribution evolves to a coarse grained distribution which is uniform with respect to the given measurement resolution.<sup>29</sup>

The upshot is that if one argues against coarse graining, as Carnap and Callender do, on the basis of its 'subjectivity' alone then one allows the Gibbsian to escape the criticism through the above three loopholes. It is one thing to say that the probabilities of SM are purely epistemic, and another to ground these epistemic probabilities in the physics of thermal phenomena. Thus, the coarse graining method yields an entropy which is not subjective but contextual,<sup>30</sup> and the more serious criticism of the coarse-

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<sup>28</sup>Note the striking similarity here to the open system approach and the caveat that this procedure is not *genuinely* random.

<sup>29</sup>See Ridderbos (*ibid.*, 72).

<sup>30</sup>The distinction between these two adjectives was, unfortunately, blurred because of careless readings of many authorities in physics. Thus for example, Heisenberg (1970, 38) writes:

Gibbs was the first to introduce a physical concept which can only be applied to an object when our knowledge is incomplete.

and Born (1964, 72) adds:

Irreversibility is therefore a consequence of the explicit introduction of ignorance into the fundamental laws.

grained entropy lies not in its ‘subjectivity’ but in the fact that this concept of entropy is foreign to the project of constructing a *dynamical* model for thermal phenomena.

### 7.2.3 The (Real) Case Against Coarse Graining

A short reminder: thermodynamic equilibrium is defined as a state in which the thermodynamic variables are stationary. Let us call the part of the theory which involves the relations between these variables in equilibrium thermostatics, and the rest of the theory which describes the relations between different equilibrium states thermodynamics.<sup>31</sup> Since TD entropy (which despite the fact that it cannot be measured directly is still a member of a distinguished small set of the thermodynamic variables) is defined only in equilibrium, it ‘plays’ its thermodynamical ‘role’ in the relation between the entropies in two equilibrium states.<sup>32</sup>

*Prima facie* Gibbs’ approach satisfies the requirement for reproducing *thermostatics* since Gibbs’ ensembles give correct results in equilibrium states and allows one to recover the correct relations between the thermodynamic variables. Yet this achievement loses much of its appeal as soon as one recalls that the original project was to do so on the basis of the underlying dynamics.

In TD it is meaningful to say that a certain individual system, say, a gas in a box, occupies an equilibrium state. But in Gibbs’ approach an equilibrium ensemble contains *by definition* individual systems which are far away from equilibrium. Without further criteria for identifying the ensemble components it remains unclear how to relate in *dynamical* terms the average quantities the equilibrium ensemble yields with the thermodynamic variables which apply to an *individual* system. Since Gibbs’ micro-canonical distribution generates empirically verified predictions, the question here is not *whether* but *why* such relation holds.<sup>33</sup>

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Some may regard these quotes and the acceptance of Gibbs’s approach they advocate as yet another distressing effect that QM has had upon the foundations of physics.

<sup>31</sup>Although also here the TD trajectories trace ‘quasi-static’ processes, that is, infinitely slow transitions from one equilibrium state to another.

<sup>32</sup>If the process which connects two equilibrium states is *not* quasi-static no thermodynamic trajectory can trace it. Nevertheless the entropy difference between the two states is still a well defined quantity.

<sup>33</sup>Leeds (1989) goes further and argues that the question is not why but rather why do Gibbs’ averages work for one observable quickly, and for another slowly. The remarkable

The gap between Gibbs’ ensembles and the underlying dynamics becomes wider when we move from thermostatics to thermodynamics. We have already mentioned the problem with Gibbs’ fine-grained entropy: there exists no way to connect two fine-grained entropies in different equilibrium states with Hamilton’s equations. This is the price we pay when in order to circumvent the famous reversibility and recurrence objections we define Gibbs’ entropy as a function of a probability distribution of a fictitious *ensemble* of systems, rather than of an individual system.<sup>34</sup> Unfortunately, in paying this price we simply abandon the original goal which was to account for thermal phenomena with the micro-dynamics.

Presumably, those who insist on maintaining Gibbs’ fine-grained entropy can live with the lack of dynamical justification for its verified predictions in thermostatics. Yet even they must admit that Gibbs’ coarse-grained entropy must be abandoned if it yields *false* predictions in thermodynamics.

Recall that coarse-graining is invoked because – due to Liouville’s theorem – the fine-grained entropy cannot evolve into a uniform distribution in phase space which is the mark of ‘true’ equilibrium. As a result an alternative concept of equilibrium is introduced in which only an “appearance” of equilibrium is obtained. Let us call this “apparent” equilibrium ‘quasi-equilibrium’.<sup>35</sup> This ‘quasi-equilibrium’ distribution indeed gives rise to the same values of macroscopic variables that define the thermodynamic state of the system as does the fine-grained distribution and for all practical purposes the two definitions are empirically indistinguishable. The fine-grained entropy, however, is still subject to the dynamical laws which preserve the correlations between the system’s micro-components and reflect the hidden ‘order’ in the system. These correlations are ignored in ‘quasi-equilibrium’, and the discrepancy between the ‘true’ and ‘quasi’ equilibria becomes evident when one is able to control the micro-components of the system, either directly or indirectly.

As already mentioned in chapter five (section 5.4), the famous ‘spin-echo’ experiments exemplify exactly such case of indirect control. Since in these experiments the first RF signal is induced after the spins have reached ‘quasi-equilibrium’, the echo produced by their alignment *after* the

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fact is that unless one assumes (non-physical) strict ergodicity the microcanonical probability distribution is even not unique, that is it is not the only one which is preserved under the dynamics. See Earman and Redei (1996).

<sup>34</sup>See Callender (*ibid.*, 352) for a lucid formalization of the problem.

<sup>35</sup>The term was coined by Blatt (1959, 749).

first signal comes as a complete surprise to the coarse-graining method which must regard such innocent velocity reversal a violation of the second law.<sup>36</sup>

Another facet of the same problem arises when one recalls that the fine-grained distribution – subject as it is to Hamilton’s laws – is also susceptible to the consequences of Poincaré’s recurrence theorem.<sup>37</sup> In thermodynamics such recurrence will result in decreasing TD entropy. It is true that, as Boltzmann remarked to Zermelo, we should live that long to observe such a state, but what is important here is that the coarse-grained entropy – increasing monotonically in time as it is – *never* decreases, hence cannot account for such true violation of the second law which according to Hamilton’s equations is possible *in principle*.<sup>38</sup>

Summarizing, Gibbs’ coarse-graining approach fails in two ways. First, as the spin-echo experiments show it predicts a violation of the second law when there is none. Second, with its insistence on a monotonically increasing function of entropy it fails to predict such violation when there is one. Both failures stem from the simple fact that the Gibbs’ approach, in its attempt to free itself from the dynamical restrictions imposed on an individual system, becomes *irrelevant* to the individual system, hence has little to do with the micro-dynamical origins of thermal phenomena. Consequently, if one’s aim is to construct a counterpart for TD entropy in classical mechanics one must abandon Gibbs’ coarse-grained entropy and look elsewhere.

#### 7.2.4 Boltzmann

It has become somewhat fashionable to resurrect L. Boltzmann’s old neglected concept of entropy, especially the reconstructed post- $H$ -theorem entropy recently championed by authorities in statistical physics.<sup>39</sup> Boltzmann introduces a concept of entropy twice along his career: first when he derives the  $H$ -theorem, and second, when he defends this theorem against the reversibility and recurrence objections of Lochsmitz and Zermelo.<sup>40</sup> Both concepts are statistical in character, yet they differ in the origins of the probabilistic assumptions introduced into the underlying dynamics:<sup>41</sup> In the  $H$ -theorem it is an assumption about continuous randomization of molecules’

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<sup>36</sup>Ridderbos and Redhead (1998).

<sup>37</sup>See Appendix B.

<sup>38</sup>Callender (1999, 366).

<sup>39</sup>E.g., Lebowitz (1994); Gallavoti (1999); and Goldstein (2001).

<sup>40</sup>See Klein (1973) for an account of the evolution of Boltzmann’s ideas.

<sup>41</sup>See chapter five (section 5.1).



collisions (the ‘molecular chaos’ assumption) which is necessary for the derivation of a stationary Maxwell-Boltzmann velocity distribution; in the post- $H$ -theorem case it an assumption of equiprobability of microstates combined with pure combinatory.

Although the former concept of entropy has been described by some, e.g., Price (1996) as ‘a dead horse’, it is the one that is more related to the dynamics of the system hence is much closer in spirit to Boltzmann’s original goal – that of constructing a mechanical counterpart to TD entropy.<sup>42</sup> Setting this involved issue aside, I want to concentrate here on Boltzmann’s later concept, the one which appears as an epitaph on his tomb in Vienna’s Central Cemetery.

Contrary to Gibbs’s ensemble approach, Boltzmann’s entropy  $S_B$  is defined for the actual microstate  $\mathbf{x}$  of an individual system which corresponds to a macrostate  $M(\mathbf{x})$ . The latter, in turn, is compatible with many different microstates. In order to *count* how many microstates are compatible with a given macrostate we partition the 6-dimensional energy surface of the phase space of the  $N$ -particles individual system, say, an ideal gas, (this space is called  $\mu$ -space) into compartments which are macroscopically indistinguishable – they share the same thermodynamic features – and specify the number of particles in each cell. Each such specification, or *arrangements* (Boltzmann called them ‘complexions’), determines a macrostate. The  $\mu$ -space is important only for counting the number of arrangements compatible with  $M(\mathbf{x})$ . Once we determine this we are able to associate with each  $M$  a volume in  $\Gamma$ . Different arrangements yield different macrostates and these partition  $\Gamma$  into disjunctive volumes. The volumes are ‘generated’ by the projection of the Lebesgue measure onto the energy surface.<sup>43</sup> Boltzmann’s entropy is then defined as:

$$S_B = K \log |\Gamma_{M(\mathbf{x})}| + C. \quad (7.13)$$

where  $K$  is Boltzmann’s constant,  $C$  is an additive constant which depends on  $N$ , and  $|\Gamma_{M(\mathbf{x})}|$  is the volume of phase space associated with the macrostate  $M(\mathbf{x})$ .

For a gas in a box, where  $N$  is in the order of  $10^{23}$ , there are overwhelmingly more arrangements corresponding to an equilibrium state (where

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<sup>42</sup>A quick survey of the physics literature demonstrates, however, that working physicists are unimpressed of Price’s remark. Boltzmann’s  $H$  theorem gave rise to Boltzmann’s equation which is one of the most useful equations in statistical physics.

<sup>43</sup>See Appendix B.

the macro-parameters are uniformly distributed in the *physical space*, and the Maxwell-Boltzmann velocity distribution is uniformly distributed in  $\mu$ -space) than, say, to a state in which most of the gas is confined to a certain corner of the box with nonuniform distributions. Thus, an equilibrium state occupies almost all the relevant energy surface on  $\Gamma$ . In chapter two (section 2.2.2) and in Appendix B we discuss how to translate statements about volume in phase space into probability statements. We can then say with Boltzmann that thermal equilibrium is the most probable, or the *typical*, state of a physical system.<sup>44</sup>

Gibbs' coarse-grained entropy displays one of the characteristics of TD entropy – strict non-decrease; Boltzmann's displays another – additivity. Both functions, however, are concave and extensive. The latter property allows Boltzmann's entropy to attain non-decrease *except for exceedingly rare cases*. The reason is simple. If one acknowledges the vast separation of scales between the macroscopic and the microscopic levels then after dividing  $S_B$  with the spatial volume of the system one obtains entropy per unit volume whose differences for different macrostates are of order unity. This means that if *NEQ* is a state in which a gas of  $N$  particles is confined to half a container with an external constraint and *EQ* is a state in which the same gas is spread all over the container, the *ratios* of the volumes  $|\Gamma_{EQ}|$  and  $|\Gamma_{NEQ}|$  is of the order  $2^N$ , which in the case of a gas with  $10^{23}$  particles is  $2^{10^{23}}$ . Thus, there is a probability of  $2^{-10^{23}}$  that a gas in *NEQ* would stay there once an external constraint is dropped.<sup>45</sup> Many physicists can live with that.

### 7.2.5 A Short Bookkeeping

As in the case of Gibbs' coarse-grained entropy, this cannot be the whole story. Since Boltzmann's entropy measures the number of microstates that the system *is not in* but could be in without us noticing, it serves more as a (quantitative) description than as a causal explanation to thermal phenomena. Surely it cannot be the case that the number of microstates our gas in a box *does not* occupy 'drives' the gas towards equilibrium. Considering that one's project is to construct a *mechanical* model for TD, the dynamics must play a certain role – if only to justify the probabilistic assumptions that lead to the definition of entropy as a probability measure. Furthermore,

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<sup>44</sup>Lebowitz(1994); Goldstein (2001).

<sup>45</sup>This, in fact, is the precise meaning of the term *typical*. See Goldstein (2001, 43).

Boltzmann's approach leaves us with another problem: since the dynamics of classical mechanics are TRI, unless we postulate an initial low entropy state for the universe as a whole, nothing prevents entropy from increasing also towards the past, which seems to go against our memories and experience. And although we can design low entropy states in the lab, why was the entropy of the universe low to begin with?

Notwithstanding these shortcomings which were discussed extensively in previous chapters, Boltzmann's entropy is a better starting point for a reduction project than Gibbs', simply because (1) it is defined as a function of individual systems and these are what we usually observe,<sup>46</sup> (2) it has *almost* all the properties of TD entropy, and (3) it behaves correctly.

Among its three merits, (1) is the most important since it ties Boltzmann's entropy to the underlying dynamics and this immediately leads to (3). The price, as is well known, is the '*almost*' in (2): the second law becomes a statistical law, in the spirit of Maxwell's (1995, 583) famous remark:

The second law has the same degree of truth as the statement that if you throw a thumbful of water into the sea you cannot get the same thumbful of water out again.

Callender (*ibid.*, 371), however, adds another feature: (4) Boltzmann's entropy can be extended to the quantum regime since the volume of a macrostate in phase space has a natural quantum analogue, namely, the dimension of the projector on the macrostate in Hilbert space. Yet this feature is not unique to Boltzmann's entropy since Gibbs' *fine-grained* entropy has similar analogues. We move, then, to the quantum regime to meet these counterparts.

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<sup>46</sup>The term 'objective' is deliberately omitted here since although the number of microstates corresponding to a macrostate is an objective matter, there still exists a kind of coarse-graining in Boltzmann's definition, apart from the fact that if Boltzmann were to pick the velocity-position space instead of the momenta-position space his entropy definition would not have worked. It is noteworthy that Callender (*ibid.*) who attacks Gibbs' entropy on the basis of its subjectivity allows a fair amount of physically justified choice of description when his pet entropy is concerned.

## 7.3 Entropy in the Quantum World

### 7.3.1 Von Neumann's Entropy

In his famous treatises on QM von Neumann introduces his concept of quantum entropy:<sup>47</sup>

$$S_{VN} = -K \text{Tr} \rho \ln \rho , \quad (7.14)$$

and justifies his definition on a thermodynamical basis. Contrary to Gibbs' who was cautious to *identify* his concept of entropy with the thermodynamical concept and referred to it only as an "analogue", von Neumann and many other authorities in QM take  $S_{VN}$  to be *identical* with TD entropy.<sup>48</sup>

Von Neumann's quantum mechanical formalism guarantees that during a measurement  $S_{VN}$  increases.<sup>49</sup> This feature, however, does not in itself assure us that  $S_{VN}$  is indeed TD entropy or that *entropy* increases during a measurement. In order to establish that von Neumann proposes a thought experiment which heuristically equates mixed states with chemical mixtures.<sup>50</sup> This experiment leads to an arithmetical argument intended to prove that the decrease in thermodynamical entropy is compensated by an increase in  $S_{VN}$ .

Additional formal features of  $S_{VN}$  are supposed to support von Neumann's claim. Thus, for example,  $S_{VN}$  is concave and additive.<sup>51</sup> Furthermore, Peres (*ibid.*, 268) mentions its tendency towards equilibrium.<sup>52</sup> Another favourable feature is that  $S_{VN}$  formally resembles Shannon's (1948) famous concept of entropy in communication theory:

$$I = -K \sum_{n=1}^N p_n \ln p_n. \quad (7.15)$$

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<sup>47</sup>Where  $K$  is Boltzmann's constant and  $\rho$  the density matrix of the system. Von Neumann (1932/1955, ch. 5) extends an earlier work of his from 1927.

<sup>48</sup>See, e.g., Peres (1993, 270) who claims that  $S_{VN}$

...is genuine entropy, fully equivalent to that of standard thermodynamics.

<sup>49</sup>In the ideal case of a pure state represented as an ensemble of identical systems, the initial  $S_{VN}$  is zero (since by definition for a pure state  $\rho^2 = \rho$ ). Measuring another operator we transform the ensemble into a mixture in which  $\rho^2 \neq \rho$  and  $S_{VN} > 0$ .

<sup>50</sup>Von Neumann (*ibid.*, 360–379). See also Peres (1993, 260–275); Shenker (1999, 36–40); and Petz (2000, 85–90).

<sup>51</sup>Werl (1978, 237–239; 241).

<sup>52</sup>Notwithstanding its TRI evolution which Peres, interestingly, regards as advantageous.

Under the interpretation of  $p_n$  as the probability of obtaining outcome  $n$  in a spectrum of a magnitude we intend to measure,  $I$  characterizes the probability distribution  $\{p_1, \dots, p_N\}$  and can be interpreted as measuring our ignorance of the future outcome.<sup>53</sup> But as Shenker (*ibid.*, 41–42) warns us, the quantity in (7.15) is not unique and depends on the initial state and the choice of magnitude to be measured. Uniqueness can be obtained by choosing the lowest value  $I$  can assume for any complete measurement. In this special case the magnitude which minimizes  $I$  is the density matrix  $\rho$ . Thus, in this case, and only in this case,  $I = S_{VN}$ . Now, since entropy in classical SM is also defined as a function of a probability distribution and can be interpreted as a measure of ignorance, the formal similarity and the linkage to SM entropy are regarded as yet another support to the equivalence between  $S_{VN}$  and TD entropy.<sup>54</sup>

Clearly this chain of reasoning is non-trivial at best. Yet it is threatened to fall apart as soon as Shenker (*ibid.*, 42–46) and Shenker and Hemmo (2003) convincingly demonstrate that von Neumann’s argument – the only argument in the literature so far which is supposed to prove the equivalence between  $S_{VN}$  and TD entropy – is inconsistent. Furthermore, since von Neumann’s proposal is based on a process which dissipationlessly transforms mixed states into pure ones and during which  $S_{VN}$  decreases with no compensation on the TD entropy side, it follows that were  $S_{VN}$  on a par with TD entropy then von Neumann’s thought experiment itself would have been a huge *perpetuum mobile* machine of the second kind.<sup>55</sup>

The moral I wish to draw here is that the hastiness in identifying entropy and information is premature and even dangerous. It was Landauer (1961) who coined the much abused phrase ‘Information is Physical’ by relating thermodynamic irreversibility with the erasure of information from a memory device. Yet there exists a wide gap between the fact that the hard-disk in my desktop computer needs ventilation to statements such as ‘Information is the currency of nature’.<sup>56</sup> First, as Bar Hillel (1955) already points out, the concept of *semantic* information has intrinsically nothing to do with

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<sup>53</sup>Von Neumann himself does not discuss this interpretation, which is clarified, e.g., in Peres (*ibid.*, 260–264).

<sup>54</sup>Note that such inference presupposes that in classical SM there exists a valid counterpart to TD entropy.

<sup>55</sup>Shenker illustrates the *reductio ad absurdum* of von Neumann’s argument by calculating the work that such machine could have preformed: in room temperature it would have lifted 176 Kilograms by 1 meter!

<sup>56</sup>Lloyd (1989, 193).

communication or information theory. Second, if Shenker’s argument tells us something it is surely that:

It is both useful and legitimate to use  $S_{VN}$  as a quantification of the amount of information one has regarding the system’s state and the possibility of predicting results of future measurements. ... However, information and entropy are not synonymous: the present paper demonstrates that one can change while the other remains constant.<sup>57</sup>

Maintaining a clear conceptual distinction between TD entropy and information-theoretic uncertainty is, of course, consistent with acknowledging that the price for acquiring information is always an increase of entropy.<sup>58</sup> Setting aside these intriguing conceptual issues, for our purpose the foregoing is sufficient to establish that until there appears in the literature another argument in support and contrary to repeated claims,<sup>59</sup> von Neumann’s entropy cannot be regarded as a counterpart to TD entropy. The question whether QM can produce a counterpart to entropy in SM is discussed below, but it is already clear that even if it could, the transition from QM to TD is not as straightforward as von Neumann and his followers assume.<sup>60</sup> If our goal is to find a quantum analogue to this entropy we should either justify von Neumann’s claim or, again, look elsewhere.

### 7.3.2 Wigner’s Function

It is well known that the uncertainty principle makes the concept of phase space in quantum mechanics problematic. Since a particle cannot simultaneously have a well defined position and momentum, one cannot define a true phase space probability distribution for a quantum mechanical system. Nonetheless, functions which bear some resemblance to (classical) phase

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<sup>57</sup>Shenker (*ibid.*, final footnote).

<sup>58</sup>See, however, Shenker (2002) for yet another convincing argument, this time a devastating criticism of Landauer’s principle.

<sup>59</sup>E.g., Peres (1989; 1993).

<sup>60</sup>Note how inconvenient Shenker’s result is for generations of physicists who used to obtain a  $S_{FG}$  as a function of a classical probability distribution from  $S_{VN}$  just by replacing the density matrix with the phase space probability distribution and the trace with the integral in phase space. Let me restate my claim: no matter how consistent this move is – both expressions are conserved by the Liouville flow and  $S_{FG}$  can take negative values only when the uncertainty principle is violated (see next section) the claim that  $S_{VN}$  is the entropy of *thermodynamics* remains unjustified.

space distribution functions have proven to be of great use in the study of QM systems. Apart from the calculational advantage these function also shed light on the connections between classical and quantum mechanics since modulo a certain difficulty they allow to express QM averages in a form which is very similar to that for classical averages.

Before we spell out this difficulty let us note that the use of the ‘quasi-probability-distribution’ functions was originally formed by Wigner (and refined by Husimi and Moyal) as an alternative representation of a quantum mechanical state.<sup>61</sup> In particular, it can serve as an equivalent substitute for the usual density matrix formulation.<sup>62</sup> Consequently, nothing new is gained here in terms of bridging the gap between von Neumann’s entropy and TD entropy. The following, however, allows us to pin point yet another problem with quantum entropy: its relation to entropy in SM.

Wigner’s representation is a useful tool to express quantum mechanics in phase space formalism. In this representation, a quantum state is described by a Wigner function (i.e. a function of the phase space variables  $q$  and  $p$ ), and Wigner’s equation provides an evolution equation for the state which is equivalent to the quantum Liouville equation.<sup>63</sup> Wigner’s function  $W(q, p)$  is defined in terms of the density matrix  $\hat{\rho}$  for a quantum mixed state

$$W(q, p) = \frac{1}{\pi\hbar} \int_{-\infty}^{+\infty} dy \langle q - y | \hat{\rho} | q + y \rangle e^{ipy/\hbar}, \quad (7.17)$$

or in terms of the wave function  $\psi(q)$  for a pure state

$$W(q, p) = \frac{1}{\pi\hbar} \int_{-\infty}^{+\infty} dy \psi^*(q + y) \psi(q - y) e^{ipy/\hbar}, \quad (7.18)$$

and possesses many of the properties of a phase space probability distribution: it is real, normalized to unity, and, when integrated over  $q$  or  $p$ , gives the correct marginal distribution, e.g.  $\int W dp = \langle q | \hat{\rho} | q \rangle =$  spatial density.

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<sup>61</sup>Wigner (1932) and Wigner *et. al.* (1984). That this alternative is rarely mentioned or used in QM textbooks is a result of the complexity involved in the representation of, e.g., the eigenstate-eigenvalue link. See Wigner *et. al.* (*ibid.*, 132).

<sup>62</sup>Wigner’s function is actually a Fourier transform along the antidiagonals of  $\rho$ , and since this transform is invertible,  $\rho$  is recoverable from  $W$ .

<sup>63</sup>The latter reads:

$$i\hbar \frac{\partial \rho}{\partial t} = H\rho - \rho H. \quad (7.16)$$

where  $\rho$  is the density matrix and  $H$  the Hamiltonian.

Furthermore, it can be used to compute averages of any dynamical variable  $A(q, p) : \langle A \rangle = \int W A dqdp$ .<sup>64</sup>

Despite these good properties, Wigner’s function cannot be straightforwardly interpreted as a probability distribution since for certain regions in phase space it can assume negative values! This is not surprising since the uncertainty principle forbids a complete joint localization in position and momentum. If, however, one is interested, as we are, in *approximate* joint measurements of  $p$  and  $q$  one can ‘blur’ Wigner’s function over phase space regions of volume  $\sim \hbar^n$  and in so doing one obtains a probability distribution of that approximate state.<sup>65</sup>

In this case the equation of motion for Wigner’s function is given by Moyal’s bracket:

$$\{H, W\}_{mb} = -i \sin(i\hbar\{H, W\}_{pb})/\hbar \quad (7.19)$$

where  $\{H, W\}_{pb}$  is the Poisson bracket describing the classical evolution (Liouville flow) of Wigner function  $W$ , and  $H$  is the Hamiltonian.<sup>66</sup> With this equation of motion it becomes almost possible to interpret the motion of quantum states as following quasi-classical trajectories on phase space.

Why ‘almost’? Because the ‘blurring’ of  $W$  is still not sufficient to ensure a straightforward interpretation of  $W$  (or  $\rho$ ) as a classical probability distribution since the state we wish to consider might be an *entangled* state. In other words,  $\rho$  might contain interference terms and if we wish to interpret it as a probability distribution we must first eliminate these. In other words, we must first solve the measurement problem!

We have arrived to the first positive result so far. A solution to the measurement problem would eliminate the interference terms in  $\rho$  either by a physical collapse (in the GRW framework) or by an apparent collapse (in the no-collapse theories powered by decoherence) hence would allow us to make progress in the attempts to define a quantum counterpart to SM entropy. In the Gibbsian case what necessitates this is the need for a (quasi-classical) probability distribution on phase space; In the Boltzmannian case

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<sup>64</sup>Note however that, since some terms in  $A(q, p)$  may not commute, it is necessary to establish a non-ambiguous correspondence between classical variables and quantum operators. This is known as Weyl’s rule. See Wigner *et. al.* (*ibid.*, 132).

<sup>65</sup>See Wallace (2001) and references therein.

<sup>66</sup>See Appendix B.



– it is the need to ensure that the system *is* in a given macrostate.<sup>67</sup> In both frameworks one must diagonalize  $\rho$  in order to make sense of the quantum probabilities and *a fortiori* of the transition from QM to SM.<sup>68</sup>

As mentioned in chapter six (section 6.3) the case of quantum chaos and celestial mechanics has recently provided a playground for the GRW and the decoherence approaches to demonstrate their ability in generating quasi-classical trajectories in phase space.<sup>69</sup> Remarkably, when a system is open to interaction with its environment decoherence ensures that the rate of von Neumann’s entropy production approximates the rate of the dynamical entropy production (the customary ‘currency’ in classical chaos).

Even more remarkable is the fact that this move has also contributed to the evaporation of some of the generic problems of classical SM, e.g., the measure-zero problem. Recall that in classical SM under the standard measure on phase space many results hold except for a measure-zero subset of phase space points.<sup>70</sup> How can we assign zero probability to these points when other measures assign them non-zero measures?<sup>71</sup> Sklar would have nothing to worry about in the case of QM: the measure-zero subset has no analogue in Wigner’s representation since *every* state occupies a phase space region with nonzero standard measure and individual points have no physical meaning. Thus, contrary to classical SM, any dynamical result applying to a nonzero measure region on phase space will apply to *all* states. This, moreover, is not mere artefact of Wigner’s representation. In QM in general – and thus in the actual world – there is no sense in localizing phase space

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<sup>67</sup>As Hemmo and Shenker (2003) remind us, “in the Boltzmann framework it is part of the parcel that the system actually *be* in a given microstate and *a fortiori* in a given macrostate.”

<sup>68</sup>Note that without such solution even von Neumann’s entropy itself can be given neither a Gibbsian interpretation nor a *Boltzmannian* one, the latter being a division of the diagonal elements of  $\rho$  into sets corresponding to different macrostates. See Hemmo and Shenker (*ibid.*)

<sup>69</sup>Agreed, the models presented by Zurek (1998) and Vitali and Grigolini (1998) are nothing but toy models but they are quite sufficient as a possibility proof. In particular, they exemplify the closed/open system dichotomy and its role in recovering CM from QM.

<sup>70</sup>Sklar (1993, 182–188) is a long cry of despair of this problem.

<sup>71</sup>Recall that our choice of a measure is usually made on grounds of convenience. Given a probability distribution we can represent it by any measure since if the probability of finding a system in a region  $\mathcal{R}$  in phase space is given by  $\int_{\mathcal{R}} f d\mu$  where  $f$  is a probability distribution and  $\mu$  a measure, any modifications of  $\mu$  can be compensated for by modifications of  $f$ . See Wallace (2001, sec. 3.3).

points on such a small scale.<sup>72</sup>

### 7.3.3 Another, (Shorter), Bookkeeping

Let us summarize the results so far. Contrary to what distinguished physicists claim, in QM there still exists no justified *direct* counterpart for TD entropy. In the case of SM entropies, however, the situation is more involved. Here the possibility of generating such counterpart is mediated by a necessary solution to the measurement problem. Once this solution is established, however, it opens the way to counterparts for either Boltzmann's entropy or Gibbs' fine-grained entropy.

In the first case, one can construct an analogue for the concept of phase space volume associated with a given macrostate (1) directly, as Callender (*ibid.*, 371) suggests, with the notion of the dimension of the projector on the macrostate in Hilbert space, or (2) indirectly with the notion of the classical phase space volume generated by the microstates that are compatible with the macrostates. In the second case a function of a probability distribution can be constructed either with von Neumann's entropy or with Wigner's function. Note, moreover, that a solution of the measurement problem also frees these functions from the restrictions of Liouville's theorem since in the decoherence approach (when accompanied by no-collapse interpretations) the dynamics are effectively non-linear. The question remains whether the novel dynamics can connect two Gibbs' entropies in two equilibrium states.

Finally, if one believes that SM entropies such as Boltzmann's entropy or the dynamically-free improved Gibbs' fine-grained entropy are valid counterparts to TD entropy as defined by Clausius, one can proudly claim that QM offers an *indirect* counterpart to TD entropy which is additive, concave, extensive, and even non-decrease.

## 7.4 Taking Sides?

Our goal was to investigate the inventory of entropies in the domains of TD, SM, and QM. We saw that TD entropy is a well-defined concept. Problems start when one wishes to construct a mechanical analogue to this concept. The underlying dynamical laws then constrain one to introduce probabilistic assumptions with respect to the initial conditions which accompany the laws

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<sup>72</sup>Wallace (*ibid.*).

since SM entropy, if defined for an individual system, cannot increase either for all initial states (the reversibility objection) or for all times (the recurrence objection). Ways about this problem, such as Gibbs' coarse graining, were examined and found wanting. We thus remained with two SM candidates for entropy: Boltzmann's entropy  $S_B$ , and Gibbs' fine-grained entropy  $S_{FG}$ , which notwithstanding their partial agreement are founded on quite distinct conceptual grounds. In the classical realm, moreover, the former is more appealing since it is defined for an individual system and it behaves (almost always) correctly while the latter – defined as it is for a fictitious ensemble of systems – is frozen and the attempts to unfreeze it are foreign to the original goal of constructing a mechanical model to TD entropy based on Hamiltonian dynamics.

When we moved to the quantum regime we saw that there still exists no justified direct counterpart to TD entropy. What QM could offer were indirect counterparts to  $S_B$  and  $S_{FG}$ . Such offer, however, came with a price: we first had to solve the measurement problem. In doing so we discovered that the effort was worth our while since (1) some generic problems of classical SM such as the measure-zero problem evaporated; (2)  $S_{FG}$  was finally unfrozen; and (3) as we are about to discover, the original goal of constructing a *purely* mechanical model for TD entropy, free from external non-dynamical probabilistic assumptions can be fulfilled.

Well, we have certainly narrowed the possibilities as we now have to choose between collapse and decoherence, that is, between the GRW theory and open system approach; between chance and ignorance.<sup>73</sup>

The GRW approach to the measurement problem – regarding as it is the wave function as representing an *individual system* – aims to recover Boltzmann's concepts of entropy and equilibrium. If Albert's (1994; 2001) dynamical hypothesis is correct, then the GRW jumps – the chancy probabilities for the collapse transition – *reproduce* the probabilities of the classical trajectories on phase space calculated from the standard statistical mechanical measure for any given macrostate of the system.<sup>74</sup> As we have seen in section 7.2.4, this measure implies in turn that a thermodynamical normal behaviour is a stable property, that is, that an equilibrium state

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<sup>73</sup>Note that the kind of ignorance introduced by the open system approach is completely orthogonal to the ignorance Gibbs' coarse graining method is usually accused of. In this case the ignorance is a natural, even physical, result of the dynamics of a physical system and has nothing to do with contextual measurement resolutions.

<sup>74</sup>Hemmo and Shenker (2001; 2003).

is overwhelmingly more probable than non-equilibrium state and that the transition from the latter to the former is a transition from an improbable state to a probable one.

Contrary to classical SM, in order to reproduce the Boltzmannian account the GRW theory need not refer to an *a priori* postulate of equiprobability or to any other postulate regarding a probability distribution on initial states. Since the transition probabilities of the GRW are genuinely stochastic, whether Albert’s dynamical hypothesis is true or not, and *a fortiori* whether the standard measure of classical SM is the correct measure or not, becomes an *empirical* issue with no recourse whatsoever to initial states or probability distributions thereof.

In the decoherence approach, on the other hand, one regards the quantum state as representing an ensemble, and not an individual system, hence the Gibbsian framework is the appropriate SM reference. First one interprets  $\rho$  as a mixture and  $W$  as probability distribution. Second, one uses Gibbs’ concept of *fine-grained* equilibrium as a stationary probability distribution over phase space towards which  $W$  approaches.<sup>75</sup>

In chapter five (sections 5.4 and 5.5) we discussed the conceptual difficulties that the quantum decoherence approach faces in general and in particular in the context of reproducing thermodynamic phenomena. In this chapter we spelled out some of the technical facets of these difficulties, namely, the problematic interpretations of  $\rho$  or  $W$  as probability distributions. But once we supplement quantum decoherence with no-collapse *interpretations* of QM the extra dynamical laws of these interpretations allow us to interpret the reduced state as a probability distribution over the components of the wave function and to regard it as an ‘effective’ state of the system.

Hemmo and Shenker (*ibid.*) propose to apply decoherence (powered by no-collapse interpretations) also in the *Boltzmannian* context. In doing so they suggest that the open system approach reproduces Boltzmann’s concepts of entropy and equilibrium to the extent the GRW theory does.

Their idea is that once macroscopic superpositions are suppressed by

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<sup>75</sup>Recall that in the quantum chaos models of celestial mechanics the interactions with the environment unfreeze the dynamics and allows  $W$  to spread in phase space, and, as a result to increase the otherwise conserved entropy of von Neumann in a rate which remarkably approximate the increase rate of dynamical entropy for classical chaotic systems. See Zurek and Paz (1994); Zurek (*ibid.*).

decoherence and an effective reduced state is ensured, the coherent states (which – entangled least as they are – represent the most stable states under the time evolution when the latter includes the decoherence interaction) ensure that the interference terms in  $\rho$  wash out and re-interfere only when the wave function spread in position becomes larger than the coherence length, a point in which decoherence operates again.

The result is that in successive times along the time-evolution of the system the coherent states diagonalize  $\rho$ . Now, if the dynamics of the certain no-collapse interpretation we apply are such that the transition probabilities between two successive effective states are *stochastic*, that is, if the two-times correlation is not 1 – 1, then given a dynamical hypothesis similar to that of Albert, these transition probabilities play exactly the same role played by the GRW jumps.<sup>76</sup>

Setting aside the deep conceptual consequence of this proposal, i.e., the unavoidable dichotomy between reality and appearance and the choice of the *latter* as the subject matter of our most fundamental theory,<sup>77</sup> until now only modal interpretations among the no-collapse theories demonstrate genuine stochastic transition probabilities which given the interaction with the environment, are independent of the total evolution of the system.<sup>78</sup> In the many worlds interpretation the status of the transition probabilities is still under dispute, and in Bohmian mechanics the transition probabilities are not genuinely stochastic since the trajectory of the quantum system depends on the (deterministic) dynamics and on the initial conditions. The recovery of thermodynamics with Bohmian mechanics is thus very similar to classical SM.<sup>79</sup>

Of course, since all no-collapse theories are TRI the ultimate reason for

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<sup>76</sup>Hemmo and Shenker (*ibid.*) regard the remarkable results of Zurek and co. in quantum chaos as supporting their dynamical hypothesis, yet one should recall that the quantum chaos results are given in the Gibbsian framework, and although the concepts of entropy in Boltzmann and in Gibbs approaches are usually regarded as yielding similar results in equilibrium, they are quite distinct. One relevant difference is that in the Boltzmannian account individual systems fluctuate *away from* equilibrium while in the Gibbsian account they fluctuate *in* equilibrium and the latter is stable over time. Furthermore, For Zurek's results to give support to their dynamical hypothesis Hemmo and Shenker must assume that von Neumann's entropy is TD entropy, and as we have seen, this is questionable.

<sup>77</sup>See chapter five (section 5.5).

<sup>78</sup>Bacciagalupi and Dickson (1999). Note that the 'openness' of the system to an interaction with the environment is crucial to this independence.

<sup>79</sup>No wonder that many hard headed Bohmians are also Boltzmannians...

the approach to equilibrium lies in the initial conditions, yet these are now *dynamical* rather than thermodynamical, that is, they are the conditions for decoherence to occur. Once these are granted and once the system is open, its thermodynamic behaviour may be recovered. Yet contrary to the GRW theory where the total evolution of the wave function is non TRI, in the open system approach if the evolution of the total wave function is such that *recoherence* should occur, it would occur regardless of the stochastic character of the transition probabilities. To the attentive reader this comes as no surprise: chance and asymmetries *in* time, as we have argued in chapter four, are independent issues, and only an inquiry into the foundations of physics can bring them together or keep them far a part.

Can we take sides and end this chapter with yet another heretic move in the foundations of SM?<sup>80</sup> Not yet. But we have demonstrated that the notions of chance and ignorance are on a par again, and the metaphysical differences between them are waiting to be turned experimental.<sup>81</sup> Until then, both contribute to the foundations of SM. The analysis of their connection with TD, however, is still missing. This task is undertaken next.

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<sup>80</sup>No offence, but the tradition of describing all the possible solutions to a certain problem in the foundations of SM and then leaving matters undecided is known in the corridors of philosophy departments as “Sklarism”.

<sup>81</sup>The term ‘experimental metaphysics’ was coined by Abner Shimony when J.S. Bell formulated his famous inequality and paved the road to Aspect’s experiment and the analysis of EPR paradox. In our case, two possible experiments involving spin echoes and light gases are discussed in Albert (2001) and in Hemmo and Shenker (*ibid.*).