

# Preface

In 1902, after three decades that Ludwig Boltzmann formulated the first version of standard statistical mechanics, Josiah Willard Gibbs shares, in the Preface of his superb *Elementary Principles in Statistical Mechanics* [1]: “*Certainly, one is building on an insecure foundation . . .*” After such words by Gibbs, it is, still today, uneasy to feel really comfortable regarding the foundations of statistical mechanics from first principles. At the time that I take the decision to write the present book, I would certainly second his words. Several interrelated facts contribute to this inclination.

First, the verification of the notorious fact that all branches of physics deeply related with theory of probabilities, such as statistical mechanics and quantum mechanics, have exhibited, along history and up to now, endless interpretations, reinterpretations, and controversies. All this fully complemented by philosophical and sociological considerations. As one among many evidences, let us mention the eloquent words by Gregoire Nicolis and David Daems [2]: “*It is the strange privilege of statistical mechanics to stimulate and nourish passionate discussions related to its foundations, particularly in connection with irreversibility. Ever since the time of Boltzmann it has been customary to see the scientific community vacillating between extreme, mutually contradicting positions.*”

Second, I am inclined to think that, together with the central geometrical concept of *symmetry*, virtually nothing more basically than *energy* and *entropy* deserves the qualification of *pillars* of modern physics. Both concepts are amazingly subtle. However, energy has to do with *possibilities*, whereas entropy with the *probabilities* of those possibilities. Consequently, the concept of entropy is, epistemologically speaking, one step further. One might remember, for instance, the illustrative dialog that Claude Elwood Shannon had with John von Neumann [3]: “*My greatest concern was what to call it. I thought of calling it “information,” but the word was overly used, so I decided to call it “uncertainty.” When I discussed it with John von Neumann, he had a better idea. Von Neumann told me, “You should call it entropy, for two reasons. In the first place your uncertainty function has been used in statistical mechanics under that name, so it already has a name. In the second place, and more important, nobody knows what entropy really is, so in a debate you will always have the advantage.*” It certainly is frequently that we hear and read diversified opinions about what *should* and what *should not* be considered as “*the physical entropy*,” its connections with heat, information, and so on.

Third, the dynamical foundations of the standard, Boltzmann–Gibbs (*BG*) statistical mechanics are, mathematically speaking, *not* yet fully established. It is known that, for classical systems, exponentially diverging sensitivity to the initial conditions (i.e., positive Lyapunov exponents almost everywhere, which typically imply mixing and ergodicity, properties that are consistent with Boltzmann’s celebrated “molecular chaos hypothesis”) is a *sufficient* property for having a meaningful statistical theory. More precisely, one expects that this property implies, for many-body Hamiltonian systems attaining thermal equilibrium, central features such as the celebrated exponential weight, introduced and discussed in the 1870s by Ludwig Boltzmann (very especially in his 1872 [5] and 1877 [6] papers) in the so called  $\mu$ -space, thus recovering, as particular instance, the velocity distribution published in 1860 by James Clerk Maxwell [7]. More generally, the exponential divergence typically leads to the exponential weight in the *full* phase space, the so-called  $\Gamma$ -space first proposed by Gibbs. However, are hypothesis such as this exponentially diverging sensitivity *necessary*? In the first place, are they, in some appropriate logical chain, *necessary* for having *BG* statistical mechanics? I would say *yes*. But are they also *necessary* for having a valid statistical mechanical description at all for *any* type of thermodynamic-like systems?<sup>1</sup> I would say *no*. In any case, it is within this belief that I write the present book. All in all, if such is today the situation for the successful, undoubtedly correct for a very wide class of systems, universally used, and centennial *BG* statistical mechanics and its associated thermodynamics, what can we then expect for its possible generalization only 20 years after its first proposal, in 1988?

Fourth, – last but not least – no logical-deductive mathematical procedure exists, nor will presumably ever exist, for proposing a new physical theory or for generalizing a pre-existing one. It is enough to think about Newtonian mechanics, which has already been generalized along at least two completely different (and compatible) paths, which eventually led to the theory of relativity and to quantum mechanics. This fact is consistent with the evidence that there is no unique way of generalizing a coherent set of axioms. Indeed, the most obvious manner of generalizing it is to replace one or more of its axioms by weaker ones. And this can be done in more than one manner, sometimes in infinite manners. So, if the prescriptions of logics and mathematics are helpful only for analyzing the *admissibility* of a given generalization, how generalizations of physical theories, or even scientific discoveries in general, occur? Through all types of heuristic procedures, but mainly – I would say – through *metaphors* [11]. Indeed, theoretical and experimental scientific progress occurs all the time through all types of logical and heuristic procedures, but the particular progress involved in the generalization of a physical theory immensely, if not essentially, relies on some kind of metaphor.<sup>2</sup> Well-known examples are the idea of Erwin Schroedinger of generalizing Newtonian mechanics through a *wave*-like

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<sup>1</sup> For example, we can read in a recent paper by Giulio Casati and Tomaz Prosen [9] the following sentence: “While exponential instability is sufficient for a meaningful statistical description, it is not known whether or not it is also necessary.”

<sup>2</sup> I was first led to think about this by Roald Hoffmann in 1995.

equation inspired by the phenomenon of optical interference, and the discovery by Friedrich August Kekule of the *cyclic* structure of benzene inspired by the shape of the mythological Ouroboros. In other words, generalizations not only use the classical logical procedures of *deduction* and *induction*, but also, and overall, the specific type of inference referred to as *abduction* (or *abductive reasoning*), which plays the most central role in Charles Sanders Peirce's *semiotics*. The procedures for theoretically proposing a generalization of a physical theory somehow crucially rely on the construction of what one may call a *plausible scenario*. The scientific value and universal acceptability of any such a proposal are of course ultimately dictated by its successful verifiability in natural and/or artificial and/or social systems. Having made all these considerations the best I could, I hope that it must by now be very transparent for the reader why, in the beginning of this Preface, I evoked Gibbs' words about the fragility of the basis on which we are founding.

The word "*nonextensive*" that – after some hesitation – I eventually adopted, in the title of the book and elsewhere, to refer to the present specific generalization of *BG* statistical mechanics may – and occasionally *does* – cause some confusion, and surely deserves clarification. The whole theory is based on a single concept, namely the *entropy* noted  $S_q$  which, for the *entropic index*  $q$  equal to unity, reproduces the standard *BG* entropy, here noted  $S_{BG}$ . The traditional functional  $S_{BG}$  is said to be *additive*. Indeed, for a system composed of any two (probabilistically) *independent* subsystems, the entropy  $S_{BG}$  of the sum coincides with the sum of the entropies. The entropy  $S_q$  ( $q \neq 1$ ) violates this property, and is therefore *nonadditive*. As we see, entropic additivity depends, from its very definition, only on the functional form of the entropy in terms of probabilities. The situation is generically quite different for the thermodynamic concept of *extensivity*. An entropy of a system or of a subsystem is said *extensive* if, for a large number  $N$  of its elements (probabilistically *independent or not*), the entropy is (asymptotically) proportional to  $N$ . Otherwise, it is *nonextensive*. This is to say, extensivity depends on *both* the mathematical form of the entropic functional *and* the correlations possibly existing within the elements of the system. Consequently, for a (sub)system whose elements are either independent or weakly correlated, the additive entropy  $S_{BG}$  is extensive, whereas the nonadditive entropy  $S_q$  ( $q \neq 1$ ) is nonextensive. In contrast, however, for a (sub)system whose elements are generically strongly correlated, the additive entropy  $S_{BG}$  can be nonextensive, whereas the nonadditive entropy  $S_q$  ( $q \neq 1$ ) can be extensive for a special value of  $q$ . Probabilistic systems exist such that  $S_q$  is *not* extensive for *any* value of  $q$ , either  $q = 1$  or  $q \neq 1$ . All these statements are illustrated in the body of the book.<sup>3</sup> We shall also see that, consistently, the index  $q$  appears to characterize

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<sup>3</sup> During more than one century, physicists have primarily addressed weakly interacting systems, and therefore the entropic form which satisfies the thermodynamical requirement of extensivity is  $S_{BG}$ . A regretful consequence of this fact is that entropic *additivity* and *extensivity* have been practically considered as synonyms in many communities, thus generating all kinds of confusions and inadvertences. For example, our own book *Nonextensive Entropy—Interdisciplinary Applications* [69] should definitively have been more appropriately entitled *Nonadditive Entropy—Interdisciplinary Applications*! Indeed, already in its first chapter, an example is shown where the nonadditive entropy  $S_q$  ( $q \neq 1$ ) is extensive.

*universality classes of nonadditivity*, by phrasing this concept similarly to what is done in the standard theory of critical phenomena. Within each class, one expects to find infinitely many dynamical systems.

Coming back to the name *nonextensive statistical mechanics*, would it not be more appropriate to call it *nonadditive statistical mechanics*? Certainly yes, if one focuses on the entropy that is being used. However, there is, on one hand, the fact that the expression *nonextensive statistical mechanics* is by now spread in thousands of papers. There is, on the other hand, the fact that important systems whose approach is expected to benefit from the present generalization of the BG theory are long-range-interacting many-body Hamiltonian systems. For such systems, the total energy is well known to be nonextensive, even if the extensivity of the entropy can be preserved by conveniently choosing the value of the index  $q$ .

Still at the linguistic and semantic levels, should we refer to  $S_q$  as an *entropy* or just as an *entropic functional* or *entropic form*? And, even before that, why should such a minor-looking point have any relevance in the first place? The point is that, in physics, since more than one century, only one entropic functional is considered “physical” in the thermodynamical sense, namely the *BG* one. In other areas, such as cybernetics, control theory, nonlinear dynamical systems, information theory, many other (well over 20!) entropic functionals have been studied and/or used as well. In the physical community only the *BG* form is undoubtedly admitted as physically meaningful because of its deep connections with thermodynamics. So, what about  $S_q$  in this specific context? A variety of thermodynamical arguments – extensivity, Clausius inequality, first principle of thermodynamics, and others – that are presented later on, definitively point  $S_q$  as a physical entropy in a quite analogous sense that  $S_{BG}$  surely is. Let us further elaborate this point.

*Complexity* is nowadays a frequently used yet poorly defined – at least quantitatively speaking – concept. It tries to embrace a great variety of scientific and technological approaches of all types of natural, artificial, and social systems. A name, *plectics*, has been coined by Murray Gell-Mann to refer to this emerging science [12]. One of the main – necessary but by no means sufficient – features of complexity has to do with the fact that both very ordered and very disordered systems are, in the sense of plectics, considered to be *simple*, not *complex*. Ubiquitous phenomena, such as the origin of life and languages, the growth of cities and computer networks, citations of scientific papers, co-authorships and co-actorships, displacements of living beings, financial fluctuations, turbulence, are frequently considered to be complex phenomena. They all seem to occur close, in some sense, to the frontier between order and disorder. Most of their basic quantities exhibit *nonexponential* behaviors, very frequently *power-laws*. It happens that the distributions and other relevant quantities that emerge naturally within the frame of nonextensive statistical mechanics are precisely of this type, becoming of the exponential type in the  $q = 1$  limit. One of the most typical dynamical situations has to do with the *edge of chaos*, occurring in the frontier between regular motion and standard chaos. Since these two typical regimes would clearly be considered “simple” in the sense of plectics, one is strongly tempted to consider as “complex” the regime in between, which has some aspects of the disorder of strong chaos but also some of the order lurking

nearby.<sup>4</sup> Nonextensive statistical mechanics turns out to be appropriate precisely for that intermediate region, thus suggesting that the entropic index  $q$  could be a convenient manner for quantifying some relevant aspects of complexity, surely not in all cases but probably so far vast classes of systems. Regular motion and chaos are time analogs for the space configurations occurring respectively in crystals and fluids. In this sense, the edge of chaos would be the analog of quasi-crystals, glasses, spin-glasses, and other amorphous, typically metastable structures. One does not expect statistical concepts to be intrinsically useful for regular motions and regular structures. On the contrary, one naturally tends to use probabilistic concepts for chaos and fluids. These probabilistic concepts and their associated entropy,  $S_{BG}$ , would typically be the realm of  $BG$  statistical mechanics and standard thermodynamics. It appears that, in the marginal cases, or at least in very many of them, between great order and great disorder, the statistical procedures can *still* be used. However, the associated natural entropy would not anymore be the  $BG$  one, but  $S_q$  with  $q \neq 1$ . It then appears quite naturally the scenario within which  $BG$  statistical mechanics is the microscopic thermodynamical description properly associated with Euclidean geometry, whereas nonextensive statistical mechanics would be the proper counterpart which has privileged connections with (multi)fractal and similar, hierarchical, statistically scale-invariant, structures (at least asymptotically speaking). As already mentioned, a paradigmatic case would be those nonlinear dynamical systems whose largest Lyapunov exponent is neither negative (easily predictable systems) nor positive (strong chaos) but vanishing instead, e.g., the edge of chaos (weak chaos<sup>5</sup>). Standard, equilibrium critical phenomena also deserve a special comment. Indeed, I have always liked to think and say that “criticality is a little window through which one can see the nonextensive world.” Many people have certainly had similar insights. Alberto Robledo, Filippo Caruso, and I have recently exhibited some rigorous evidences – to be discussed later on – along this line. *Not* that there is anything wrong with the usual and successful use of  $BG$  concepts to discuss the neighborhood of criticality in cooperative systems at thermal equilibrium! But, if one wants to make a delicate quantification of some of the physical concepts *precisely at the critical point*, the nonextensive language appears to be a privileged one for this task. It may be so for many anomalous systems. Paraphrasing Angel Plastino’s (A. Plastino Sr.) last statement in his lecture at the 2003 Villasimius meeting, “for different sizes of screws one must use different screwdrivers”!

A proposal of a generalization of the  $BG$  entropy as the physical basis for dealing, in statistical mechanical terms, with some classes of complex systems might –

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<sup>4</sup> It is frequently encountered nowadays the belief that complexity emerges typically at the edge of chaos. For instance, the final words of the Abstract of a lecture delivered in September 2005 by Leon O. Chua at the Politecnico di Milano were “*Explicit mathematical criteria are given to identify a relatively small subset of the locally-active parameter region, called the edge of chaos, where most complex phenomena emerge.*” [14].

<sup>5</sup> In the present book, the expression “weak chaos” is used in the sense of a sensitivity to the initial conditions diverging with time slower than exponentially, and *not* in other senses used currently in the theory of nonlinear dynamical systems.

in the view of many – in some sense imply in a new paradigm, whose validity may or may not be further validated by future progress and verifications. Indeed, we shall argue in the entire book that  $q$  is determined a priori by the microscopic dynamics of the system. This is in some sense less innocuous than it looks at first sight. Indeed, this means that the entropy to be used for thermostistical purposes would be *not universal* but would *depend on the system* or, more precisely, *on the nonadditive universality class to which the system belongs*. Whenever a new scientific viewpoint is proposed, either correct or wrong, it usually attracts quite extreme opinions. One of the questions that is regularly asked is the following: “Do I really need this? Is it not possible to work all this out just with the concepts that we already have, and that have been lengthily tested?”. This type of question is rarely easy to answer, because it involves the proof without ambiguity that some given result can *by no means* be obtained within the traditional theory. However, let me present an analogy, basically due to Michel Baranger, in order to clarify at least one of the aspects that are relevant for this nontrivial problem. Suppose one only knows how to handle straight lines and segments and wants to calculate areas delimited by curves. Does one really need the Newton–Leibnitz differential and integral calculus? Well, one might approach the result by approximating the curve with polygonals, and that works reasonably well in most cases. However, if one wants to better approach reality, one would consider more and more, shorter and shorter, straight segments. But one would ultimately want to take an *infinity* of such infinitely small segments. If one does so, then one has precisely jumped into the standard differential and integral calculus! How big was that step epistemologically speaking is a matter of debate, but its practicality is out of question. The curve that is handled might, in particular, be a straight line itself (or a finite number of straight pieces). In this case, there is of course no need to do the limiting process. Let me present a second analogy, this one primarily due to Angel Ricardo Plastino (A. Plastino Jr.). It was known by ancient astronomers that the apparent orbits of stars are *circles*, form that was considered geometrically “perfect.” The problematic orbits were those of the planets, for instance that of Mars. Ptolemy proposed a very ingenious way out, the *epicycles*, i.e., circles turning around circles. The predictions became of great precision, and astronomers along centuries developed, with sensible success, the use of dozens of epicycles, each one on top of the previous one. It remained so until the proposal of Johannes Kepler: the orbits are well described by *ellipses*, a form which generalizes the circle by having an extra parameter, the *eccentricity*. The eccentricities of the various planets were determined through fitting with the observational data. We know today, through Newtonian mechanics, that it would in principle be possible to determine a priori those eccentricities (the entire orbits, in fact) *if* we knew all positions and velocities of the celestial bodies and masses at some time in the past, and *if* we had a colossal computer which would be able to handle such data. Not having in fact that information, nor the computer, astronomers just fit, by using however the correct functional forms, i.e., the Keplerian ellipses. In few years, virtually all European astronomers abandoned the use of the complex Ptolemaic epicycles and adopted the simple Keplerian orbits. We know today, through Fourier transform, that the periodic motion on *one* ellipse is totally equivalent to an *infinite* number of specific



circular epicycles. So we can proceed either way. It is clear, however, that an ellipse is by far more practical and concise, even if in principle it can be thought as very many circles. We must concomitantly “pay the price” of an extra parameter, the eccentricity.

Newton’s decomposition of white light into the rainbow colors, not only provided a deeper insight on the nature of what we know today to classically be electromagnetic waves, but also opened the door to the discovery of infrared and ultraviolet. While trying to follow the methods of this great master, it is my cherished hope that the present, nonextensive generalization of Boltzmann–Gibbs statistical mechanics, may provide a deeper understanding of the standard theory, in addition to proposing some extension of the domain of applicability of the methods of statistical mechanics. The book is written at a graduate course level, and some basic knowledge of quantum and statistical mechanics, as well of thermodynamics, is assumed. The style is however slightly different from a conventional textbook, in the sense that not *all* the results that are presented are proved. The quick ongoing development of the field does not yet allow for such ambitious task. Various relevant points of the theory are still only partially known and understood. So, here and there we are obliged to proceed by heuristic arguments. The book is unconventional also in the sense that here and there historical and other side remarks are included as well. Some sections of the book, the most basic ones, are presented with all details and intermediate steps; some others, more advanced or quite lengthy, are presented only through their main results, and the reader is referred to the original publications to know more. We hope however that a unified perception of statistical mechanics, its background, and its basic concepts does emerge.

The book is organized in four parts, namely Part I—*Basics* or *How the theory works*, Part II—*Foundations* or *Why the theory works*, Part III—*Applications* or *What for the theory works*, and Part IV—*Last (but not least)*. The first part constitutes a pedagogical introduction to the theory and its background (Chapters 1, 2, and 3). The second part contains the state of the art in its dynamical foundations, in particular how the index (indices)  $q$  can be obtained, in some paradigmatic cases, from microscopic first principles or, alternatively, from mesoscopic principles (Chapters 4, 5, and 6). The third part is dedicated to list brief presentations of typical applications of the theory and its concepts, or at least of its functional forms, as well as possible extensions existing in the literature (Chapter 7). Finally, the fourth part constitutes an attempt to place the present – intensively evolving, open to further contributions, improvements, corrections, and insights [13] – theory into contemporary science, by addressing some frequently asked or still unsolved current issues (Chapter 8). An Appendix with useful formulae has been added at the end, as well as another one discussing escort distributions and  $q$ -expectation values.

Towards this end, it is a genuine pleasure to warmly acknowledge the contributions of M. Gell-Mann, *maître à penser*, with whom I have had frequent and delightfully deep conversations on the subject of nonextensive statistical mechanics... as well as on many others. Very many other friends and colleagues have substantially contributed to the ideas, results, and figures presented in this book. Those contributions range from insightful questions or remarks – sometimes fairly

critical – to entire mathematical developments and seminal ideas. Their natures are so diverse that it becomes an impossible task to duly recognize them all. So, *faute de mieux*, I decided to name them in alphabetical order, being certain that I am by no means doing justice to their enormous and varied intellectual importance. In all cases, my gratitude could not be deeper. They are S. Abe, G.F.J. Ananos, F.C. Alcaraz, C. Anteneodo, N. Ay, G. Baker Jr., F. Baldovin, M. Baranger, C. Beck, I. Bediaga, G. Bemsiki, A.B. Bishop, H. Blom, B.M. Boghosian, E. Bonderup, J.P. Boon, E.P. Borges, L. Borland, E. Brezin, B.J.C. Cabral, M.O. Caceres, S.A. Cannas, A. Carati, M. Casas, G. Casati, N. Caticha, A. Chame, P.-H. Chavanis, E.G.D. Cohen, A. Coniglio, M. Coutinho Filho, E.M.F. Curado, S. Curilef, S.A. Dias, A. Erzan, J.D. Farmer, R. Ferreira, M.A. Fuentes, P.-G. de Gennes, A. Giansanti, P. Grigolini, D.H.E. Gross, G.R. Guerberoff, R. Hanel, H.J. Haubold, R. Hersh, H.J. Herrmann, H.J. Hilhorst, R. Hoffmann, L.P. Kadanoff, G. Kaniadakis, T.A. Kaplan, S. Kawasaki, T. Kodama, D. Krakauer, P.T. Landsberg, V. Latora, C.M. Lattes, E.K. Lenzi, S.V.F. Levy, M.L. Lyra, S.D. Mahanti, A.M. Mariz, J. Marsh, R. Maynard, G.F. Mazenko, R.S. Mendes, L.C. Mihalcea, L.G. Moyano, J. Naudts, K. Nelson, F.D. Nobre, J. Nogales, F.A. Oliveira, P.M.C. Oliveira, I. Oppenheim, A.W. Overhauser, G. Parisi, A. Plastino, A.R. Plastino, A. Pluchino, D. Prato, P. Quarati, S.M.D. Queiros, A.K. Rajagopal, A. Rapisarda, M.A. Rego-Monteiro, A. Robledo, A. Rodriguez, S. Ruffo, G. Ruiz, S.R.A. Salinas, Y. Sato, V. Schwammle, L.R. da Silva, R.N. Silver, A.M.C. Souza, H.E. Stanley, D.A. Stariolo, D. Stauffer, S. Steinberg, R. Stinchcombe, H. Suyari, H.L. Swinney, F.A. Tamarit, S. Thurner, U. Tirnakli, R. Toral, A.C. Tsallis, A.F. Tsallis, S. Umarov, M.E. Vares, M.C.S. Vieira, C. Vignat, J. Villain, B. Widom, G. Wilk, H.O. Wio, I.I. Zovko. Unavoidably, I must have forgotten to mention some – this idea started developing more than two decades ago! –: to them my most genuine apologies. Finally, as in virtually all the fields of science and very especially during the first stages of any new development, there are also a few colleagues whose intentions have not been – I confess – very transparent to me. But they have nevertheless – perhaps even unwillingly – contributed to the progress of the ideas that are presented in this book. They surely know who they are. My gratitude goes to them as well: it belongs to human nature to generate fruitful ideas through all types of manners.

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Finally, some of the figures that are presented in the present book have been reproduced from various publications indicated case by case. I gratefully acknowledge the gracious authorization from their authors to do so.

In the mind of its author, a book, like a living organism, never stops evolving.

*Rio de Janeiro and Santa Fe – New Mexico, through the period 2004–2008*

*C. T.*



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