

# Introduction to Nonextensive Statistical Mechanics

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APPROACHING A COMPLEX WORLD

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Constantino Tsallis



Springer

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*To my family,  
whose love is the roots of my dreams*

# 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 Schrödinger of generalizing Newtonian mechanics through a *wave*-like

<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 definitely 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 undoubtfully 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, *plexics*, 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 –

<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 thermostatistical 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 polygons, 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. Bemski, 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.

Along the years I have relevantly benefited from the partial financial support of various Agencies, especially the Brazilian CNPq, FAPERJ, PRONEX/MCT and CAPES, the USA NSF, SFI, SI International and AFRL, the Italian INFN and INFM, among others. I am indebted to all of them.

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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# **Part I**

## **Basics or How the Theory Works**

# Chapter 1

## Historical Background and Physical Motivations

*Beauty is the first test:  
there is no permanent place in the world for ugly mathematics.*  
G.H. Hardy  
(*A Mathematician's Apology*, 1941)

### 1.1 Introduction

Let us consider the free *surface* of a glass covering a table. And let us idealize it as being *planar*. What is its *volume*? Clearly *zero* since it has no height. An uninteresting answer to an uninteresting question. What is its *length*? Clearly *infinity*. One more uninteresting answer to another uninteresting question. Now, if we ask what is its *area*, we will have a meaningful answer, say  $2 \text{ m}^2$ . A *finite* answer. Not zero, not infinity – correct but poorly informative features. A *finite* answer for a measurable quantity, as expected from good theoretical physics, good experimental physics, and good mathematics. Who “told” us that the interesting question for this problem was the *area*? *The system did!* Its planar geometrical nature did. If we were focusing on a fractal, the interesting question would of course be its measure in  $d_f$  dimensions,  $d_f$  being the corresponding *fractal* or *Hausdorff dimension*. Its measure in any dimension  $d$  larger than  $d_f$  is zero, and in any dimension smaller than  $d_f$  is infinity. Only the measure at precisely  $d_f$  dimensions yields a *finite* number. For instance, if we consider an ideal 10 cm long straight segment, and we proceed through the celebrated Cantor-set construction (i.e., eliminate the central third of the segment, and then also eliminate the central third of each of the two remaining thirds, and hypothetically continue doing this for ever) we will ultimately arrive to a remarkable geometrical set – the triadic Cantor set – which is embedded in a one-dimensional space but whose Lebesgue measure is zero. The fractal dimension of this set is  $d_f = \ln 2 / \ln 3 = 0.6309\dots$ . Therefore, the interesting information about our present hypothetical system is that its measure is  $(10 \text{ cm})^{0.6309\dots} \simeq 4.275 \text{ cm}^{0.6309}$ . And, interestingly enough, the *nature* of this valuable geometric information was dictated by the system itself!

This entire book is written within precisely this philosophy: *it is the natural (or artificial or social) system itself which, through its geometrical-dynamical*

*properties, determines the specific informational tool – entropy – to be meaningfully used for the study of its (thermo) statistical properties.* The reader surely realizes that this epistemological standpoint somehow involves what some consider as a kind of new paradigm for statistical mechanics and related areas. Indeed, the physically important entropy – a crucial concept – is *not* thought as being an universal functional that is given once for ever, but it rather is a delicate and powerful concept to be carefully constructed for classes of systems. In other words, we adopt here the viewpoint that the – simultaneously aesthetic and fruitful – way of thinking about this is the existence of *universality classes of systems*. These systems share the *same* functional connection between the entropy and the set of probabilities of their microscopic states. The most known such universality class is that which we shall refer to as the Boltzmann–Gibbs (*BG*) one. Its associated entropy is given (for a set of  $W$  discrete states) by

$$S_{BG} = -k \sum_{i=1}^W p_i \ln p_i , \quad (1.1)$$

with

$$\sum_{i=1}^W p_i = 1 , \quad (1.2)$$

and where  $k$  is some conventional positive constant. This constant is taken to be Boltzmann constant  $k_B$  in thermostatistics, and is usually taken equal to unity for informational or computational purposes. In this book we shall use, without further clarification, one or the other of these two conventions, depending on the particular convenience. The reader will unambiguously detect which convention we are using within a specific context. For the particular case of *equal probabilities* (i.e.,  $p_i = 1/W, \forall i$ ), Eq. (1.1) becomes

$$S_{BG} = k \ln W , \quad (1.3)$$

which is carved on Boltzmann’s grave in Vienna by suggestion of Planck. This celebrated expression, as well as Eq. (1.1), has been used in a variety of creative manners by Planck, Einstein, von Neumann, Shannon, Szilard, Tisza, and others. Equation (1.1) has the following remarkable property. If we compose two *probabilistically independent* subsystems  $A$  and  $B$  (with numbers of states respectively denoted by  $W_A$  and  $W_B$ ), i.e., such that the joint probabilities factorize,  $p_{ij}^{A+B} = p_i^A p_j^B (\forall(i, j))$ , the entropy  $S_{BG}$  is *additive*<sup>1</sup> [4]. By this we mean that

$$S_{BG}(A + B) = S_{BG}(A) + S_{BG}(B) , \quad (1.4)$$

---

<sup>1</sup> The important mathematical distinction between *additive* and *extensive* is addressed later on.

where

$$S_{BG}(A + B) \equiv -k \sum_{i=1}^{W_A} \sum_{j=1}^{W_B} p_{ij}^{A+B} \ln p_{ij}^{A+B} \quad (\text{with } W = W_A W_B), \quad (1.5)$$

$$S_{BG}(A) \equiv -k \sum_{i=1}^{W_A} p_i^A \ln p_i^A, \quad (1.6)$$

and

$$S_{BG}(B) \equiv -k \sum_{j=1}^{W_B} p_j^B \ln p_j^B. \quad (1.7)$$

Expression (1.1) was first proposed (for simple continuous systems) by Boltzmann [5,6] in the 1870s, and was then refined by Gibbs [1] for more general systems. It is the basis of the usual *BG* statistical mechanics. In particular, its optimization under appropriate constraints (that we shall describe later on) yields, for a system in *thermal equilibrium* with a thermostat at *temperature T*, the celebrated *BG factor or weight*, namely

$$p_i = \frac{e^{-\beta E_i}}{Z_{BG}} \quad (1.8)$$

with

$$\beta \equiv 1/kT, \quad (1.9)$$

$$Z_{BG} \equiv \sum_{j=1}^W e^{-\beta E_j}, \quad (1.10)$$

and where  $\{E_i\}$  denotes the *energy spectrum* of the system, i.e., the *eigenvalues* of the Hamiltonian of the system with the adopted boundary conditions;  $Z_{BG}$  is referred to as the *partition function*.

Expressions (1.1) and (1.8) are the landmarks of *BG* statistical mechanics, and are vastly and successfully used in physics, chemistry, mathematics, computational sciences, engineering, and elsewhere. Since their establishment, about 130 years ago, they constitute fundamental pieces of contemporary physics. Though notoriously applicable in very many systems and situations, we believe that they need to be modified (generalized) in others, in particular in most of the so-called *complex systems* (see, for instance, [12, 15–18]). We believe, in other words, that they are *not universal*, as somehow implicitly (or explicitly) thought until not long ago by many physicists. They *must* have in fact a restricted domain of validity, *as any other human intellectual construct*. As Newtonian mechanics, nonrelativistic quantum mechanics, special relativity, Maxwell electromagnetism, and all others. The basic purpose

of this book is precisely to explore – the best that our present knowledge allows – for what systems and conditions the *BG* concepts become either inefficiently applicable or nonapplicable at all, and what might be done in such cases, or at least in (apparently wide) classes of them. The possibility of some kind of generalization of *BG* statistical concepts, or at least some intuition about the restricted validity of such concepts, already emerged, in one way or another, in the mind of various physicists or mathematicians. This is, at least, what one might be led to think from the various statements that we reproduce in the next section.

## 1.2 Background and Indications in the Literature

We recall here interesting points raised along the years by various thinkers on the theme of the foundations and domain of validity of the concepts that are currently used in standard statistical mechanics.

Boltzmann himself wrote, in his 1896 *Lectures on Gas Theory* [19], the following words: (*The bold faces in this and subsequent quotations are mine.*)

When the distance at which two gas molecules interact with each other noticeably is vanishingly small relative to the average distance between a molecule and its nearest neighbor – or, as one can also say, when the **space occupied by the molecules (or their spheres of action) is negligible compared to the space filled by the gas** – then the fraction of the path of each molecule during which it is affected by its interaction with other molecules is vanishingly small compared to the fraction that is rectilinear, or simply determined by external forces. [...] The gas is “ideal” in all these cases.

Boltzmann is here referring essentially to the hypothesis of *ideal* gas. It shows nevertheless how clear it was in his mind the relevance of the *range* of the interactions for the thermostatistical theory he was putting forward.

Gibbs, in the Preface of his celebrated 1902 *Elementary Principles in Statistical Mechanics – Developed with Especial Reference to the Rational Foundation of Thermodynamics* [1], wrote the following touching words:

Certainly, **one is building on an insecure foundation**, who rests his work on hypotheses concerning the constitution of matter.

**Difficulties of this kind have deterred the author from attempting to explain the mysteries of nature**, and have forced him to be contented with the more modest aim of deducing some of the more obvious propositions relating to **the statistical branch of mechanics**.

In these lines, Gibbs not only shares with us his epistemological distress about the foundations of the science that himself, Maxwell and Boltzmann are founding. He also gives a precious indication that, in his mind, this unknown foundation would certainly come *from mechanics*. Everything indicates that this was also the ultimate understanding of Boltzmann, who – unsuccessfully – tried his entire life (the so-called *Boltzmann’s program*) to derive statistical mechanics from Newtonian mechanics. In fact, Boltzmann’s program remains unconcluded until today!

As we see next, the same understanding permeates in the words of Einstein that we cite, from his 1910 paper [20]:

Usually  $W$  is set equal to the number of ways (complexions) in which a state, which is incompletely defined in the sense of a molecular theory (i.e., coarse grained), can be realized. To compute  $W$  one needs a complete theory (something such as a complete molecular-mechanical theory) of the system. For that reason it appears to be **doubtful whether Boltzmann's principle alone**, i.e., without a complete molecular-mechanical theory (Elementary theory) **has any real meaning**. **The equation  $S = k \log W + \text{const. appears [therefore]}$** , without an Elementary theory – or however one wants to say it – **devoid of any meaning from a phenomenological point of view**.

By *Boltzmann's principle* – expression coined apparently by Einstein himself –, the author refers precisely to the logarithmic form for the entropy that he explicitly writes down a few words later. It is quite striking the crucial role that Einstein attributes to microscopic dynamics for giving a clear sense to that particular form for the entropy.

Coming back to Gibbs's book [1], in page 35 he wrote:

In treating of the canonical distribution, we shall always suppose the multiple integral in equation (92) [*the partition function, as we call it nowadays*] to have a **finite** value, as otherwise the coefficient of probability vanishes, and **the law of distribution becomes illusory**. This will exclude certain cases, but not such apparently, as will affect the value of our results with respect to their bearing on thermodynamics. It will exclude, for instance, cases in which the system or parts of it can be distributed in unlimited space [...]. **It also excludes many cases in which the energy can decrease without limit, as when the system contains material points which attract one another inversely as the squares of their distances**. [...]. For the purposes of a general discussion, it is sufficient to call attention to the assumption implicitly involved in the formula (92).

Clearly, Gibbs is well aware that the theory he is developing has limitations. It does not apply to anomalous cases such as gravitation.

Enrico Fermi, in his 1936 *Thermodynamics* [23], wrote:

The entropy of a system composed of several parts is **very often** equal to the sum of the entropies of all the parts. This is true if the energy of the system is the sum of the energies of all the parts and if the work performed by the system during a transformation is equal to the sum of the amounts of work performed by all the parts. Notice that **these conditions are not quite obvious** and that in some cases **they may not be fulfilled**. Thus, for example, in the case of a system composed of two homogeneous substances, it will be possible to express the energy as the sum of the energies of the two substances only if we can neglect the surface energy of the two substances where they are in contact. The surface energy can generally be neglected only if the two substances are not very finely subdivided; otherwise, **it can play a considerable role**.

So, Fermi says “very often,” which virtually implies “not always!”

Ettore Majorana, mysteriously missing since 25 March 1938, wrote [24]:

This is mainly because entropy is an additive quantity as the other ones. In other words, the entropy of a system composed of several **independent** parts is equal to the sum of entropy of each single part. [...] Therefore one considers all possible internal determinations as equally probable. This is indeed a **new hypothesis** because the universe, which is far from being in the same state forever, is subjected to continuous transformations. We will therefore **admit as an extremely plausible working hypothesis, whose far consequences could sometime not be verified, that all the internal states of a system are a priori equally**

**probable** in specific physical conditions. **Under this hypothesis**, the *statistical ensemble* associated to each macroscopic state  $A$  turns out to be completely defined.

As Fermi, Majorana leaves the door open to other, nonstandard, possibilities, which could not be inconsistent with the methods of statistical mechanics.

Claude Elwood Shannon, in his 1948/1949 *The Mathematical Theory of Communication* [25], justified the logarithmic entropy  $k \ln W$  in these plain terms:

It is practically more **useful**. [...] It is nearer to our **intuitive** feeling as to the proper measure. [...] It is **mathematically** more **suitable**. [...].

And, after stating the celebrated axioms that yield, as unique answer, the entropy (1.1), he wrote:

This theorem and the assumptions required for its proof **are in no way necessary** for the present theory. It is **given chiefly to lend a certain plausibility** to some of our later definitions. **The real justification of these definitions, however, will reside in their implications.**

It is certainly remarkable how wide Shannon leaves the door open to other entropies than the one that he brilliantly used.

Laszlo Tisza wrote, in 1961, in his *Generalized Thermodynamics* [26]:

**The situation is different for the additivity postulate  $P\ a2$ , the validity of which cannot be inferred from general principles.** We have to require that **the interaction energy between thermodynamic systems be negligible**. This assumption is closely related to the homogeneity postulate  $P\ d1$ . From the molecular point of view, **additivity** and homogeneity can be expected to be **reasonable approximations** for systems containing many particles, **provided that the intermolecular forces have a short range character**.

Peter Landsberg wrote, in 1978/1990, in his *Thermodynamics and Statistical Mechanics* [27]:

**The presence of long-range forces causes important amendments to thermodynamics, some of which are not fully investigated as yet.**

And in 1984 he added [28]

[...] in the case of systems with long-range forces and which are therefore nonextensive (in some sense) **some thermodynamic results do not hold**. [...] The failure of some thermodynamic results, normally taken to be standard for black hole and other nonextensive systems has recently been discussed. [...] If two identical black holes are merged, the presence of long-range forces in the form of gravity leads to a more complicated situation, and **the entropy is nonextensive**.

Nico van Kampen, in his 1981 *Stochastic Processes in Physics and Chemistry* [29], wrote:

Actually an additional stability criterion is needed, see M.E. Fisher, Archives Rat. Mech. Anal. **17**, 377 (1964); D. Ruelle, *Statistical Mechanics: Rigorous Results* (Benjamin, New York 1969). A collection of point particles with **mutual gravitation** is an example where this criterion **is not satisfied**, and for which therefore **no statistical mechanics exists**.

L.G. Taff wrote in his 1985 *Celestial Mechanics* [30]:

[...] This means that the **total energy of any finite collection of self-gravitating mass points does not have a finite, extensive** (e.g., proportional to the number of particles)

**lower bound. Without such a property there can be no rigorous basis for the statistical mechanics of such a system** (Fisher and Ruelle 1966). Basically it is that simple. One can **ignore the fact** that one knows that there is no rigorous basis for one's computer manipulations; one can **try to improve the situation**, or one can **look for another job**.

Needless to say that the very existence of the present book constitutes but an attempt *to improve the situation!*

The same point is addressed by W.C. Saslaw in his 1985 *Gravitation Physics of Stellar and Galactic Systems* [31]:

When interactions are important **the thermodynamic parameters may lose their simple intensive and extensive properties** for subregions of a given system. [...] **Gravitational systems**, as often mentioned earlier, do not saturate and so **do not have an ultimate equilibrium state**.

Radu Balescu, in his 1975 *Equilibrium and Nonequilibrium Statistical Mechanics* [32], wrote:

It therefore appears from the present discussion that **the mixing property of a mechanical system is much more important for the understanding of statistical mechanics than the mere ergodicity**. [...] A detailed rigorous study of the way in which the concepts of mixing and the concept of **large numbers of degrees of freedom** influence the macroscopic laws of motion **is still lacking**.

David Ruelle wrote in page 1 of his 1978 *Thermodynamical Formalism* [33] (and maintains in page 1 of his 2004 Edition):

The formalism of equilibrium statistical mechanics – which we shall call *thermodynamic formalism* – has been developed since G.W. Gibbs to describe the properties of certain physical systems. [...] While **the physical justification of the thermodynamic formalism remains quite insufficient**, this formalism has proved remarkably successful at explaining facts.

**The mathematical investigation of the thermodynamic formalism is in fact not completed:** the theory is a young one, with emphasis still more on imagination than on technical difficulties. This situation is reminiscent of pre-classic art forms, where inspiration has not been castrated by the necessity to conform to standard technical patterns. We hope that some of this juvenile freshness of the subject will remain in the present monograph!

He wrote also, in page 3:

**The problem of why the Gibbs ensemble describes thermal equilibrium** (at least for "large systems") when the above physical identifications have been made **is deep and incompletely clarified**.

The basic identification he is referring to is between  $\beta$  and the inverse temperature. Consistently, the first equation in both editions (page 3) is dedicated to define the entropy to be associated with a probability measure. The *BG* form is introduced after the words "we define its *entropy*" without any kind of justification or physical motivation.

The same theme is retaken by Floris Takens in the 1991 *Structures in Dynamics* [34]. Takens wrote:

The values of  $p_i$  are determined by the following **dogma**: if the energy of the system in the  $i$ th state is  $E_i$  and if the temperature of the system is  $T$  then:  $p_i = e^{-E_i/kT}/Z(T)$ ,

where  $Z(T) = \sum_i e^{-E_i/kT}$ , (this last constant is taken so that  $\sum_i p_i = 1$ ). This choice of  $p_i$  is called the *Gibbs distribution*. **We shall give no justification for this dogma**; even a physicist like Ruelle disposes of this question as “deep and incompletely clarified”.

We know that mathematicians sometimes use the word “dogma” when they do not have the theorem. Indeed, this is not widely known, but still today no theorem exists, to the best of our knowledge, stating the necessary and sufficient microscopic conditions for being legitimate the use of the celebrated *BG weight*!

Roger Balian wrote in his 1982/1991 *From Microphysics to Macrophysics* [35]:

These various quantities are connected with one another through thermodynamic relations which make their extensive or intensive nature obvious, as soon as **one postulates**, for instance, for a fluid, **that the entropy**, considered as a function of the volume  $\Omega$  and of the constants of motion such as  $U$  and  $N$ , is **homogeneous of degree 1**:  $S(x\Omega, xU, xN) = xS(\Omega, U, N)$  (Eq. (5.43)). [...] Two **counter-examples** will help us to feel why **extensivity is less trivial than it looks**. [...] A complete justification of the Laws of thermodynamics, starting from statistical physics, requires a proof of the extensivity (5.43), a property which was **postulated** in macroscopic physics. This proof is difficult and appeals to **special conditions which must be satisfied by the interactions between the particles**.

John Maddox wrote, in 1993, an article suggestively entitled *When entropy does not seem extensive* [36]. He focused on a paper by Mark Srednicki [37] where the entropy of a black hole is addressed. Maddox writes:

Everybody who knows about entropy knows that it is an extensive property, such as mass or enthalpy. [...] Of course, there is more than that to entropy, which is also a measure of disorder. Everybody also agrees on that. But **how is disorder measured?** [...] So why is the entropy of a black hole proportional to the square of its radius, and **not** to the cube of it? **To its surface area rather than to its volume?**

These comments and questions are of course consistent with the so-called black-hole Hawking entropy, whose value *per unit area* equals  $1/(4\hbar Gk_B^{-1}c^{-3})$ , a remarkable combination of four universal constants.

A suggestive paper by van Enter, Fernandez, and Sokal appeared in 1993. It is entitled *Regularity Properties and Pathologies of Position-Space Renormalization-Group Transformations: Scope and Limitations of Gibbsian Theory* [38]. We transcribe here a few fragments of its content. From its Abstract:

We provide a careful, and, we hope, pedagogical, overview of the theory of Gibbsian measures as well as (**the less familiar**) **non-Gibbsian measures**, emphasizing the distinction between these two objects and the **possible occurrence of the latter in different physical situations**.

And from its Section 6.1.4 *Toward a Non-Gibbsian Point of View*:

Let us close with some general remarks on the **significance of (non-)Gibbsianness and (non)quasilocality in statistical physics**. Our first observation is that **Gibbsianness has heretofore been ubiquitous in equilibrium statistical mechanics because it has been put in by hand**: nearly all measures that physicists encounter are Gibbsian because **physicists have decided to study Gibbsian measures!** However, we now know that natural operations on Gibbs measures can sometimes lead out of this class. [...] **It is thus of great interest to study which types of operations preserve, or fail to preserve, the Gibbsianness (or quasilocality) of a measure. This study is currently in its infancy.**

[...] More generally, **in areas of physics where Gibbsianness is not put in by hand, one should expect non-Gibbsianness to be ubiquitous.** This is probably the case in nonequilibrium statistical mechanics.

**Since one cannot expect all measures of interest to be Gibbsian, the question then arises whether there are weaker conditions that capture some or most of the “good” physical properties characteristic of Gibbs measures.** For example, the stationary measure of the voter model appears to have the critical exponents predicted (under the hypothesis of Gibbsianness) by the Monte Carlo renormalization group, even though this measure is provably non-Gibbsian.

**One may also inquire whether there is a classification of non-Gibbsian measures according to their “degree of non-Gibbsianness”.**

The authors make in this paper no reference whatsoever to nonextensive statistical mechanics (proposed in fact 5 years earlier [39]). It will nevertheless become evident that, interestingly enough, several among their remarks neatly apply to the content of the present book. Particularly, it will become obvious that  $(q - 1)$  represents a possible measure of “non-Gibbsianness,” where  $q$  denotes the entropic index to be soon introduced.

From the viewpoint of the dynamical foundations of statistical mechanics, a recent remark (already quoted in the Preface of this book) by Giulio Casati and Tomaz Prosen [9] is worth to be reproduced at this point:

While exponential instability is **sufficient** for a meaningful statistical description, it is not known whether or not it is also **necessary**.

Let us anticipate that it belongs to the aim of the present book to convince the reader precisely that it is *not* necessary: power-law instability appears to do the job similarly well, if we consistently adopt the appropriate entropy.

Many more statements exist in the literature along similar lines. But we believe that the ones that we have selected are enough (both in quality and quantity!) for depicting, at least in an “impressionistic” way, the epistemological scenario within which we are evolving. A few basic interrelated points that emerge include:

(i) No strict physical or mathematical reason exists (or, at least, is known) for not exploring the possible generalization of the *BG* entropy and its consequences.

(ii) The *BG* entropy and any of its possible generalizations should conform to the microscopical dynamical features of the system, very specifically to properties such as sensitivity to the initial conditions and mixing. The relevant rigorous necessary and sufficient conditions are still unknown. The ultimate justification of any physical entropy is expected to come from microscopic dynamics and detailed geometrical conditions.

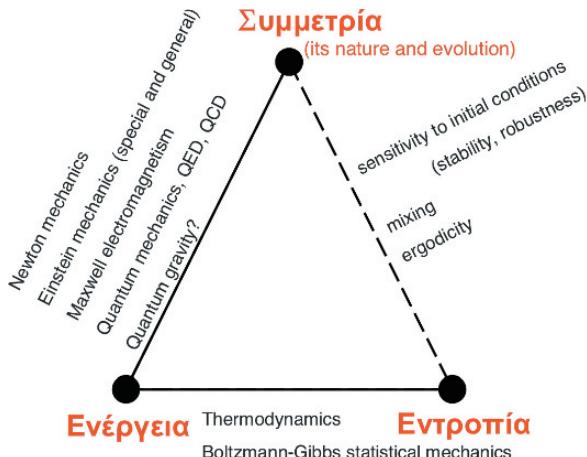
(iii) No physical or mathematical reason exists (or, at least, is known) for not exploring, in natural, artificial and even social systems, distributions differing from the *BG* one, very specifically for stationary or quasi-stationary states differing from thermal equilibrium, such as metastable states, and other nonequilibrium ones.

(iv) Long-range microscopic interactions (and long-range microscopic memory), as well as interactions exhibiting severe (e.g., nonintegrable attractive) singularities at the origin, appear as a privileged field for the exploration and understanding of anomalous thermostatistical behavior.

### 1.3 Symmetry, Energy, and Entropy

At this point, let us focus on some connections between three key concepts of physics, namely *symmetry*, *energy*, and *entropy*: see Fig. 1.1. According to Plato, symmetry sits in *Topos Ouranos* (heavens), where sit all branches of mathematics – science of structures –. In contrast, energy and entropy sit in *Physis* (nature). Energy deals with the *possibilities* of the system; entropy deals with the *probabilities* of those possibilities. It is fair to say that energy is a quite subtle physical concept. Entropy is based upon the ingredients of energy, and therefore is, epistemologically speaking, one step further. It is most likely because of this feature that entropy emerged, in the history of physics, well after energy. A coin has two faces, and can therefore fall in two possible manners, head and tail (if we disconsider the very unlike possibility that it falls on its edge). This is the world of the possibilities for this simple system. The world of its probabilities is more delicate. *Before* throwing the coin (assumed *fair* for simplicity), the entropy equals  $\ln 2$ . *After* throwing it, *it still equals  $\ln 2$  for whoever has not seen the result* (or just does not know it), whereas *it equals zero for whoever has seen the outcome* (or knows it). This example neatly illustrates the *informational nature* of the concept.

Let us now address the connections. Those between symmetry and energy are long and well known. Galilean invariance of the equations is central to Newtonian mechanics. Its simplest form of energy can be considered to be the kinetic one of a point particle, namely  $p^2/2m$ ,  $p$  being the *linear momentum*, and  $m$  the *mass*. This energy, although having an unique form, is *not universal*; indeed it depends on the mass of the system. If we replace now the Galilean invariance by the Lorentzian one, this drastically changes the form itself of the kinetic energy, which now becomes  $(p^2c^2 + m_0^2c^4)^{1/2}$ ,  $c$  being the speed of light in vacuum, and  $m_0$  the mass at rest. In



**Fig. 1.1** Connections between symmetry, energy, and entropy. QED and QCD respectively denote *quantum electrodynamics* and *quantum chromodynamics*.

other words, this change of symmetry is far from innocuous; it does nothing less than changing Newtonian mechanics into special relativity! Maxwell electromagnetism is, as well known, deeply related to this same Lorentzian invariance, as well as to gauge invariance. The latter plays, in turn, a central role in quantum electrodynamics and quantum field theory. Quantum chromodynamics also is deeply related to symmetry properties. And so is expected to be quantum gravity, whenever it becomes reality. Summarizing, the deep connections between symmetry and energy are standard knowledge in contemporary physics. Changes in one of them are concomitantly followed by changes in the other one.

What about the connections between energy and entropy? Well, also these are quite known. They naturally emerge in thermodynamics (the possibility and manners for transforming work into heat, and the other way around). This obviously reflects on *BG* statistical mechanics itself.

But, what can we say about the possible connections between symmetry (its nature and evolution) and entropy? This topic has remained basically unchanged and virtually unexplored during more than one century! *Why?* Hard to know. However, it is allowed to suspect that this intellectual lethargy comes, on one hand, from the “sloppiness” of the concept of entropy, and, on the other one, from the remarkable fact that the unique functional form that has been used in thermal equilibrium-like physics is the *BG* one (Eq. (1.8) and its continuum or quantum analogs), which depends only on one of the universal constants, namely Boltzmann constant  $k_B$ . Within this intellectual landscape, generation after generation, the idea installed in the mind of very many physicists that the physical entropy *must* be universal, and that it is of course the *BG* one. In the present book, we try to convince the reader that it is *not* so, that many types of entropy can be physically and mathematically meaningful. Moreover, we shall argue that dynamical concepts such as the time-dependence of the sensitivity to the initial conditions, mixing, and the associated occupancy and visitation networks they may cause in phase-space, have so strong effects, that even the functional form of the entropy must, in some occasions, be modified. The *BG* entropy will then still have a highly privileged position. It surely is the correct one when the microscopic nonlinear dynamics is controlled by *positive* Lyapunov exponents, hence *strong* chaos. If the system is such that strong chaos is absent (typically because the maximal Lyapunov exponent vanishes), then the physical entropy to be used appears to be a different one.

## 1.4 A Few Words on the Foundations of Statistical Mechanics

A mechanical foundation of statistical mechanics from *first principles* should essentially include, in one way or another, the following main steps [40].

(i) Adopt a *microscopic dynamics*. This dynamics typically is deterministic, i.e., without any phenomenological noise or stochastic ingredient, so that the foundation may be considered as *from first principles*. This dynamics could be Newtonian, or quantum, or relativistic mechanics (or some other mechanics to be found in fu-

ture) of a many-body system composed by say  $N$  interacting elements or fields. It could also be conservative or dissipative coupled maps, or even cellular automata. Consistently, time  $t$  could be continuous or discrete. The same is valid for space. The quantity which is defined in space-time could itself be continuous or discrete. For example, in quantum mechanics, the quantity is a complex continuous variable (the wave function) defined in a continuous space-time. On the other extreme, we have cellular automata, for which all three relevant variables – time, space, and the quantity therein defined – are discrete. In the case of a Newtonian mechanical system of particles, we may think of  $N$  Dirac delta functions localized in continuous spatial positions which depend on a continuous time.

Langevin-like equations (and associated Fokker-Planck-like equations) are typically considered not microscopic, but *mesoscopic* instead. The reason of course is the fact that they include at their very formulation, i.e., in an essential manner, some sort of (stochastic) noise. Consequently, they should not be used as a starting point if we desire the foundation of statistical mechanics to be from first principles.

(ii) Then assume some set of *initial conditions* and let the system evolve in time. These initial conditions are defined in the so-called *phase-space* of the microscopic configurations of the system, for example Gibbs'  $\Gamma$  space for a Newtonian  $N$ -particle system (the  $\Gamma$  space for point masses has  $2dN$  dimensions if the particles live in a  $d$ -dimensional space). These initial conditions typically (but not necessarily) involve one or more constants of motion. For example, if the system is a conservative Newtonian one of point masses, the initial total energy and the initial total linear momentum ( $d$  dimensional vector) are such constants of motion. The total angular momentum might also be a constant of motion. It is quite frequent to use coordinates such that both total linear momentum and total angular momentum vanish.

If the system consists of conservative coupled maps, the initial hypervolume of an ensemble of initial conditions near a given one is preserved through time evolution. By the way, in physics, such coupled maps are frequently obtained through Poincaré sections of Newtonian dynamical systems.

(iii) After some *sufficiently long evolution time* (which typically depends on both  $N$  and the spatial range of the interactions), the system might approach some *stationary* or *quasi-stationary* macroscopic state.<sup>2</sup> In such a state, the various regions of phase-space are being visited with some probabilities. This set of probabilities either does not depend anymore on time or depends on it very slowly. More precisely, if it depends on time, it does so on a scale much longer than the microscopic time scale. The visited regions of phase-space that we are referring to typically correspond to a partition of phase-space with a degree of (coarse or fine) graining that we adopt for specific purposes. These probabilities can be either insensitive or, on the contrary, very sensitive to the ordering in which  $t \rightarrow \infty$  (*asymptotic*) and  $N \rightarrow \infty$  (*thermodynamic*) limits are taken. This can depend on various aspects such as the range of

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<sup>2</sup> When the system exhibits some sort of *aging*, the expression *quasi-stationary* is preferable to *stationary*.

the interactions, or whether the system is on the ordered or on the disordered side of a continuous phase transition. Generically speaking, the influence of the ordering of  $t \rightarrow \infty$  and  $N \rightarrow \infty$  limits is typically related to some kind of breakdown of symmetry, or of ergodicity, or the alike.

The simplest nontrivial dynamical situation is expected to occur for an isolated many-body short-range-interacting classical Hamiltonian system (microcanonical ensemble); later on we shall qualify when an interaction is considered *short-ranged* in the present context. In such a case, the typical microscopic (nonlinear) dynamics is expected to be *strongly chaotic*, in the sense that the maximal Lyapunov exponent is positive. Such a system would necessarily be *mixing*, i.e., it would quickly visit virtually all the accessible phase-space (more precisely, very close to almost all the accessible phase-space) for almost *any* possible initial condition. Furthermore, it would necessarily be *ergodic* with respect to some measure in the full phase-space, i.e., *time averages* and *ensemble averages* would coincide. In most of the cases this measure is expected to be uniform in phase-space, i.e., the *hypothesis of equal probabilities* would be satisfied.

A slightly more complex situation is encountered for those systems which exhibit a continuous phase transition. Let us consider the simple case of a ferromagnet which is invariant under inversion of the hard axis of magnetization, e.g., the  $d = 3$  XY classical nearest-neighbor ferromagnetic model on simple cubic lattice. If the system is in its disordered (paramagnetic) phase, the limits  $t \rightarrow \infty$  and  $N \rightarrow \infty$  commute, and the entire phase-space is expected to be equally well visited. If the system is in its ordered (ferromagnetic) phase, the situation is expected to be more subtle. The  $\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty}$  set of probabilities is, as before, equally distributed all over the entire phase-space *for almost any initial condition*. But this is not expected to be so for the  $\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty}$  set of probabilities. The system probably lives, in this case, only in half of the entire phase-space. Indeed, if the initial condition is such that the initial magnetization is *positive*, even infinitesimally positive (for instance, under the presence of a vanishingly small external magnetic field), then the system is expected to be ergodic *but only in the half phase-space associated with positive magnetization*; the other way around occurs if the initial magnetization is *negative*. This illustrates, already in this simple example, the importance that the ordering of those two limits can have.

A considerably more complex situation is expected to occur, if we consider a long-range-interacting model, e.g., the same  $d = 3$  XY classical ferromagnetic model on simple cubic lattice as before, but now with a coupling constant which decays with distance as  $1/r^\alpha$ , where  $r$  is the distance measured in crystal units, and  $0 \leq \alpha \leq d$  (the nearest-neighbor model that we just discussed corresponds to  $\alpha \rightarrow \infty$ , which is the extreme case of the *short-ranged* domain  $\alpha > d$ ). The  $0 \leq \alpha/d \leq 1$  model also appears to have a continuous phase transition. In the disordered phase, the system possibly is ergodic over the entire phase-space. But in the ordered phase the result can strongly depend on the ordering of the two limits. The  $\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty}$  set of probabilities corresponds to the system living in the entire phase-space. In contrast, the  $\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty}$  set of probabilities for the same (conveniently scaled) total energy might be considerably more complex. It seems that, for this ordering, phase-space exhibits at least two macroscopic basins

of attraction. One of them leads essentially to half of the same phase-space where the system lives in the  $\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty}$  ordering, i.e., the half phase-space which is associated with a sign for the magnetization which coincides with the sign of the initial magnetization. The other basin of attraction could well correspond to living in a very complicated, hierarchical-like, geometrical structure. This structure could be a zero Lebesgue measure one (in the full multidimensional phase-space), somewhat similar to that of an airlines company, say Air France, whose central hub is located in Paris, or Continental Airlines, whose central hub is located in Houston. The specific *location* of the structure in phase-space would depend on the particular initial condition within that special basin of attraction, but the *geometrical-dynamical nature* of the structure would be virtually the same for any initial condition within that basin of attraction. At this point, let us warn the reader that the scenario that we have depicted here is only conjectural, and remains to be proved. It is however based on various numerical evidences (see, e.g., [41, 44, 45, 50] and references therein). It is expected to be caused by a possibly *vanishing* maximal Lyapunov exponent. In other words, one would possibly have, instead of strong, only *weak* chaos.

(iv) Now let us focus further on the specific role played by the *initial conditions*. If the system is strongly chaotic, hence mixing, hence ergodic, this point is irrelevant. We can make or not averages over initial conditions, we can take almost any initial condition, the outcome for sufficiently long times will be the same, in the sense that the set of probabilities in phase-space will be the same. But if the system is only weakly chaotic, the result can drastically change from initial condition to initial condition. If two initial conditions belong to the same “basin of attraction,” the difference at the macroscopic level could be quite irrelevant. If they belong however to different basins of attraction, the results can be sensibly different. For some purposes we might wish to stick to a specific initial condition within a certain class of initial conditions. For other purposes, we might wish to average over all initial conditions belonging to a given basin of attraction, or even over all possible initial conditions of the entire phase-space. The macroscopic result obtained after averaging might considerably differ from that corresponding to a single initial condition.

(v) Last but not least, the mathematical form of the *entropy functional* must be addressed. Strictly speaking, if we have deduced (from microscopic dynamics) the probabilities to be associated with every cell in phase-space, we can in principle calculate useful averages of *any* physical quantity of interest which is defined in that phase-space. In this sense, we do not need to introduce an entropic functional which is defined precisely in terms of those probabilities. Especially if we take into account that *any* set of physically relevant probabilities can be obtained through *extremization* (typically *maximization*) of an infinite number of entropic functionals (monotonically depending one onto the other), given any set of physically and mathematically meaningful constraints. However, if we wish to make contact with classical thermodynamics, we certainly need to know the mathematical form of such entropic functional. This functional is expected to match, in the appropriate limits, the classical, macroscopic, entropy ‘*a la Clausius*. In particular, one expects it to satisfy the Clausius property of extensivity, i.e., essentially to be proportional to the

weight or mass of the system. In statistical mechanical terms, we expect it to be proportional to  $N$  for large  $N$ .<sup>3</sup>

The foundations of any statistical mechanics are, as already said, expected to cover basically all of the above points. There is a wide-spread vague belief among physicists that these steps have already been satisfactorily accomplished since long for the standard, *BG* statistical mechanics. *This is not so!* Not so surprising after all, given the enormity of the corresponding task! For example, as already mentioned, at this date, there is no available deduction, from and only from microscopic dynamics, of the celebrated *BG* exponential weight (1.8). Neither exists the deduction from microscopic dynamics of the *BG* entropy (1.1).

For standard systems, there is not a single reasonable doubt about the correctness of the expressions (1.1) and (1.8) and of their relationships. But, from the logical-deductive viewpoint, there is still pretty much work to be done! This is, in fact, kind of easy to notice. Indeed, all the textbooks, without exception, introduce the *BG* factor and/or the entropy  $S_{BG}$  in some kind of phenomenological manner, or as self-evident, or within some axiomatic formulation. None of them introduces them as (and only as) a rational consequence of Newtonian, or quantum mechanics, using theory of probabilities. This is in fact sometimes referred to as the *Boltzmann program*. Boltzmann himself died without succeeding its implementation. Although important progress has been accomplished in these last 130 years, Boltzmann program still remains in our days as a basic intellectual challenge. Were it not the genius of scientists like Boltzmann and Gibbs, were we to exclusively depend on mathematically well-constructed arguments, one of the monuments of contemporary physics – *BG* statistical mechanics – would not exist!

Many anomalous natural, artificial, and social systems exist for which *BG* statistical concepts appear to be inapplicable. Typically because they live in peculiar stationary or quasi stationary states that are quite different from thermal equilibrium, where *BG* statistics reigns. Nevertheless, as we shall see, some of them can still be handled within statistical mechanical methods, but with a more general entropy, namely  $S_q$ , to be introduced later on [39, 59, 60].

It should be clear that, whatever is not yet mathematically justified in *BG* statistical mechanics, it is even less justified in the generalization to which the present book is dedicated. In addition to this, some of the points that are relatively well understood in the standard theory can be still unclear in its generalization. In other words, the theory we are presenting here is still in intense evolution (sets of reviews can be found in [62, 64–76]).

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<sup>3</sup> Let us anticipate that it has been recently shown [55–58] that, if we impose a Poissonian distribution for visitation times in phase-space, in addition to the first and second principles of thermodynamics, we obtain the *BG* functional form for the entropy. If a conveniently deformed Poissonian distribution is imposed instead, we obtain the  $S_q$  functional form. These results in themselves *cannot* be considered as a justification from first principles of the *BG*, or of the nonextensive, statistical mechanics. Indeed, the visitation distributions are phenomenologically introduced, and the first and second principles are just imposed. This connection is nevertheless extremely clarifying, and can help producing a full justification.

# Chapter 2

## Learning with Boltzmann–Gibbs Statistical Mechanics

Πᾶν μέτρον ἀριστον [78]  
Kleoboulos of Lindos (6th century B.C.)

### 2.1 Boltzmann–Gibbs Entropy

#### 2.1.1 Entropic Forms

The entropic forms (1.1) and (1.3) that we have introduced in Chapter 1 correspond to the case where the (microscopic) states of the system are *discrete*. There are, however, cases in which the appropriate variables are *continuous*. For these, the *BG* entropy takes the form

$$S_{BG} = -k \int dx p(x) \ln[\sigma p(x)], \quad (2.1)$$

with

$$\int dx p(x) = 1, \quad (2.2)$$

where  $x/\sigma \in \mathbb{R}^D$ ,  $D \geq 1$  being the dimension of the full space of microscopic states (called *Gibbs Γ phase-space* for classical Hamiltonian systems). Typically  $x$  carries physical units. The constant  $\sigma$  carries the same physical units as  $x$ , so that  $x/\sigma$  is a dimensionless quantity (we adopt from now on the notation  $[x] = [\sigma]$ , hence  $[x/\sigma] = 1$ ). For example, if we are dealing with an isolated classical  $N$ -body Hamiltonian system of point masses interacting among them in  $d$  dimensions, we may use  $\sigma = \hbar^{Nd}$ . This standard choice comes of course from the fact that, at a sufficiently small scale, Newtonian mechanics becomes incorrect and we must rely on quantum mechanics. In this case,  $D = 2dN$ , where each of the  $d$  pairs of components of momentum and position of each of the  $N$  particles has been taken

into account (we recall that  $[momentum][position] = [\hbar]$ ). For the case of *equal probabilities* (i.e.,  $p(x) = 1/\Omega$ , where  $\Omega$  is the hypervolume of the admissible  $D$ -dimensional space), we have

$$S_{BG} = k \ln(\Omega/\sigma). \quad (2.3)$$

A particular case of  $p(x)$  is the following one:

$$p(x) = \sum_{i=1}^W p_i \Delta(x - x_i) \quad (W \equiv \Omega/\sigma), \quad (2.4)$$

where  $\Delta(x - x_i)$  denotes a normalized uniform distribution centered on  $x_i$  and whose “width” is  $\sigma$  (hence its height is  $1/\sigma$ ). In this case, Eqs. (2.1), (2.2) and (2.3) precisely recover Eqs. (1.1), (1.2) and (1.3).

In both discrete and continuous cases that we have addressed until now, we were considering classical systems in the sense that all physical observables are real quantities and *not operators*. However, for intrinsically quantum systems, we must generalize the concept. In that case, the *BG* entropic form is to be written (as first introduced by von Neumann) in the following manner:

$$S_{BG} = -k \operatorname{Tr} \rho \ln \rho, \quad (2.5)$$

with

$$\operatorname{Tr} \rho = 1, \quad (2.6)$$

where  $\rho$  is the *density matrix* acting on a  $W$ -dimensional Hilbert vectorial space (typically associated with the solutions of the Schroedinger equation with the chosen boundary conditions; in fact, quite frequently we have  $W \rightarrow \infty$ ).

A particular case of  $\rho$  is when it is *diagonal*, i.e., the following one:

$$\rho_{ij} = p_i \delta_{ij}, \quad (2.7)$$

where  $\delta_{ij}$  denotes Kroenecker’s delta function. In this case, Eqs. (2.5) and (2.6) exactly recover Eqs. (1.1) and (1.2).

All three entropic forms (1.1), (2.1), and (2.5) will be generically referred in the present book as *BG-entropy* because they are all based on a logarithmic measure for *disorder*. Although we shall use one or the other for specific purposes, we shall mainly address the simple form expressed in Eq. (1.1).

## 2.1.2 Properties

### 2.1.2.1 Non-negativity

If we know with *certainty* the state of the system, then  $p_{i_0} = 1$ , and  $p_i = 0, \forall i \neq i_0$ . Then it follows that  $S_{BG} = 0$ , where we have taken into account that  $\lim_{x \rightarrow 0}(x \ln x) = 0$ . In any other case, we have  $p_i < 1$  for at least two different values of  $i$ . We can therefore write Eq. (1.1) as follows:

$$S_{BG} = -k\langle \ln p_i \rangle = k \left\langle \ln \frac{1}{p_i} \right\rangle, \quad (2.8)$$

where  $\langle \dots \rangle \equiv \sum_{i=1}^W p_i(\dots)$  is the standard *mean value*. Since  $\ln(1/p_i) > 0 (\forall i)$ , it clearly follows that  $S_{BG}$  is *positive*.

### 2.1.2.2 Maximal at Equal Probabilities

Energy is a concept which definitively takes into account the physical nature of the system. *Less so, in some sense, the BG entropy.*<sup>1</sup> This entropy depends of course on the total number of possible microscopic configurations of the system, but it is insensitive to its specific physical support; it only takes into account the (abstract) probabilistic information on the system. Let us make a trivial illustration: a spin that can be up or down (with regard to some external magnetic field), a coin that comes head or tail, and a computer bit which can be 0 or 1 are all equivalent for the concept of entropy. Consequently, entropy is expected to be a functional which is *invariant with regard to any permutations of the states*. Indeed, expression (1.1) exhibits this invariance through the form of a sum. Consequently, if  $W > 1$ , the entropy must have an extremum (maximum or minimum), and this must occur for equal probabilities. Indeed, this is the unique possibility for which the entropy is invariant with regard to the permutation of *any two* states. It is easy to verify that it is a maximum, and not a minimum. In fact, the identification as a maximum (and not a minimum) will become obvious when we shall prove, later on, that  $S_{BG}$  is a *concave* functional. Of course, the expression that  $S_{BG}$  takes for equal probabilities has already been indicated in Eq. (1.3).

### 2.1.2.3 Expansibility

Adding to a system new possible states with *zero* probability should not modify the entropy. This is precisely what is satisfied by  $S_{BG}$  if we take into account the

<sup>1</sup> This statement is to be revisited for the more general entropy  $S_q$ . Indeed, as we shall see, the index  $q$  does depend on some universal aspects of the physical system, e.g., the type of inflection of a dissipative unimodal map, or, possibly, the type of power-law decay of long-range interactions for Hamiltonian systems.

already-mentioned property  $\lim_{x \rightarrow 0} (x \ln x) = 0$ . So, we have that

$$S_{BG}(p_1, p_2, \dots, p_W, 0) = S_{BG}(p_1, p_2, \dots, p_W). \quad (2.9)$$

### 2.1.2.4 Additivity

Let  $\mathcal{O}$  be a physical quantity associated with a given system, and let  $A$  and  $B$  be two probabilistically independent subsystems. We shall use the term *additive* if and only if  $\mathcal{O}(A + B) = \mathcal{O}(A) + \mathcal{O}(B)$ . If so, it is clear that if we have  $N$  equal systems, then  $\mathcal{O}(N) = N\mathcal{O}(1)$ , where the notation is self-explanatory. A weaker condition is  $\mathcal{O}(N) \sim N\Omega$  for  $N \rightarrow \infty$ , with  $0 < |\Omega| < \infty$ , i.e.,  $\lim_{N \rightarrow \infty} \mathcal{O}(N)/N$  is finite (generically  $\Omega \neq \mathcal{O}(1)$ ). In this case, the expression *asymptotically additive* might be used. Clearly, any observable, which is additive with regard to a given composition law, is asymptotically additive (with  $\Omega = \mathcal{O}(1)$ ), but the opposite is not necessarily true.

It is straightforwardly verified that, if  $A$  and  $B$  are *independent*, i.e., if the *joint probability* satisfies  $p_{ij}^{A+B} = p_i^A p_j^B$  ( $\forall(ij)$ ), then

$$S_{BG}(A + B) = S_{BG}(A) + S_{BG}(B). \quad (2.10)$$

Therefore, the entropy  $S_{BG}$  is *additive*.

### 2.1.2.5 Concavity

Let us assume two arbitrary and different probability sets, namely  $\{p_i\}$  and  $\{p'_i\}$ , associated with a single system having  $W$  states. We define an *intermediate* probability set as follows:

$$p''_i = \lambda p_i + (1 - \lambda)p'_i \quad (\forall i; 0 < \lambda < 1). \quad (2.11)$$

The functional  $S_{BG}(\{p_i\})$  (or any other functional in fact) is said *concave if and only if*

$$S_{BG}(\{p''_i\}) > \lambda S_{BG}(\{p_i\}) + (1 - \lambda)S_{BG}(\{p'_i\}). \quad (2.12)$$

This is indeed satisfied by  $S_{BG}$ . The proof is straightforward. Because of its *negative second derivative*, the (continuous) function  $-x \ln x$  ( $x > 0$ ) satisfies

$$-p''_i \ln p''_i > \lambda(-p_i \ln p_i) + (1 - \lambda)(-p'_i \ln p'_i) \quad (\forall i; 0 < \lambda < 1). \quad (2.13)$$

Applying  $\sum_{i=1}^W$  on both sides of this inequality, we immediately obtain Eq. (2.12), i.e., the *concavity* of  $S_{BG}$ .

### 2.1.2.6 Lesche-Stability or Experimental Robustness

An entropic form  $S(\{p_i\})$  (or any other functional of the probabilities, in fact) is said *Lesche-stable* or *experimentally robust* [79] if and only if it satisfies the following continuity property. Two probability distributions  $\{p_i\}$  and  $\{p'_i\}$  are said *close* if they satisfy the metric property:

$$D \equiv \sum_{i=1}^W |p_i - p'_i| \leq d_\epsilon, \quad (2.14)$$

where  $d_\epsilon$  is a small real number. Then, experimental robustness is verified if, for any  $\epsilon > 0$ , a  $d_\epsilon$  exists such that  $D \leq d_\epsilon$  implies

$$R \equiv \left| \frac{S(\{p_i\}) - S(\{p'_i\})}{S_{max}} \right| < \epsilon, \quad (2.15)$$

where  $S_{max}$  is the maximal value that the entropic form can achieve (assuming its extremum corresponds to a maximum and not a minimum). For  $S_{BG}$  the maximal value is of course  $\ln W$ .

Condition (2.15) should be satisfied under all possible situations, including for  $W \rightarrow \infty$ . This implies that the condition

$$\lim_{d_\epsilon \rightarrow 0} \lim_{W \rightarrow \infty} \left| \frac{S(\{p_i\}) - S(\{p'_i\})}{S_{max}} \right| = 0 \quad (2.16)$$

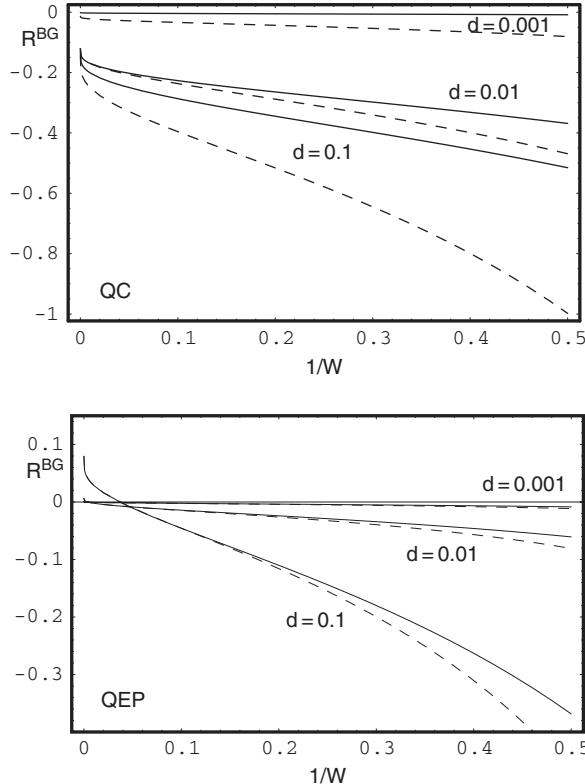
should also be satisfied, in addition to  $\lim_{W \rightarrow \infty} \lim_{d_\epsilon \rightarrow 0} \left| \frac{S(\{p_i\}) - S(\{p'_i\})}{S_{max}} \right| = 0$ , which is of course always satisfied.

What this property essentially guarantees is that *similar* experiments performed onto *similar* physical systems should provide *similar* results (i.e., a small percentage discrepancy) for the measured physical functionals. Lesche showed [79] that  $S_{BG}$  is experimentally robust, whereas the Renyi entropy  $S_q^R \equiv \frac{\ln \sum_{i=1}^W p_i^q}{1-q}$  is not. See Fig. 2.1.

It is in principle possible to use, as a concept for *distance*, a quantity different from that used in Eq. (2.14). We could use for instance the following definition:

$$D_\mu \equiv \left[ \sum_{i=1}^W |p_i - p'_i|^\mu \right]^{1/\mu} \quad (\mu > 0). \quad (2.17)$$

Equation (2.14) corresponds to  $\mu = 1$ . The Pythagorean metric corresponds to  $\mu = 2$ . What about other values of  $\mu$ ? It happens that only for  $\mu \geq 1$  the triangular inequality is satisfied, and consequently it does constitute a metric. Still, why not



**Fig. 2.1** Illustration of the Lesche-stability of  $S_{BG}$ .  $QC$  and  $QEP$  stand for *quasi-certainty* and *quasi-equal-probabilities*, respectively (see details in [110, 113]).

using values of  $\mu > 1$ ? Because, only for  $\mu = 1$ , the distance  $D$  does *not* depend on  $W$ , which makes it appropriate for a generic property [80].

We come back in Section 3.2.2 onto this interesting property introduced by Lesche.

### 2.1.2.7 Shannon Uniqueness Theorem

Let us assume that an entropic form  $S(\{p_i\})$  satisfies the following properties:

$$(i) \quad S(\{p_i\}) \text{ is a continuous function of } \{p_i\}; \quad (2.18)$$

$$(ii) \quad S(p_i = 1/W, \forall i) \text{ monotonically increases with the total number of possibilities } W; \quad (2.19)$$

$$(iii) \quad S(A + B) = S(A) + S(B) \quad \text{if } p_{ij}^{A+B} = p_i^A p_j^B \forall (i, j), \quad (2.20)$$

$$\begin{aligned}
&\text{where } S(A + B) \equiv S(\{p_{ij}^{A+B}\}), \quad S(A) \equiv S(\{p_i^A\}) \quad (p_i^A \equiv \sum_{j=1}^{W_B} p_{ij}^{A+B}), \\
&\text{and } \quad S(B) \equiv S(\{p_j^B\}) \quad (p_j^B \equiv \sum_{i=1}^{W_A} p_{ij}^{A+B}); \\
(iv) \quad &S(\{p_i\}) = S(p_L, p_M) + p_L S(\{p_i/p_L\}) + p_M S(\{p_i/p_M\}) \quad (2.21) \\
\text{with} \quad &p_L \equiv \sum_{L \text{ terms}} p_i, \quad p_M \equiv \sum_{M \text{ terms}} p_i, \\
&L + M = W, \text{ and } p_L + p_M = 1.
\end{aligned}$$

Then and only then [25]

$$S(\{p_i\}) = -k \sum_{i=1}^W p_i \ln p_i \quad (k > 0). \quad (2.22)$$

### 2.1.2.8 Khinchin Uniqueness Theorem

Let us assume that an entropic form  $S(\{p_i\})$  satisfies the following properties:

$$(i) \quad S(\{p_i\}) \text{ is a continuous function of } \{p_i\}; \quad (2.23)$$

$$(ii) \quad S(p_i = 1/W, \forall i) \text{ monotonically increases with the total number of possibilities } W; \quad (2.24)$$

$$(iii) \quad S(p_1, p_2, \dots, p_W, 0) = S(p_1, p_2, \dots, p_W); \quad (2.25)$$

$$(iv) \quad S(A + B) = S(A) + S(B|A), \quad (2.26)$$

$$\text{where } S(A + B) \equiv S(\{p_{ij}^{A+B}\}), \quad S(A) \equiv S(\{p_i^A\}) \quad (p_i^A \equiv \sum_{j=1}^{W_B} p_{ij}^{A+B}),$$

$$\text{and the conditional entropy } S(B|A) \equiv \sum_{i=1}^{W_A} p_i^A S(\{p_{ij}^{A+B}/p_i^A\}).$$

Then and only then [81]

$$S(\{p_i\}) = -k \sum_{i=1}^W p_i \ln p_i \quad (k > 0). \quad (2.27)$$

### 2.1.2.9 Composability

A dimensionless entropic form  $S(\{p_i\})$  (i.e., whenever expressed in appropriate conventional units, e.g., in units of  $k$ ) is said *composable* if the entropy  $S(A + B)$  corresponding to a system composed of two *independent* subsystems  $A$  and  $B$  can be expressed in the form

$$S(A + B) = F(S(A), S(B); \{\eta\}), \quad (2.28)$$

where  $F(x, y; \{\eta\})$  is a function which, besides depending symmetrically on  $(x, y)$ , depends on a (typically small) set of universal indices  $\{\eta\}$ . In other words, it does *not* depend on the microscopic configurations of  $A$  and  $B$ . Equivalently, we are able to macroscopically calculate the entropy of the composed system without any need of entering into the knowledge of the microscopic states of the subsystems. This property appears to be a natural one for an entropic form if we desire to use it as a basis for a statistical mechanics which would naturally connect to thermodynamics.

The  $BG$  entropy is composable since it satisfies Eq. (2.10). In other words, we have  $F(x, y) = x + y$ . Since  $S_{BG}$  is nonparametric, no index exists.

### 2.1.2.10 Sensitivity to the Initial Conditions, Entropy Production per Unit Time, and a Pesin-Like Identity

For a one-dimensional dynamical system (characterized by the variable  $x$ ) the sensitivity to the initial conditions  $\xi$  is defined as follows:

$$\xi \equiv \lim_{\Delta x(0) \rightarrow 0} \frac{\Delta x(t)}{\Delta x(0)}. \quad (2.29)$$

It can be shown [82, 83] that  $\xi$  paradigmatically satisfies the equation

$$\frac{d\xi}{dt} = \lambda_1 \xi, \quad (2.30)$$

whose solution is given by

$$\xi = e^{\lambda_1 t}. \quad (2.31)$$

(The meaning of the subscript 1 will become transparent later on). If the *Lyapunov exponent*  $\lambda_1 > 0$  ( $\lambda_1 < 0$ ), the system will be said to be *strongly chaotic (regular)*. The case where  $\lambda_1 = 0$  is sometimes called *marginal* and will be extensively addressed later on.

At this point let us briefly review, without proof, some basic notions of nonlinear dynamical systems. If the system is  $d$ -dimensional (i.e., it evolves in a phase-space whose  $d$ -dimensional Lebesgue measure is finite), it has  $d$  Lyapunov exponents:  $d_+$  of them are positive,  $d_-$  are negative, and  $d_0$  vanish, hence  $d_+ + d_- + d_0 = d$ . Let us order them all from the largest to the smallest:  $\lambda_1^{(1)} \geq \lambda_1^{(2)} \geq \dots \geq \lambda_1^{(d_+)} > \lambda_1^{(d_++1)} = \lambda_1^{(d_++2)} = \dots = \lambda_1^{(d_++d_0)} = 0 > \lambda_1^{(d_++d_0+1)} \geq \lambda_1^{(d_++d_0+2)} \geq \dots \geq \lambda_1^{(d)}$ . An infinitely small *segment* (having then a well defined one-dimensional Lebesgue measure) diverges like  $e^{\lambda_1^{(1)} t}$ ; this precisely is the case focused in Eq. (2.31). An infinitely small *area* (having then a well defined two-dimensional Lebesgue measure) diverges like  $e^{(\lambda_1^{(1)} + \lambda_1^{(2)}) t}$ . An infinitely small volume diverges like  $e^{(\lambda_1^{(1)} + \lambda_1^{(2)} + \lambda_1^{(3)}) t}$ , and so on. An infinitely small  $d$ -dimensional hypervolume evolves like  $e^{[\sum_{r=1}^d \lambda_1^{(r)}] t}$ . If

the system is *conservative*, i.e., if the infinitely small  $d$ -dimensional hypervolume remains constant with time, then it follows that  $\sum_{r=1}^d \lambda_1^{(r)} = 0$ . An important particular class of conservative systems is constituted by the so-called *symplectic* ones. For these,  $d$  is an even integer, and the Lyapunov exponents are coupled two by two as follows:  $\lambda_1^{(1)} = -\lambda_1^{(d)} \geq \lambda_1^{(2)} = -\lambda_1^{(d-1)} \geq \dots \geq \lambda_1^{(d_+)} = -\lambda_1^{(d_++d_0+1)} \geq \lambda_1^{(d_++1)} = \dots = \lambda_1^{(d_++d_0)} = 0$ . Consistently, such systems have  $d_+ = d_-$  and  $d_0$  is an even integer. The most popular illustration of symplectic systems is the Hamiltonian systems. They are conservative, which precisely is what the classical Liouville theorem states!

Do all these degrees of freedom contribute, as time evolves, to the erratic exploration of the phase-space? *No, they do not.* Only those associated with the  $d_+$  positive Lyapunov exponents, and some of the  $d_0$  vanishing ones, do. Consistently, it is only these which contribute to our loss of information, as time evolves, about the location in phase-space of a set of initial conditions. As we shall see, these remarks enable an intuitive understanding to the so-called Pesin identity, that we will soon state.

Let us now address the interesting question of the *BG* entropy production as time  $t$  increases. More than one entropy production can be defined as a function of time. Two basic choices are the so-called *Kolmogorov–Sinai entropy* (or *KS entropy rate*) [84], based on a single trajectory in phase-space, and the one associated to the evolution of an *ensemble of initial conditions*. We shall preferentially use here the latter, because of its sensibly higher computational tractability. In fact, excepting for pathological cases, they both coincide.

Let us schematically describe the *Kolmogorov–Sinai entropy rate* concept or *metric entropy* [83, 84, 286]. We first partition the phase-space in two regions, noted  $A$  and  $B$ . Then we choose a generic initial condition (the final result will not depend on this choice) and, applying the specific dynamics of the system at equal and finite time intervals  $\tau$ , we generate a long string (infinitely long in principle), say  $ABBAABBABA\dots$ . Then we analyze words of length  $l = 1$ . In our case, there are only two such words, namely  $A$  and  $B$ . The analysis consists in running along the string a window whose width is  $l$ , and determining the probabilities  $p_A$  and  $p_B$  of the words  $A$  and  $B$ , respectively. Finally, we calculate the entropy  $S_{BG}(l = 1) = -p_A \ln p_A - p_B \ln p_B$ . Then we repeat for words whose length equals  $l = 2$ . In our case, there are four such words, namely  $AA, AB, BA, BB$ . Running along the string a  $l = 2$  window letter by letter, we determine the probabilities  $p_{AA}, p_{AB}, p_{BA}, p_{BB}$ , hence the entropy  $S_{BG}(l = 2) = -p_{AA} \ln p_{AA} - p_{AB} \ln p_{AB} - p_{BA} \ln p_{BA} - p_{BB} \ln p_{BB}$ . Then we repeat for  $l = 3, 4, \dots$  and calculate the corresponding values for  $S_{BG}(l)$ . We then choose another two-partition, say  $A'$  and  $B'$ , and repeat the whole procedure. Then we do in principle for all possible two partitions. Then we go to three partitions, i.e., the alphabet will be now constituted by three letters, say  $A, B$ , and  $C$ . We repeat the previous procedure for  $l = 1$  (corresponding to the words  $A, B, C$ ), then for  $l = 2$  (corresponding to the words  $AA, AB, AC, BA, BB, BC, CA, CB, CC$ ), etc. Then we run windows with  $l = 3, 4, \dots$ . We then consider a different three-partition, say  $A', B',$  and  $C' \dots$ . Then we consider four-partitions, and so on. Of all these entropies we retain the *supremum*. In the appropriate limits of infinitely fine partitions and

$\tau \rightarrow 0$  we obtain finally the largest rate of increase of the  $BG$  entropy. This is basically the Kolmogorov–Sinai entropy rate.

It is not necessary to insist on how deeply inconvenient this definition can be for any computational implementation! Fortunately, a different type of entropy production can be defined [85], whose computational implementation is usually very simple. It is defined as follows. First partition the phase-space into  $W$  little cells (normally equal in size) and denote them with  $i = 1, 2, \dots, W$ . Then randomly place  $M$  initial conditions in one of those  $W$  cells (if  $d_+ \geq 1$ , normally the result will not depend on this choice). And then follow, as time evolves, the number of points  $M_i(t)$  in each cell ( $\sum_{i=1}^W M_i(t) = M$ ). Define the probability set  $p_i(t) \equiv M_i(t)/M$  ( $\forall i$ ), and calculate finally  $S_{BG}(t)$  through Eq. (1.1). The *entropy production per unit time* is defined as

$$K_1 \equiv \lim_{t \rightarrow \infty} \lim_{W \rightarrow \infty} \lim_{M \rightarrow \infty} \frac{S_{BG}(t)}{t}. \quad (2.32)$$

The Pesin identity [86], or more precisely the Pesin-like identity that we shall use here, states, for large classes of dynamical systems [85],

$$K_1 = \sum_{r=1}^{d_+} \lambda_1^{(r)}. \quad (2.33)$$

As it will become gradually clear along the book, this relationship (and its  $q$ -generalization) will play an important role in the determination of the particular entropic form which is adequate for a given nonlinear dynamical system.

## 2.2 Kullback–Leibler Relative Entropy

In many problems the question arises on how different are two probability distributions  $p$  and  $p^{(0)}$ ; for reasons that will become clear soon,  $p^{(0)}$  will be referred to as the *reference*. It becomes therefore interesting to define some sort of “distance” between them. One possibility is of course the distance introduced in Eq. (2.17). In other words, for say continuous distributions, we can use

$$D_\mu(p, p^{(0)}) \equiv \left[ \int dx |p(x) - p^{(0)}(x)|^\mu \right]^{1/\mu} \quad (\mu > 0). \quad (2.34)$$

In general we have that  $D_\mu(p, p^{(0)}) = D_\mu(p^{(0)}, p)$ , and that  $D_\mu(p, p^{(0)}) = 0$  if and only if  $p(x) = p^{(0)}(x)$  almost everywhere. We remind, however, that the triangular inequality is satisfied only for  $\mu \geq 1$ . Therefore, only then the distance constitutes a metric. If  $p(x) = \sum_{i=1}^W p_i \Delta(x - x_i)$  and  $p^{(0)}(x) = \sum_{i=1}^W p_i^{(0)} \Delta(x - x_i)$ , (see Eq. (2.4)) Eq. (2.34) leads to

$$D_\mu(p, p^{(0)}) \equiv \left[ \sum_{i=1}^W |p_i - p_i^{(0)}|^\mu \right]^{1/\mu} \quad (\mu > 0), \quad (2.35)$$

which exactly recovers Eq. (2.17).

For some purposes, this definition of distance is quite convenient. For others, the *Kullback–Leibler entropy* [87] has been introduced (see, for instance, [88, 92] and references therein). It is occasionally called *cross entropy*, or *relative entropy*, or *mutual information*, and it is defined as follows:

$$I_1(p, p^{(0)}) \equiv \int dx p(x) \ln \left[ \frac{p(x)}{p^{(0)}(x)} \right] = - \int dx p(x) \ln \left[ \frac{p^{(0)}(x)}{p(x)} \right]. \quad (2.36)$$

It can be proved, by using  $\ln r \geq 1 - 1/r$  (with  $r \equiv p(x)/p^{(0)}(x) > 0$ ), that  $I_1(p, p^{(0)}) \geq 0$ , the equality being valid if and only if  $p(x) = p^{(0)}(x)$  almost everywhere. It is clear that in general  $I_1(p, p^{(0)}) \neq I_1(p^{(0)}, p)$ . This inconvenience is sometimes overcome by using the symmetrized quantity  $[I_1(p, p^{(0)}) + I_1(p^{(0)}, p)]/2$ .

$I_1(p, p^{(0)})$  (like the distance (2.34)) has the property of being invariant under variable transformation. Indeed, if we make  $x = f(y)$ , the measure preservation implies  $p(x)dx = \tilde{p}(y)dy$ . Since  $p(x)/p^{(0)}(x) = \tilde{p}(y)/\tilde{p}^{(0)}(y)$ , we have  $I_1(p, p^{(0)}) = I_1(\tilde{p}, \tilde{p}^{(0)})$ , which proves the above-mentioned invariance. The *BG* entropy in its continuous (*not* in its discrete) form  $S_{BG} = - \int dx p(x) \ln p(x)$  lacks this important property. Because of this fact, the *BG* entropy is advantageously replaced, in some calculations, by the Kullback–Leibler one. Depending on the particular problem, the referential distribution  $p^{(0)}(x)$  is frequently taken to be a standard distribution such as the uniform, or Gaussian, or Lorentzian, or Poisson or *BG* ones. When  $p^{(0)}(x)$  is chosen to be the uniform distribution on a compact support of Lebesgue measure  $W$ , we have the relation

$$I_1(p, 1/W) = \ln W - S_{BG}(p). \quad (2.37)$$

Because of relations of this kind, the minimization of the Kulback–Leibler entropy is sometimes used instead of the maximization of the Boltzmann–Gibbs–Shannon entropy.

Although convenient for a variety of purposes,  $I_1(p, p^{(0)})$  has a disadvantage. It is needed that  $p(x)$  and  $p^{(0)}(x)$  simultaneously vanish, if they do so for certain values of  $x$  (this property is usually referred to as being *absolutely continuous*). Indeed, it is evident that otherwise the quantity  $I_1(p, p^{(0)})$  becomes ill-defined. To overcome this difficulty, a different distance has been defined along the lines of the Kullback–Leibler entropy. We refer to the so-called *Jensen–Shannon divergence*. Although interesting in many respects, its study would take us too far from our present line. Details can be seen in [93, 94] and references therein.

Let us mention also that, for discrete probabilities, definition (2.36) leads to

$$I_1(p, p^{(0)}) \equiv \sum_{i=1}^W p_i \ln \left[ \frac{p_i}{p_i^{(0)}} \right] = - \sum_{i=1}^W p_i \ln \left[ \frac{p_i^{(0)}}{p_i} \right]. \quad (2.38)$$

Various other interesting related properties can be found in [95, 96].

## 2.3 Constraints and Entropy Optimization

The most simple entropic optimization cases are those worked out in what follows.

### 2.3.1 *Imposing the Mean Value of the Variable*

In addition to

$$\int_0^\infty dx p(x) = 1, \quad (2.39)$$

we might know the mean value of the variable, i.e.,

$$\langle x \rangle \equiv \int_0^\infty dx x p(x) = X^{(1)}. \quad (2.40)$$

By using the Lagrange method to find the optimizing distribution, we define

$$\Phi[p] \equiv - \int_0^\infty dx p(x) \ln p(x) - \alpha \int_0^\infty dx p(x) - \beta^{(1)} \int_0^\infty dx x p(x), \quad (2.41)$$

and then impose  $\delta\Phi[p]/\delta p(x) = 0$ . We straightforwardly obtain  $1 + \ln p_{opt} + \alpha + \beta^{(1)}x = 0$  (*opt* stands for *optimal*), hence

$$p_{opt} = \frac{e^{-\beta^{(1)}x}}{\int_0^\infty dx e^{-\beta^{(1)}x}} = \beta^{(1)} e^{-\beta^{(1)}x}, \quad (2.42)$$

where we have used condition (2.39) to eliminate the Lagrange parameter  $\alpha$ . By using condition (2.40), we obtain the following relation for the Lagrange parameter  $\beta^{(1)}$ :

$$\beta^{(1)} = \frac{1}{X^{(1)}}, \quad (2.43)$$

hence, replacing in (2.42),

$$p_{opt} = \frac{e^{-x/X^{(1)}}}{X^{(1)}}. \quad (2.44)$$

### 2.3.2 Imposing the Mean Value of the Squared Variable

Another simple and quite frequent case is when we know that  $\langle x \rangle = 0$ . In such case, in addition to

$$\int_{-\infty}^{\infty} dx p(x) = 1, \quad (2.45)$$

we might know the mean value of the squared variable, i.e.,

$$\langle x^2 \rangle \equiv \int_{-\infty}^{\infty} dx x^2 p(x) = X^{(2)} > 0. \quad (2.46)$$

By using, as before, the Lagrange method to find the optimizing distribution, we define

$$\Phi[p] \equiv - \int_{-\infty}^{\infty} dx p(x) \ln p(x) - \alpha \int_{-\infty}^{\infty} dx p(x) - \beta^{(2)} \int_{-\infty}^{\infty} dx x^2 p(x), \quad (2.47)$$

and then impose  $\delta\Phi[p]/\delta p(x) = 0$ . We straightforwardly obtain  $1 + \ln p_{opt} + \alpha + \beta^{(2)}x^2 = 0$ , hence

$$p_{opt} = \frac{e^{-\beta^{(2)}x^2}}{\int_{-\infty}^{\infty} dx e^{-\beta^{(2)}x^2}} = \sqrt{\frac{\beta^{(2)}}{\pi}} e^{-\beta^{(2)}x^2}, \quad (2.48)$$

where we have used condition (2.45) to eliminate the Lagrange parameter  $\alpha$ .

By using condition (2.46), we obtain the following relation for the Lagrange parameter  $\beta^{(2)}$ :

$$\beta^{(2)} = \frac{1}{2X^{(2)}}, \quad (2.49)$$

hence, replacing in (2.48),

$$p_{opt} = \frac{e^{-x^2/(2X^{(2)})}}{\sqrt{2\pi X^{(2)}}}. \quad (2.50)$$

We thus see the very basic connection between Gaussian distributions and *BG* entropy.

### 2.3.3 Imposing the Mean Values of both the Variable and Its Square

Let us unify here the two preceding subsections. We impose

$$\int_{-\infty}^{\infty} dx p(x) = 1 \quad (2.51)$$

and, in addition to this, we know that

$$\langle x \rangle \equiv \int_{-\infty}^{\infty} dx x p(x) = X^{(1)}, \quad (2.52)$$

and

$$\langle (x - \langle x \rangle)^2 \rangle \equiv \int_{-\infty}^{\infty} dx (x - \langle x \rangle)^2 p(x) = X^{(2)} - (X^{(1)})^2 \equiv M^{(2)} > 0. \quad (2.53)$$

By using once again the Lagrange method, we define

$$\begin{aligned} \Phi[p] \equiv & - \int_{-\infty}^{\infty} dx p(x) \ln p(x) - \alpha \int_{-\infty}^{\infty} dx p(x) \\ & - \beta^{(1)} \int_{-\infty}^{\infty} dx x p(x) - \beta^{(2)} \int_{-\infty}^{\infty} dx (x - \langle x \rangle)^2 p(x), \end{aligned} \quad (2.54)$$

and then impose  $\delta\Phi[p]/\delta p(x) = 0$ . We straightforwardly obtain  $1 + \ln p_{opt} + \alpha + \beta^{(1)}x + \beta^{(2)}(x - \langle x \rangle)^2 = 0$ , hence

$$p_{opt} = \frac{e^{-\beta^{(1)}x - \beta^{(2)}(x - \langle x \rangle)^2}}{\int_{-\infty}^{\infty} dx e^{-\beta^{(1)}x - \beta^{(2)}(x - \langle x \rangle)^2}} = \sqrt{\frac{\beta^{(2)}}{\pi}} e^{-\beta^{(2)}(x - \langle x \rangle)^2}, \quad (2.55)$$

where we have used condition (2.51) to eliminate the Lagrange parameter  $\alpha$ . By using conditions (2.52) and (2.53), we obtain the following relations for the Lagrange parameters  $\beta^{(1)}$  and  $\beta^{(2)}$ :

$$\beta^{(1)} = \frac{1}{X^{(1)}}, \quad (2.56)$$

and

$$\beta^{(2)} = \frac{1}{2[X^{(2)} - (X^{(1)})^2]}. \quad (2.57)$$

Replacing (2.57) in (2.55), we finally obtain

$$p_{opt} = \frac{e^{-\frac{(x-X^{(1)})^2}{2[X^{(2)}-(X^{(1)})^2]}}}{\sqrt{2\pi[X^{(2)}-(X^{(1)})^2]}}. \quad (2.58)$$

We see that the only effect of a nonzero mean value of  $x$  is to re-center the Gaussian.

### 2.3.4 Others

A quite general situation would be to impose, in addition to

$$\int dx p(x) = 1, \quad (2.59)$$

the constraint

$$\int dx f(x) p(x) = F, \quad (2.60)$$

where  $f(x)$  is some known function and  $F$  a known number. We obtain

$$p_{opt} = \frac{e^{-\beta f(x)}}{\int dx e^{-\beta f(x)}}. \quad (2.61)$$

It is clear that, by appropriately choosing  $f(x)$ , we can force  $p_{opt}(x)$  to be virtually *any* distribution we wish. For example, by choosing  $f(x) = |x|^\gamma$  ( $\gamma \in \mathbb{R}$ ), we obtain a generic stretched exponential  $p_{opt}(x) \propto e^{-\beta|x|^\gamma}$ ; by choosing  $f(x) = \ln x$ , we obtain for  $p_{opt}(x)$  a power law. But the use of such procedures hardly has any epistemological interest at all, since it provides no hint onto the underlying nature of the problem. Only choices such as  $f(x) = x$  or  $f(x) = x^2$  are sound since such constraints correspond to very generic informational features, namely the *location of the center* and the *width* of the distribution. Other choices are, unless some exceptional fact enters into consideration (e.g.,  $f(x)$  being a constant of motion of the system), quite ad hoc and uninteresting. Of course, this mathematical fact is by no means exclusive of  $S_{BG}$ : the same holds for virtually *any* entropic form.

## 2.4 Boltzmann–Gibbs Statistical Mechanics and Thermodynamics

There are many formal manners for deriving the *BG* entropy and its associated probability distribution for thermal equilibrium. *None of them uses exclusively first principle arguments*, i.e., arguments that entirely remain at the level of mechanics

(classical, quantum, relativistic, or any other). That surely was, as previously mentioned, one of the central scientific goals that Boltzmann pursued his entire life, but, although he probably had a strong intuition about this point, he died without succeeding. The difficulties are so heavy that even today we do not know how to do this. At first sight, this might seem surprising given the fact that  $S_{BG}$  and the  $BG$  weight enjoy the universal acceptance that we all know. So, let us illustrate our statement more precisely. Assume that we have a quite generic many-body short-range-interacting Hamiltonian. We currently know that its thermal equilibrium is described by the  $BG$  weight. What we still do not know is *how* to derive this important result from purely mechanical and statistical logical steps, i.e., without using a priori generic dynamical hypothesis such as *ergodicity*, or a priori postulating the validity of macroscopic relations such as some or all of the principles of thermodynamics. For example, Fisher et al. [97–99] proved long ago, for a vast class of short-range-interacting Hamiltonians, that the thermal equilibrium physical quantities are computable within standard  $BG$  statistical mechanics. Such a proof, no matter how precious might it be, does *not* prove also that this statistics *indeed* provides the correct description at thermal equilibrium. Rephrasing, it proves that  $BG$  statistics *can* be the correct one, but it does *not* prove that it *is* the correct one. Clearly, there is no reasonable doubt today that, for such systems,  $BG$  is the correct one. It is nevertheless instructive that the logical implications of the available proofs be outlined.

On a similar vein, even for the case of long-range-interacting Hamiltonians (e.g., infinitely-long-range interactions), the standard  $BG$  calculations can still be performed through convenient renormalizations of the coupling constants (e.g., *a la* Kac, or through the usual mean field approximation recipe of artificially dividing the coupling constant by the number  $N$  of particles raised to some appropriate power). The possibility of computability does *by no means* prove, strictly speaking, that  $BG$  statistics is the correct description. And certainly it does not enlighten us on what the necessary and sufficient *first-principle* conditions could be for the  $BG$  description to be the adequate one.

In spite of all these mathematical difficulties, at least one nontrivial example has been advanced in the literature [100] for which it has been possible to exhibit *numerically* the  $BG$  weight by *exclusively* using Newton's  $\mathbf{F} = m\mathbf{a}$  as microscopic dynamics, *with no thermostatistical assumption of any kind*.

Let us anticipate that these and worse difficulties exist for the considerably more subtle situations that will be addressed in nonextensive statistical mechanics.

In what follows, we shall conform to more traditional, though epistemologically less ambitious, paths. We shall primarily follow the Gibbs' elegant lines of first *postulating* an entropic form, and then using it, *without proof*, as the basis for a variational principle including appropriate constraints. The philosophy of such path is quite clear. It is a form of *Occam's razor*, where we use all that we know and not more than we know. This is obviously extremely attractive from a conceptual standpoint. However, that its mathematical implementation is to be done with a *given specific entropic functional* with *given specific constraints* is of course far from trivial! After 130 years of impressive success, there can be no doubt that  $BG$

concepts and statistical mechanics provide the correct connection between microscopic and macroscopic laws for a vast class of physical systems. But – we insist – the mathematically *precise* qualification of this class remains an open question.

### 2.4.1 Isolated System – Microcanonical Ensemble

In this and subsequent subsections, we briefly review *BG* statistical mechanics (see, for instance, [35]). We consider a quantum Hamiltonian system constituted by  $N$  interacting particles under specific boundary conditions, and denote by  $\{E_i\}$  its energy eigenvalues.

The microcanonical ensemble corresponds to an isolated  $N$ -particle system whose total energy  $U$  is known within some precision  $\delta U$  (to be in fact taken at its zero limit at the appropriate mathematical stage). The number of states  $i$  with  $U \leq E_i \leq U + \delta U$  is denoted by  $W$ . *Assuming* that the system is such that its dynamics leads to ergodicity at its stationary state (thermal equilibrium), we assume that all such states are equally probable, i.e.,  $p_i = 1/W$ , and the entropy is given by Eq. (1.3). The temperature  $T$  is introduced through

$$\frac{1}{T} \equiv \frac{\partial S_{BG}}{\partial U} = k \frac{\partial \ln W}{\partial U}. \quad (2.62)$$

### 2.4.2 In the Presence of a Thermostat – Canonical Ensemble

The canonical ensemble corresponds to an  $N$ -particle system defined in a Hilbert space whose dimension is noted  $W$ , and which is in longstanding thermal contact with a (infinitely large) thermostat at temperature  $T$ . Its exact energy is unknown, but its mean energy  $U$  is known since it is determined by the thermostat. We must optimize the entropy given by Eq. (1.1) with the norm constraint (1.2), and with the energy constraint

$$\sum_{i=1}^W p_i E_i = U. \quad (2.63)$$

Following along the lines of Section 2.3, we obtain the celebrated *BG* weight

$$p_i = \frac{e^{-\beta E_i}}{Z_{BG}}, \quad (2.64)$$

with the *partition function* given by

$$Z_{BG} \equiv \sum_{i=1}^W e^{-\beta E_i}, \quad (2.65)$$

the Lagrange parameter  $\beta$  being related with the temperature through  $\beta \equiv 1/(kT)$ .

We can prove also that

$$\frac{1}{T} = \frac{\partial S_{BG}}{\partial U}, \quad (2.66)$$

that the *Helmholtz free energy* is given by

$$F_{BG} \equiv U - TS_{BG} = -\frac{1}{\beta} \ln Z_{BG}, \quad (2.67)$$

and that the *internal energy* is given by

$$U = -\frac{\partial}{\partial \beta} \ln Z_{BG}. \quad (2.68)$$

In the limit  $T \rightarrow \infty$  we recover the microcanonical ensemble.

### 2.4.3 Others

The system may be exchanging with the thermostat not only energy, so that the temperature is that of the thermostat, but also particles, so that also the chemical potential is fixed by the reservoir. This physical situation corresponds to the so-called *grand-canonical ensemble*. This and other similar physical situations can be treated along the same path, as shown by Gibbs. We shall not review here these types of systems, which are described in detail in [35], for instance.

Another important physical case, which we do not review here either, is when the particles cannot be considered as distinguishable. Such is the case of *bosons* (leading to Bose–Einstein statistics), *fermions* (leading to Fermi–Dirac statistics), and the so-called *gentilions* (leading to Gentile statistics, also called *parastatistics* [101–103], which unifies those of Bose–Einstein and Fermi–Dirac).

All these various physical systems, and even others, constitute what is currently referred to as *BG statistical mechanics*, essentially because at its basis we find, in one way or another, the entropic functional  $S_{BG}$ . It is this entire theoretical body that in principle we intend to generalize in the rest of the book, through the generalization of  $S_{BG}$  itself.

# Chapter 3

## Generalizing What We Learnt: Nonextensive Statistical Mechanics

*Don Quijote me ha revelado íntimos secretos suyos que no reveló a Cervantes*

Víctor Goti

(Prólogo de *Niebla* de Miguel de Unamuno, 1935)

### 3.1 Playing with Differential Equations – A Metaphor

As we already emphasized, there is no logical-deductive procedure for generalizing *any* physical theory. This occurs through all types of paths that, in one way or another, are ultimately but metaphors. Let us present here a possible metaphor for generalizing the *BG* entropy.

The simplest ordinary differential equation can be considered to be

$$\frac{dy}{dx} = 0 \quad (y(0) = 1). \quad (3.1)$$

Its solution is

$$y = 1, \quad (3.2)$$

whose symmetric curve with regard to the bissector axis is

$$x = 1. \quad (3.3)$$

As the second simplest differential equation we might consider

$$\frac{dy}{dx} = 1 \quad (y(0) = 1). \quad (3.4)$$

Its solution is

$$y = 1 + x, \quad (3.5)$$

whose inverse function is

$$y = x - 1. \quad (3.6)$$

We may next wish to consider the following one:

$$\frac{dy}{dx} = y \quad (y(0) = 1), \quad (3.7)$$

whose solution is

$$y = e^x. \quad (3.8)$$

Its inverse function is

$$y = \ln x, \quad (3.9)$$

and satisfies of course

$$\ln(x_A x_B) = \ln x_A + \ln x_B. \quad (3.10)$$

Is it possible to unify the three differential equations we considered up to now (i.e., (3.1), (3.4), and (3.7))? Yes indeed. It is enough to consider

$$\frac{dy}{dx} = a + by \quad (y(0) = 1), \quad (3.11)$$

and play with the *two* parameters  $a$  and  $b$ . Is it possible to unify the same three differential equations with only *one* parameter? Yes indeed, . . . *out of linearity!* Just consider

$$\frac{dy}{dx} = y^q \quad (y(0) = 1; q \in \mathbb{R}). \quad (3.12)$$

Its solution is

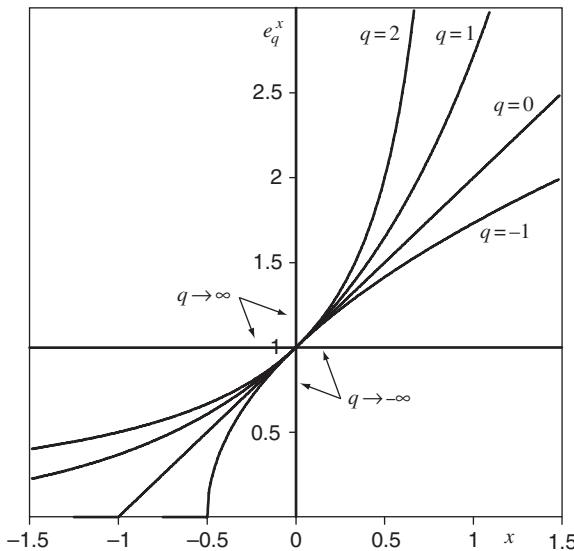
$$y = [1 + (1 - q)x]^{1/(1-q)} \equiv e_q^x \quad (e_1^x = e^x). \quad (3.13)$$

Its inverse is

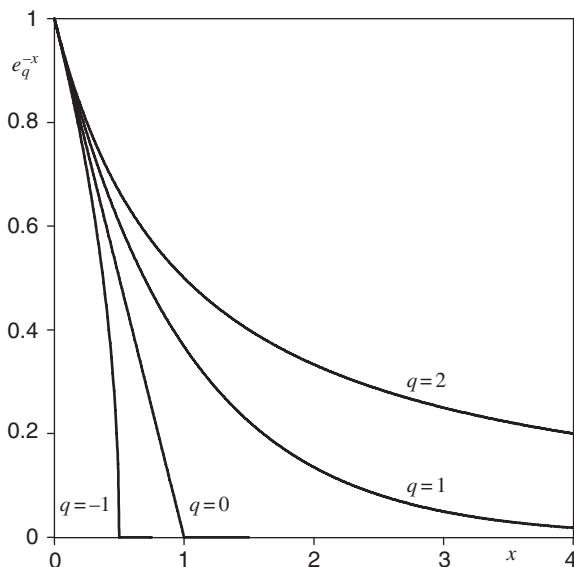
$$y = \frac{x^{1-q} - 1}{1 - q} \equiv \ln_q x \quad (x > 0; \ln_1 x = \ln x), \quad (3.14)$$

and satisfies the following property:

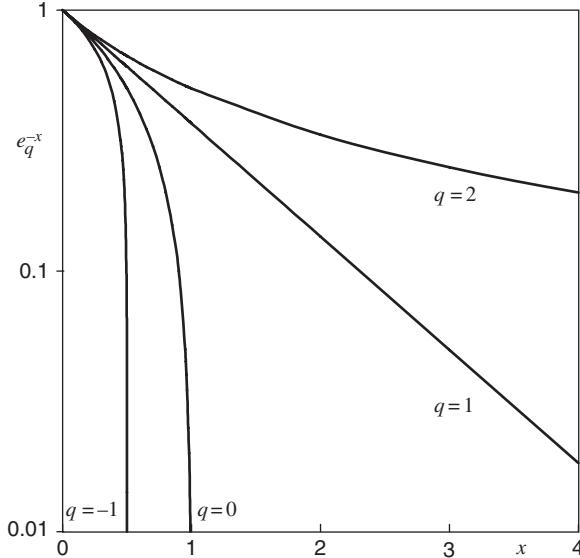
$$\ln_q(x_A x_B) = \ln_q x_A + \ln_q x_B + (1 - q)(\ln_q x_A)(\ln_q x_B). \quad (3.15)$$



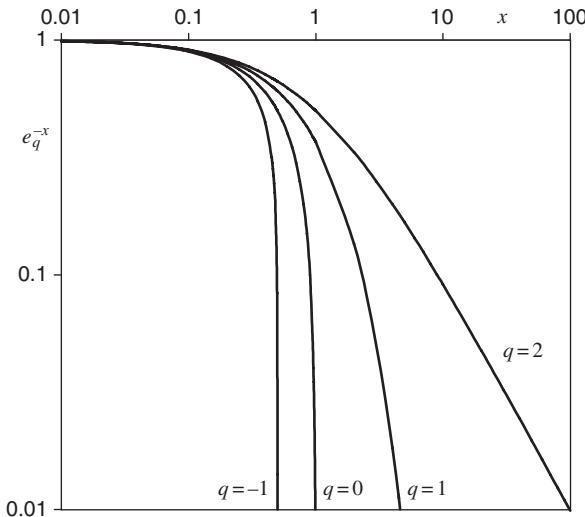
**Fig. 3.1** The  $q$ -exponential function  $e_q^x$  for typical values of  $q$ . For  $q > 1$ , it is defined in the interval  $(-\infty, (q-1)^{-1})$ ; it diverges if  $x \rightarrow (q-1)^{-1} - 0$ . For  $q < 1$ , it is defined  $\forall x$ , and vanishes for all  $x < -(1-q)^{-1}$ . In the limit  $x \rightarrow 0$ , it is  $e_q^x \sim 1 + x$  ( $\forall q$ ).



**Fig. 3.2** The  $q$ -exponential function  $e_q^{-x}$  for typical values of  $q$ : linear–linear scales. For  $q > 1$ , it vanishes like  $[(q-1)x]^{-1/(q-1)}$  for  $x \rightarrow \infty$ . For  $q < 1$ , it vanishes for  $x > (1-q)^{-1}$  (cutoff).



**Fig. 3.3** The  $q$ -exponential function  $e_q^{-x}$  for typical values of  $q$ : log–linear scales. It is convex (concave) if  $q > 1$  ( $q < 1$ ). For  $q < 1$ , it has a vertical asymptote at  $x = (1 - q)^{-1}$ .



**Fig. 3.4** The  $q$ -exponential function  $e_q^{-x}$  for typical values of  $q$ : log–log scales. For  $q > 1$ , it has an asymptotic slope equal to  $-1/(q - 1)$ .

We shall from now on refer to these two functions as the  *$q$ -exponential* and the  *$q$ -logarithm*, respectively [104]. They will play an important role through the entire theory. We may, in fact, anticipate that *virtually all* the generic expressions associated with *BG* statistics and its (nonlinear) dynamical foundations will, remarkably enough, turn out to be generalized essentially just by replacing the standard exponential and logarithm forms by the above  $q$ -generalized ones. Let us add that, whenever the  $1 + (1 - q)x$  argument of the  $q$ -exponential is negative, the function is defined to vanish. In other words, the definition is  $e_q^x \equiv [1 + (1 - q)x]_+^{1/(1-q)}$ , where  $[z]_+ = \max\{z, 0\}$ . However, for simplicity, we shall, most of the time, avoid this notation. Typical representations of the  $q$ -exponential function are illustrated in Figs. 3.1, 3.2, 3.3, and 3.4. It is immediately verified that the  $q \rightarrow -\infty$ ,  $q = 0$ , and  $q = 1$  particular instances precisely recover the cases presented in Eqs. (3.1), (3.4), and (3.7) respectively.

## 3.2 Nonadditive Entropy $S_q$

### 3.2.1 Definition

Through the metaphor presented above, and because of various other reasons that will gradually emerge, we may *postulate* the following generalization of Eq. (1.3):

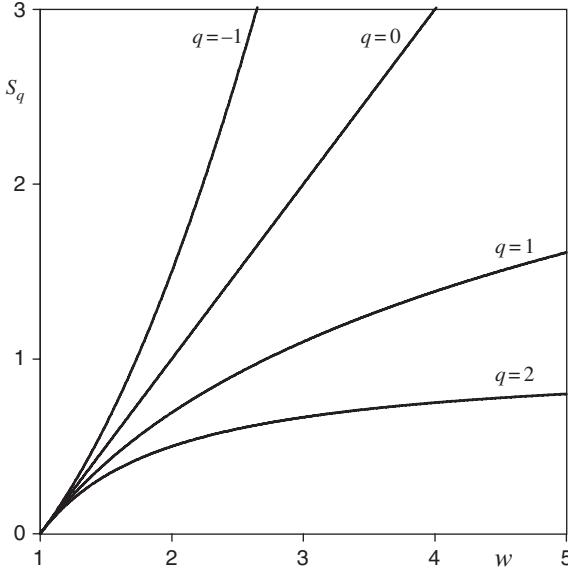
$$S_q = k \ln_q W \quad (S_1 = S_{BG}). \quad (3.16)$$

See Fig. 3.5 for the illustration of this generalization of the celebrated formula for equal probabilities. Let us address next the general case, i.e., for arbitrary  $\{p_i\}$ . We saw in Eq. (2.8) that  $S_{BG}$  can be written as the mean value of  $\ln(1/p_i)$ . This quantity is called *surprise* [105] or *unexpectedness* [106] by some authors. This is quite appropriate, in fact. If we have *certainty* ( $p_i = 1$  for some value of  $i$ ) that something will happen, when it does happen we have *no surprise*. On the opposite extreme, if something is *very unexpected* ( $p_i \simeq 0$ ), if it eventually happens, we are certainly *very surprised!* Along this line, it is certainly admissible to consider the quantity  $\ln_q(1/p_i)$  and call it  *$q$ -surprise* or  *$q$ -unexpectedness*. It then appears as quite natural to *postulate* the simultaneous generalization of Eqs. (2.8) and (3.16) as follows:

$$S_q = k \langle \ln_q(1/p_i) \rangle. \quad (3.17)$$

If we use the definition (3.14) in this expression, we straightforwardly obtain

$$S_q = k \frac{1 - \sum_{i=1}^W p_i^q}{q - 1}. \quad (3.18)$$



**Fig. 3.5** The equiprobability entropy  $S_q$  as a function of the number of states  $W$  (with  $k = 1$ ), for typical values of  $q$ . For  $q > 1$ ,  $S_q$  saturates at the value  $1/(q - 1)$  if  $W \rightarrow \infty$ ; for  $q \leq 1$ , it diverges. For  $q \rightarrow \infty$  ( $q \rightarrow -\infty$ ), it coincides with the abscissa (ordinate).

This is precisely the form *postulated* in [39] as a possible basis for generalizing  $BG$  statistical mechanics. See Table 3.1. One possible manner for checking that  $S_1 \equiv \lim_{q \rightarrow 1} S_q = S_{BG}$  is to directly replace into Eq. (3.18) the equivalence  $p_i^q = p_i p_i^{q-1} = p_i e^{(q-1)\ln p_i} \sim p_i [1 + (q - 1) \ln p_i]$ .

It turned out that this generalized entropic form, first with a *different* and then with the *same* multiplying factor, had already appeared outside the literature of physics, namely in that of cybernetics and control theory [107]. It was rediscovered independently in [39], when it was for the first time proposed as a starting point to generalize the standard statistical mechanics itself. This was done for the canonical ensemble, by optimizing  $S_q$  in the presence of an additional constraint, namely that related to the mean value of the energy. We shall focus on this calculation later on.

**Table 3.1**  $S_{BG}$  and  $S_q$  entropies ( $S_1 = S_{BG}$ )

Entropy	Equal probabilities ( $p_i = 1/W, \forall i$ )	Generic probabilities ( $\forall \{p_i\}$ )
$S_{BG}$	$k \ln W$	$-k \sum_{i=1}^W p_i \ln_{2-q} p_i = k \sum_{i=1}^W p_i \ln(1/p_i)$
$S_q$ ( $q \in \mathbb{R}$ )	$k \ln_q W$	$k \frac{1 - \sum_{i=1}^W p_i^q}{q-1} = k \sum_{i=1}^W p_i \ln_q(1/p_i)$ $= -k \sum_{i=1}^W p_i^q \ln_q p_i$ $= -k \sum_{i=1}^W p_i \ln_{2-q} p_i$

This form turns out to be in fact directly related to a generalized metric proposed in 1952 by Hardy, Littlewood and Polya [109], whose  $q = 2$  particular case corresponds to the Pythagorean metric.

A different path for arriving to the entropy (3.18) is the following one. This was in fact the original path, inspired by multifractals, that led to the postulate adopted in [39]. The entropic index  $q$  introduces a *bias* in the probabilities. Indeed, given the fact that generically  $0 < p_i < 1$ , we have that  $p_i^q > p_i$  if  $q < 1$  and  $p_i^q < p_i$  if  $q > 1$ . Therefore,  $q < 1$  (relatively) enhances the rare events, those which have probabilities close to zero, whereas  $q > 1$  (relatively) enhances the frequent events, those whose probability is close to unity. This property can be directly checked if we compare  $p_i$  with  $p_i^q / \sum_{j=1}^W p_j^q$ .

So, it appears as appealing to introduce an entropic form based on  $p_i^q$ . We want also the form to be invariant under permutations. So the simplest assumption is to consider  $S_q = f(\sum_{i=1}^W p_i^q)$ , where  $f$  is some continuous function to be found. The simplest choice is the linear one, i.e.,  $S_q = a + b \sum_{i=1}^W p_i^q$ . Since any entropy should be a measure of disorder or ignorance, we want that certainty corresponds to zero entropy. This immediately imposes  $a + b = 0$ , hence  $S_q = a(1 - \sum_{i=1}^W p_i^q)$ . But, since we are seeking for a generalization (and *not* an alternative), for  $q = 1$  we want to recover  $S_{BG}$ . Therefore, in the  $q \rightarrow 1$  limit,  $a$  must be asymptotically proportional to  $1/(q - 1)$  (we remind the equivalence indicated in the previous paragraph). The simplest way for this to occur is just to be  $a = k/(q - 1)$ , with  $k > 0$ , which immediately leads to Eq. (3.18).

We shall next address the properties of  $S_q$ . But before doing that, let us clarify a point which has a generic relevance. If  $q > 0$ , then expression (3.18) is well defined whether or not one or more states have *zero* probability. Not so if  $q < 0$ . In this case, it must be understood that the sum indicated in Eq. (3.8) runs *only* over states with *positive* probability. For simplicity, we shall not explicitly indicate this fact along the book. But it is *always* to be taken into account.

### 3.2.2 Properties

#### 3.2.2.1 Non-negativity

If we have certainty about the state of the system, then one of the probabilities equals unity, and all the others vanish. Consequently, the entropy  $S_q$  vanishes for all  $q$ .

If we do not have certainty, at least two of the probabilities are smaller than unity. Therefore, for those,  $1/p_i > 1$ , hence  $\ln_q(1/p_i) > 0, \forall i$  (see also Fig. 3.5). Consequently, using Eq. (3.17), it immediately follows that  $S_q > 0$ , for all  $q$ .

#### 3.2.2.2 Extremal at Equal Probabilities

For the same reason indicated in the *BG* case (invariance of the entropy par rapport to *any* permutation of states), at equiprobability  $S_q$  must be extremal. It turns out to be a *maximum* for  $q > 0$  and a *minimum* for  $q < 0$ . The proof will be completed

as soon as we establish that  $S_q(\{p_i\})$  is *concave* (*convex*) for  $q > 0$  ( $q < 0$ ), which will be done below. The  $q = 0$  case is marginal: the entropy is a constant. In that case we have that

$$S_0 = k(W - 1) \quad (\forall \{p_i\}) \quad (3.19)$$

### 3.2.2.3 Expansibility

It is straightforwardly verified that  $S_q$  is *expansible*,  $\forall q$ , since

$$S_q(p_1, p_2, \dots, p_W, 0) = S_q(p_1, p_2, \dots, p_W). \quad (3.20)$$

This property trivially follows from the definition (3.18) if  $q > 0$ . For  $q < 0$ , it follows from the fact that the sum in (3.18) runs only for states whose probability is positive.

### 3.2.2.4 Nonadditivity

It is straightforwardly verified that, if  $A$  and  $B$  are *independent*, i.e., if the *joint probability* satisfies  $p_{ij}^{A+B} = p_i^A p_j^B$  ( $\forall(i,j)$ ), then

$$\frac{S_q(A + B)}{k} = \frac{S_q(A)}{k} + \frac{S_q(B)}{k} + (1 - q) \frac{S_q(A)}{k} \frac{S_q(B)}{k}. \quad (3.21)$$

It is due to this property that, for  $q \neq 1$ ,  $S_q$  is said to be *nonadditive*.<sup>1</sup> However, drastic modifications occur when the subsystems  $A$  and  $B$  are correlated in a special manner. We shall see that in this case, a value of  $q$  might exist such that, either strictly or asymptotically ( $N \rightarrow \infty$ ),  $S_q(A + B) = S_q(A) + S_q(B)$ . In other words, the nonadditive entropy  $S_q$  can be extensive for  $q \neq 1$ ! This is a nontrivial issue that will be addressed in detail in Section 3.3.

Still, given the nonnegativity of  $S_q$ , it follows that, for *independent* subsystems,  $S_q(A + B) \geq S_q(A) + S_q(B)$  if  $q < 1$ , and  $S_q(A + B) \leq S_q(A) + S_q(B)$  if  $q > 1$ . Consistently, the  $q < 1$  and  $q > 1$  cases are occasionally referred in the literature as the *superadditive* and *subadditive* ones, respectively.

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<sup>1</sup> During many years, this property has been referred in the literature as *nonextensivity*. This is, in some sense, unfortunate. Indeed, it will become clear that, for a vast class of systems, a special value of  $q$  exists for which the nonadditive entropy  $S_q$  is extensive. The name “nonextensive statistical mechanics” itself had historically been coined from this property. At the level of statistical mechanics, this name is in fact not inadequate, since the Hamiltonian systems for which this theory is expected to apply are those with long-range interactions, whose total energy is precisely nonextensive in the thermodynamical sense.

### 3.2.2.5 Concavity and Convexity

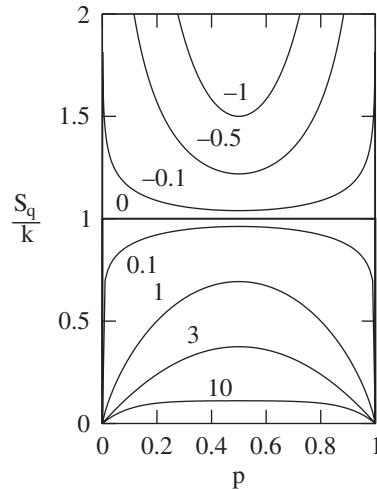
We refer to the concepts introduced in Eqs. (2.11), (2.12), and (2.13), which naturally extend for arbitrary  $q$ . The second derivative of the (continuous) function  $x(1 - x^{q-1})/(q - 1)$  is *negative (positive)* for  $q > 0$  ( $q < 0$ ). Consequently, for  $q > 0$ , we have

$$\frac{p_i''[1 - (p_i'')^{q-1}]}{q - 1} > \lambda \frac{p_i[1 - p_i^{q-1}]}{q - 1} + (1 - \lambda) \frac{p_i'[1 - (p_i')^{q-1}]}{q - 1} \quad (\forall i; 0 < \lambda < 1). \quad (3.22)$$

Applying  $\sum_{i=1}^W$  on both sides of this inequality, we immediately obtain that

$$S_q(\{p_i''\}) > \lambda S_q(\{p_i\}) + (1 - \lambda) S_q(\{p_i'\}) \quad (q > 0). \quad (3.23)$$

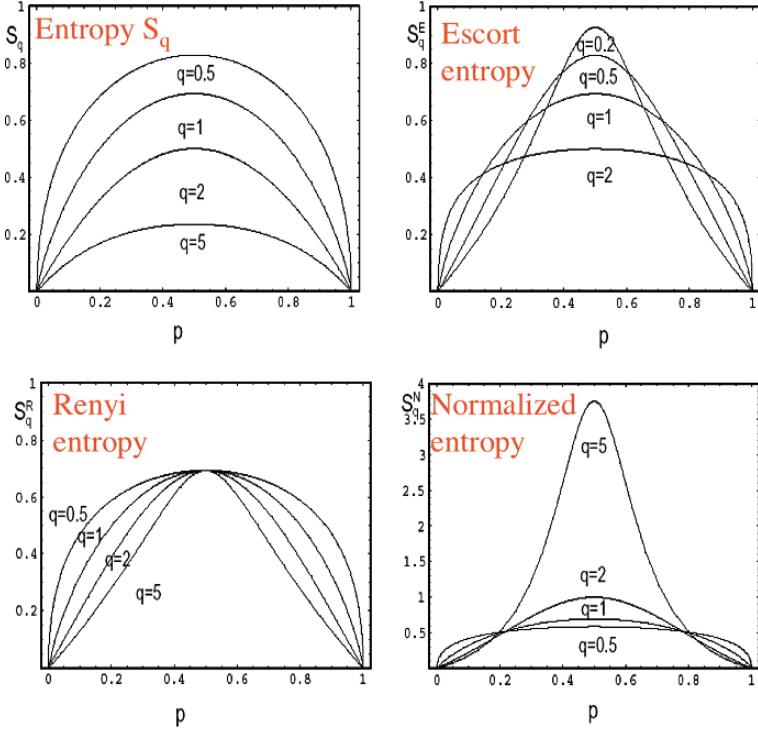
These inequalities are obviously reversed for  $q < 0$ . It is therefore proved that  $S_q$  is *concave (convex)* for  $q > 0$  ( $q < 0$ ). An immediate corollary is, as announced previously, that the case of equal probabilities corresponds to a *maximum* for  $q > 0$ , whereas it corresponds to a *minimum* for  $q < 0$ . See in Fig. 3.6 an illustration of this property. See also Fig. 3.7.



**Fig. 3.6** The  $p$ -dependence of the  $W = 2$  entropy  $S_q = [1 - p^q - (1 - p)^q]/(q - 1)$  for typical values of  $q$  (with  $S_1 = -p \ln p - (1 - p) \ln(1 - p)$ ).

### 3.2.2.6 Connection with Jackson Derivative

One century ago, the mathematician Jackson generalized [111] the concept of *derivative* of a generic function  $f(x)$ . He introduced his differential operator  $D_q$  as follows:



**Fig. 3.7** The  $p$ -dependence of the  $W = 2$  entropies  $S_q$ ,  $S_q^R$ ,  $S_q^E$ , and  $S_q^N$  [110], where the *Renyi entropy*  $S_q^R(\{p_i\}) \equiv \frac{\ln \sum_{i=1}^W p_i^q}{1-q} = \frac{\ln[1+(1-q)S_q(\{p_i\})]}{1-q}$ , the *escort entropy*  $S_q^E(\{p_i\}) \equiv S_q\left(\left\{\frac{p_i^q}{\sum_{j=1}^W p_j^q}\right\}\right) = \frac{1-(\sum_{i=1}^W p_i^{1/q})^{-q}}{q-1}$ , and the *Landsberg–Vedral–Rajagopal–Abe entropy*, or just *normalized entropy*  $S_q^N(\{p_i\}) \equiv \frac{S_q(\{p_i\})}{\sum_{i=1}^W p_i^q} = \frac{S_q(\{p_i\})}{1+(1-q)S_q(\{p_i\})}$ . We verify that, among these four entropic forms, only  $S_q$  is concave for all  $q > 0$ .

$$D_q f(x) \equiv \frac{f(qx) - f(x)}{qx - x}. \quad (3.24)$$

We immediately verify that  $D_1 f(x) = df(x)/dx$ . For  $q \neq 1$ , this operator replaces the usual (infinitesimal) *translation* operation on the abscissa  $x$  of the function  $f(x)$  by a *dilatation* operation.

Abe noticed a remarkable property [112]. In the same way that we can easily verify that

$$S_{BG} = -\frac{d}{dx} \sum_{i=1}^W p_i^x|_{x=1}, \quad (3.25)$$

we can verify that,  $\forall q$ ,

$$S_q = -D_q \sum_{i=1}^W p_i^x|_{x=1}. \quad (3.26)$$

We consider this as an inspiring property, where the usual *infinitesimal* translational operation is replaced by a *finite* operation, namely, in this case, by the one which is basic for *scale-invariance*. Since the postulation of the entropy  $S_q$  was inspired by multifractal geometry, the least one can say is that this property is most welcome.

### 3.2.2.7 Lesche-stability or Experimental Robustness

Let us start by emphasizing that this property is totally independent from concavity. For example, Renyi entropy  $S_q^R \equiv \frac{\ln \sum_{i=1}^W p_i^q}{1-q}$  is concave for  $0 < q \leq 1$  and is neither concave nor convex for  $q > 1$ . However, it is Lesche-unstable for all  $q > 0$  (excepting of course for  $q = 1$ ) [79].

It has been proved [110, 113] that the definition of experimental robustness, i.e., Eq. (2.15), is satisfied for  $S_q$  for  $q > 0$  (See Fig. 3.8).

### 3.2.2.8 Conditional Nonextensive Entropy, $q$ -expectations Values, and Escort Distributions

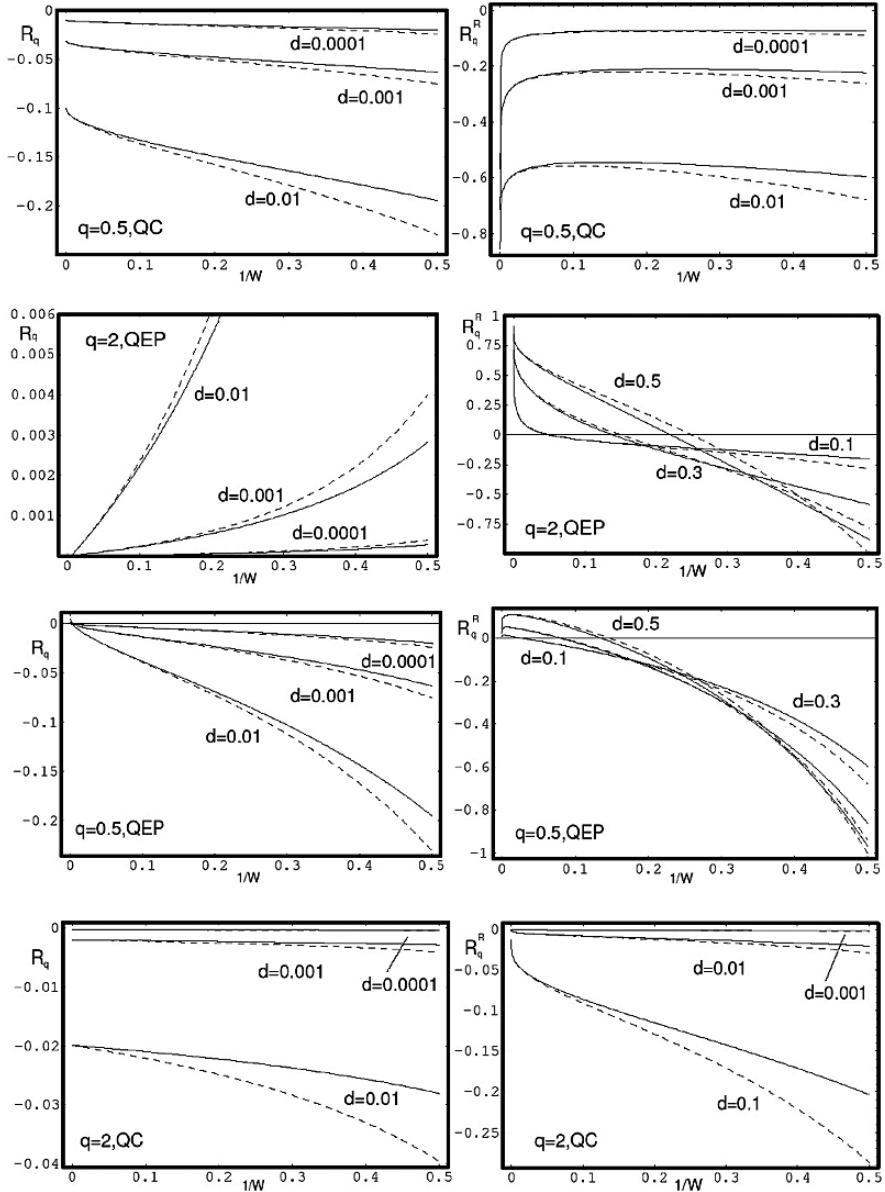
Let us consider the entropy (3.18) and divide the set of  $W$  possibilities in  $K$  nonintersecting subsets, respectively, containing  $W_1, W_2, \dots, W_K$  elements, with  $\sum_{k=1}^K W_k = W$  ( $1 \leq K \leq W$ ) [114]. We define the probabilities

$$\begin{aligned} \pi_1 &\equiv \sum_{\{W_1 \text{ terms}\}} p_i, \\ \pi_2 &\equiv \sum_{\{W_2 \text{ terms}\}} p_i, \dots \\ \pi_K &\equiv \sum_{\{W_K \text{ terms}\}} p_i, \end{aligned} \quad (3.27)$$

hence  $\sum_{k=1}^K \pi_k = 1$ . It is straightforward to verify the following property:

$$S_q(\{p_i\}) = S_q(\{\pi_k\}) + \sum_{k=1}^K \pi_k^q S_q(\{p_i/\pi_k\}), \quad (3.28)$$

where, consistently with Bayes' formula,  $\{p_i/\pi_k\}$  are the *conditional* probabilities, and satisfy  $\sum_{\{W_k \text{ terms}\}} (p_i/\pi_k) = 1$  ( $k = 1, 2, \dots, K$ ). Property (3.28) recovers, for  $q = 1$ , Shannon's celebrated *grouping* relation



**Fig. 3.8** Illustration of the dependence on  $(W, d)$  of the ratios  $R_q$  and  $R_q^R$  for the entropies  $S_q$  (left) and  $S_q^R$  (right), respectively. *QC* and *QEP* denote *quasi-certainty* and *quasi-equal-probabilities* (see the text). We see that  $\lim_{d \rightarrow 0} \lim_{W \rightarrow 1} R_q = 0$  in all four cases, whereas it is violated for  $R_q^R$  for the cases (*QC*,  $q < 1$ ) and (*QEP*,  $q > 1$ ). Not so for the two last cases, (*QC*,  $q > 1$ ) and (*QEP*,  $q < 1$ ), for which we do have  $\lim_{d \rightarrow 0} \lim_{W \rightarrow 1} R_q^R = 0$ . The dashed (continuous) curves correspond to metric  $\mu = 1$  ( $\mu = 2$ ) [110].

$$S_{BG}(\{p_i\}) = S_{BG}(\{\pi_k\}) + \sum_{k=1}^K \pi_k S_{BG}(\{p_i/\pi_k\}). \quad (3.29)$$

This property constitutes in fact the fourth axiom of the Shannon theorem.

The nonnegative entropies  $S_q(\{p_i\})$ ,  $S_q(\{\pi_k\})$ , and  $S_q(\{p_i/\pi_k\})$  depend, respectively, on  $W$ ,  $K$ , and  $W_k$  probabilities. Equation (3.28) can be rewritten as

$$S_q(\{p_i\}) = S_q(\{\pi_k\}) + \langle S_q(\{p_i/\pi_k\}) \rangle_q^{(u)}, \quad (3.30)$$

where the *unnormalized q-expectation value* ( $u$  stands for *unnormalized*) of the conditional entropy is defined as

$$\langle S_q(\{p_i/\pi_k\}) \rangle_q^{(u)} \equiv \sum_{k=1}^K \pi_k^q S_q(\{p_i/\pi_k\}), \quad (3.31)$$

Also, since the definition of  $S_q(\{\pi_k\})$  implies

$$\frac{1 + (1 - q)S_q(\{\pi_k\})}{\sum_{k'=1}^K \pi_{k'}^q} = 1, \quad (3.32)$$

Equation 3.28 can be rewritten as follows:

$$S_q(\{p_i\}) = S_q(\{\pi_k\}) + \sum_{k=1}^K \pi_k^q \frac{1 + (1 - q)S_q(\{\pi_k\})}{\sum_{k'=1}^K \pi_{k'}^q} S_q(\{p_i/\pi_k\}). \quad (3.33)$$

Consequently

$$S_q(\{p_i\}) = S_q(\{\pi_k\}) + \langle S_q(\{p_i/\pi_k\}) \rangle_q + (1 - q) S_q(\{\pi_k\}) \langle S_q(\{p_i/\pi_k\}) \rangle_q, \quad (3.34)$$

where the *normalized q-expectation value* of the conditional entropy is defined as

$$\langle S_q(\{p_i/\pi_k\}) \rangle_q \equiv \sum_{k=1}^K \Pi_k S_q(\{p_i/\pi_k\}), \quad (3.35)$$

with the *escort probabilities* [212]

$$\Pi_k \equiv \frac{\pi_k^q}{\sum_{k'=1}^K \pi_{k'}^q} \quad (k = 1, 2, \dots, K). \quad (3.36)$$

Property (3.34) is, as we shall see later on, a very useful one, and it exhibits a most important fact, namely that the definition of the nonextensive entropic form (3.18) naturally leads to normalized  $q$ -expectation values and to escort distributions.

Let us further elaborate on Eq. (3.34). It can be also rewritten in a more symmetric form, namely as

$$1 + (1 - q)S_q(\{p_i\}) = [1 + (1 - q)S_q(\{\pi_k\})][1 + (1 - q)\langle S_q(\{p_i/\pi_k\}) \rangle_q]. \quad (3.37)$$

Since the *Renyi entropy* (associated with the probabilities  $\{p_i\}$ ) is defined as  $S_q^R(\{p_i\}) \equiv (\ln \sum_{i=1}^W p_i^q)/(1 - q)$ , we can conveniently define the (monotonically increasing) function  $\mathcal{R}_q[x] \equiv \ln[1 + (1 - q)x]/[1 - q] = \ln\{[1 + (1 - q)x]^{[1/(1-q)]}\}$  (with  $\mathcal{R}_1[x] = x$ ), hence, for any distribution of probabilities, we have  $S_q^R = \mathcal{R}_q[S_q]$ . Equation (3.37) can now be rewritten as

$$\mathcal{R}_q[S_q(\{p_i\})] = \mathcal{R}_q[S_q(\{\pi_k\})] + \mathcal{R}_q[\langle S_q(\{p_i/\pi_k\}) \rangle_q], \quad (3.38)$$

or equivalently,

$$S_q^R(\{p_i\}) = S_q^R(\{\pi_k\}) + \mathcal{R}_q[\langle \mathcal{R}_q^{-1}[S_q^R(\{p_i/\pi_k\})] \rangle_q], \quad (3.39)$$

where the inverse function is defined as  $\mathcal{R}_q^{-1}[y] \equiv [(e^y)^{(1-q)} - 1]/[1 - q]$  (with  $\mathcal{R}_1^{-1}[y] = y$ ). Notice that, in general,  $\mathcal{R}_q[\langle \dots \rangle_q] \neq \langle \mathcal{R}_q[\dots] \rangle_q$ .

Everything we have said in this Section is valid for *arbitrary* partitions (in  $K$  nonintersecting subsets) of the ensemble of  $W$  possibilities. Let us from now on address the particular case where the  $W$  possibilities correspond to the joint possibilities of two subsystems  $A$  and  $B$ , having respectively  $W_A$  and  $W_B$  possibilities (hence  $W = W_A W_B$ ). Let us denote by  $\{p_{ij}\}$  the probabilities associated with the total system  $A + B$ , with  $i = 1, 2, \dots, W_A$ , and  $j = 1, 2, \dots, W_B$ . The *marginal probabilities*  $\{p_i^A\}$  associated with subsystem  $A$  are given by  $p_i^A = \sum_{j=1}^{W_B} p_{ij}$ , and those associated with subsystem  $B$  are given by  $p_j^B = \sum_{i=1}^{W_A} p_{ij}$ .  $A$  and  $B$  are said to be *independent* if and only if  $p_{ij} = p_i^A p_j^B$  ( $\forall(i, j)$ ). We can now identify the  $K$  subsets which we were previously analyzing with the  $W_A$  possibilities of subsystem  $A$ , hence the probabilities  $\{\pi_k\}$  correspond to  $\{p_i^A\}$ . Consistently, Eq. (3.34) implies now

$$S_q[A + B] = S_q[A] + S_q[B|A] + (1 - q)S_q[A]S_q[B|A], \quad (3.40)$$

where  $S_q[A + B] \equiv S_q(\{p_{ij}\})$ ,  $S_q[A] \equiv S_q(\{p_i^A\})$  and the conditional entropy

$$S_q[B|A] \equiv \frac{\sum_{i=1}^{W_A} (p_i^A)^q S_q[B|A_i]}{\sum_{i=1}^{W_A} (p_i^A)^q} \equiv \langle S_q[B|A_i] \rangle_q, \quad (3.41)$$

where

$$S_q[B|A_i] \equiv \frac{1 - \sum_{j=1}^{W_B} (p_{ij}/p_i^A)^q}{q - 1} \quad (i = 1, 2, \dots, W_A), \quad (3.42)$$

with  $\sum_{j=1}^{W_B} (p_{ij}/p_i^A) = 1$ . Symmetrically, Eq. (3.40) can be also written as

$$S_q[A + B] = S_q[B] + S_q[A|B] + (1 - q)S_q[B]S_q[A|B]. \quad (3.43)$$

If  $A$  and  $B$  are independent, then  $p_{ij} = p_i^A p_j^B (\forall i, j)$ , hence  $S_q[A|B] = S_q[A]$  and  $S_q[B|A] = S_q[B]$ , therefore both Eqs. (3.40) and (3.43) yield the well-known pseudo-additivity property of the nonadditive entropy  $S_q$ , namely

$$S_q[A + B] = S_q[A] + S_q[B] + (1 - q)S_q[A]S_q[B]. \quad (3.44)$$

We thus see that Eqs. (3.40) and (3.43) nicely compress into *one* property two important properties of the entropic form  $S_q$ , namely Eqs. (3.28) and (3.44). Some of the axiomatic implications of these relations have been discussed by Abe [115].

### 3.2.2.9 Santos Uniqueness Theorem

The Santos theorem [117] generalizes that of Shannon (addressed in Section 2.1.2).

Let us assume that an entropic form  $S(\{p_i\})$  satisfies the following properties:

$$(i) \quad S(\{p_i\}) \text{ is a continuous function of } \{p_i\}; \quad (3.45)$$

$$(ii) \quad S(p_i = 1/W, \forall i) \text{ monotonically increases with the total number of possibilities } W; \quad (3.46)$$

$$(iii) \quad \frac{S(A + B)}{k} = \frac{S(A)}{k} + \frac{S(B)}{k} + (1 - q) \frac{S(A)}{k} \frac{S(B)}{k} \quad (3.47)$$

if  $p_{ij}^{A+B} = p_i^A p_j^B \forall (i, j)$ , with  $k > 0$ ;

$$(iv) \quad S(\{p_i\}) = S(p_L, p_M) + p_L^q S(\{p_i/p_L\}) + p_M^q S(\{p_i/p_M\}) \quad (3.48)$$

$$\text{with } p_L \equiv \sum_{L \text{ terms}} p_i, \quad p_L \equiv \sum_{M \text{ terms}} p_i,$$

$$L + M = W, \text{ and } p_L + p_M = 1.$$

Then and only then [117]

$$S(\{p_i\}) = k \frac{1 - \sum_{i=1}^W p_i^q}{q - 1}. \quad (3.49)$$

### 3.2.2.10 Abe Uniqueness Theorem

The Abe theorem [115] generalizes that of Khinchin (addressed in Section 2.1.2).

Let us assume that an entropic form  $S(\{p_i\})$  satisfies the following properties:

(i)  $S(\{p_i\})$  is a continuous function of  $\{p_i\}$ ; (3.50)

(ii)  $S(p_i = 1/W, \forall i)$  monotonically increases with the total number of possibilities  $W$ ; (3.51)

(iii)  $S(p_1, p_2, \dots, p_W, 0) = S(p_1, p_2, \dots, p_W)$ ; (3.52)

$$(iv) \frac{S(A+B)}{k} = \frac{S(A)}{k} + \frac{S(B|A)}{k} + (1-q)\frac{S(A)}{k}\frac{S(B|A)}{k} \quad (3.53)$$

where  $S(A+B) \equiv S(\{p_{ij}^{A+B}\})$ ,  $S(A) \equiv S(\{\sum_{j=1}^{W_B} p_{ij}^{A+B}\})$ , and the

$$\text{conditional entropy } S(B|A) \equiv \frac{\sum_{i=1}^{W_A} (p_i^A)^q S(\{p_{ij}^{A+B}/p_i^A\})}{\sum_{i=1}^{W_A} (p_i^A)^q} \quad (k > 0)$$

Then and only then [115]<sup>2</sup>

$$S(\{p_i\}) = k \frac{1 - \sum_{i=1}^W p_i^q}{q-1}. \quad (3.54)$$

Notice that, interestingly enough, what enters in the definition of the conditional entropy is the escort distribution, and *not* the original one.

### 3.2.2.11 Composability

The entropy  $S_q$  is, like the  $BG$  one, composable (see also [116]). Indeed, it satisfies Eq. (3.21). In other words, we have  $F(x, y; q) = x + y + (1-q)x y$ .

The Renyi entropy  $S_q^R$  is composable since it is additive. In other words, in that case we have  $F(x, y; q) = x + y$ .

As examples of the various *noncomposable* entropic forms that exist in the literature, we may cite the Curado entropy  $S^C$  [120] and the Anteneodo–Plastino entropy  $S^{AP}$  [121]. Since these two forms have some quite interesting mathematical properties, it would be thermodynamically valuable in principle to construct entropies following along the lines of these ones, but which would be composable instead.

### 3.2.2.12 Sensitivity to the Initial Conditions, Entropy Production Per Unit Time, and the $q$ -generalized Pesin-Like Identity

Let us focus on a one-dimensional nonlinear dynamical system (characterized by the variable  $x$ ) whose Lyapunov exponent  $\lambda_1$  vanishes (e.g., the *edge of chaos* for typical unimodal maps such as the logistic one). The sensitivity to the initial conditions  $\xi$  defined in Eq. (2.29) is *conjectured* to satisfy the equation

<sup>2</sup> The possibility of existence of such a theorem through the appropriate generalization of Khinchin's fourth axiom had already been considered by Plastino and Plastino [118, 119]. Abe established [115] the precise form of this generalized fourth axiom, and proved the theorem.

$$\frac{d\xi}{dt} = \lambda_q \xi^q, \quad (3.55)$$

whose solution is given by

$$\xi = e^{\lambda_q t}. \quad (3.56)$$

The paradigmatic case corresponds to  $\lambda_q > 0$  and  $q < 1$ . In this case we have

$$\xi \propto t^{1/(1-q)} \quad (t \rightarrow \infty), \quad (3.57)$$

(see also [122–126]) and we refer to it as *weak chaos*, in contrast to *strong chaos*, associated with positive  $\lambda_1$ . To be more precise, Eq. (3.56) has been proved to be the *upper bound* of an entire family of such relations at the edge of chaos of unimodal maps. For each specific (strongly or weakly) chaotic one-dimensional dynamical system, we generically expect to have a couple  $(q_{sen}, \lambda_{q_{sen}})$  (where *sen* stands for *sensitivity*) such that we have

$$\xi = e^{\lambda_{q_{sen}} t}. \quad (3.58)$$

Clearly, strong chaos is recovered here as the particular instance  $q_{sen} = 1$ .

Let us now address the interesting question of the  $S_q$  entropy production as time  $t$  increases. By using  $S_q$  instead of  $S_{BG}$ , we could follow the same steps already indicated in Section 2.1.2, and attempt the definition of a  $q$ -generalized Kolmogorov–Sinai entropy rate. We will not follow along this line, but we shall rather  $q$ -generalize the entropy production  $K_1$  introduced in Section 2.1.2. We define now

$$K_q \equiv \lim_{t \rightarrow \infty} \lim_{W \rightarrow \infty} \lim_{M \rightarrow \infty} \frac{S_q(t)}{t}. \quad (3.59)$$

We *conjecture* that generically an unique value of  $q$  exists, noted  $q_{ent}$  (where *ent* stands for *entropy*) such that (the upper bound of)  $K_{q_{ent}}$  is *finite* (i.e., positive), whereas  $K_q$  vanishes (diverges) for  $q > q_{ent}$  ( $q < q_{ent}$ ).

We further conjecture for one-dimensional systems that

$$q_{ent} = q_{sen}, \quad (3.60)$$

and that

$$K_{q_{ent}} = K_{q_{sen}} = \lambda_{q_{sen}}. \quad (3.61)$$

As already mentioned, strong chaos is recovered as a particular case, and we obtain the Pesin-like identity  $K_1 = \lambda_1$ . Conjectures (3.58), (3.60), and (3.61) were first introduced in [127], and have been analytically proved and/or numerically verified

in a considerable number of examples [128–133, 139–142, 146, 147, 150, 153]. We shall lengthily come back onto these questions in Chapter 5.

If our weakly chaotic system has  $v$  positive  $q$ -generalized Lyapunov coefficients  $\lambda_{q_{sen}^{(1)}}, \lambda_{q_{sen}^{(2)}}, \dots, \lambda_{q_{sen}^{(v)}}$ , we expect [172]

$$\frac{1}{1 - q_{ent}} = \sum_{k=1}^v \frac{1}{1 - q_{sen}^{(k)}}. \quad (3.62)$$

This yields, if all the  $q_{sen}^{(k)}$  are equal,

$$q_{ent} = 1 - \frac{1 - q_{sen}}{v}. \quad (3.63)$$

If  $v = 1$ , we recover Eq. (3.60). If  $q_{sen} = 0$ , we obtain

$$q_{ent} = 1 - \frac{1}{v}. \quad (3.64)$$

### 3.3 Correlations, Occupancy of Phase-Space, and Extensivity of $S_q$

#### 3.3.1 A Remark on the Thermodynamical Limit

Let us assume a classical mechanical many-body system characterized by the following Hamiltonian:

$$\mathcal{H} = K + V = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i \neq j} V(r_{ij}), \quad (3.65)$$

where the two-body potential energy  $V(r)$  presents no mathematical difficulties near the origin  $r = 0$  (e.g., in the  $r \rightarrow 0$  limit, either it is repulsive, or, if it is attractive, it is nonsingular or at least integrable), and which behaves at long distances ( $r \rightarrow \infty$ ) like

$$V(r) \sim -\frac{A}{r^\alpha} \quad (A > 0; \alpha \geq 0). \quad (3.66)$$

A typical example would be the  $d = 3$  Lennard–Jones gas model, for which  $\alpha = 6$ . Were it not the strong singularity at the origin, another example would have been Newtonian  $d = 3$  gravitation, for which  $\alpha = 1$ .

Let us analyze the characteristic average potential energy  $U_{pot}$  per particle

$$\frac{U_{pot}(N)}{N} \propto -A \int_1^\infty dr r^{d-1} r^{-\alpha}, \quad (3.67)$$

where we have integrated from a typical distance (taken equal to unity) on. This is the typical energy one would calculate within a *BG* approach. We see immediately that this integral *converges* for  $\alpha/d > 1$  (hereafter referred to as *short-range interactions* for classical systems) but *diverges* for  $0 \leq \alpha/d \leq 1$  (hereafter referred to as *long-range interactions*). This already indicates that something anomalous might happen.<sup>3</sup> By the way, it is historically fascinating the fact that Gibbs himself was aware of the possibility of such difficulty! (see, in Section 1.2, Gibbs' remarks concerning long-range interactions).

On a vein slightly differing from the standard *BG* recipe, which would demand integration up to infinity in Eq. (3.67), let us assume that the  $N$ -particle system is roughly homogeneously distributed within a limited sphere. Then Eq. (3.67) has to be replaced by the following one:

$$\frac{U_{pot}(N)}{N} \propto -A \int_1^{N^{1/d}} dr r^{d-1} r^{-\alpha} = -\frac{A}{d} N^*, \quad (3.68)$$

with

$$N^* \equiv \frac{N^{1-\alpha/d} - 1}{1 - \alpha/d} = \ln_{\alpha/d} N \sim \begin{cases} \frac{1}{\alpha/d - 1} & \text{if } \alpha/d > 1; \\ \ln N & \text{if } \alpha/d = 1; \\ \frac{N^{1-\alpha/d}}{1 - \alpha/d} & \text{if } 0 < \alpha/d < 1. \end{cases} \quad (3.69)$$

Therefore, in the  $N \rightarrow \infty$  limit,  $\frac{U_{pot}(N)}{N}$  approaches a constant ( $\propto -A/(\alpha - d)$ ) if  $\alpha/d > 1$ , and diverges like  $N^{1-\alpha/d}/(1 - \alpha/d)$  if  $0 \leq \alpha/d < 1$  (it diverges logarithmically if  $\alpha/d = 1$ ).<sup>4</sup> In other words, the energy is *extensive for short-*

<sup>3</sup> This is essentially the very same reason for which virtually all statistical mechanics textbooks discuss paradigmatic systems like a particle in a square well, the harmonic oscillator, the rigid rotator, and a spin 1/2 in the presence of an external magnetic field, *but not the Hydrogen atom!* All these simple systems, including of course the Hydrogen atom, are discussed in the quantum mechanics textbooks. But, in what concerns statistical mechanics, the Hydrogen atom constitutes an illustrious absence. Amazingly enough, and in spite of the existence of an almost centennial related literature [160–171], this highly important system passes without comments in almost all the textbooks on thermal statistics. The – understandable but not justifiable – reason of course is that, since the system involves the long-range Coulombian attraction between electron and proton, the energy spectrum exhibits an accumulation point at the ionization energy (frequently taken to be zero), which makes the *BG* partition function to diverge.

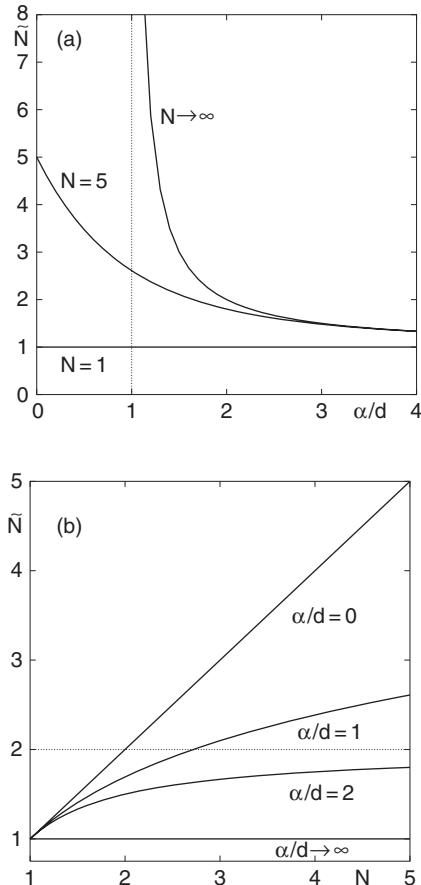
<sup>4</sup> These results turn out afterwards to be consistent with those discussed in relation to Eq. (1.67) of [340], in the frame of how strongly can  $N$  random variables be correlated, and be still applicable to the standard Central Limit Theorem, in the sense of the corresponding attractor be a Gaussian distribution.

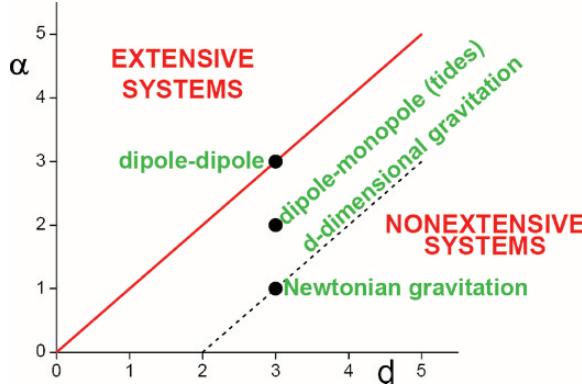
range interactions ( $\alpha/d > 1$ ), and nonextensive for long-range interactions ( $0 \leq \alpha/d \leq 1$ ). Satisfactorily enough, Eqs. (3.69) recover the characterization with Eq. (3.67) in the limit  $N \rightarrow \infty$ , but they have the great advantage of providing, for finite  $N$ , a finite value. This fact will be now shown to enable to properly scale the macroscopic quantities in the thermodynamic limit ( $N \rightarrow \infty$ ), for all values of  $\alpha/d \geq 0$  (See Figs. 3.9 and 3.10).

A totally similar situation occurs if we have, playing the role of Hamiltonian 3.65, say  $N$  coupled rotators localized on a lattice. We further detail this case later on.

We are now prepared to address the thermodynamical consequences of the microscopic interactions being short- or long-ranged ([173], and references within [174]). To present a slightly more general illustration, we shall assume from now on that our homogeneous and isotropic classical fluid is made by magnetic particles. Its Gibbs free energy is then given by

**Fig. 3.9** The rescaling function  $\tilde{N}(N, \alpha/d) \equiv N^*(N, \alpha/d) + 1$  vs.  $\alpha/d$  for typical values of  $N$  (a), and vs.  $N$  for typical values of  $\alpha/d$  (b). For fixed  $\alpha/d \geq 0$ ,  $\tilde{N}$  monotonically increases with  $N$  increasing from 1 to  $\infty$ ; for fixed  $N > 1$ ,  $\tilde{N}$  monotonically decreases for  $\alpha/d$  increasing from 0 to  $\infty$ .  $\tilde{N}(N, 0) = N$ , thus recovering the Mean Field Approximation usual rescaling;  $\lim_{N \rightarrow \infty} \tilde{N}$  diverges for  $0 \leq \alpha/d \leq 1$ , thus separating the extensive from the nonextensive region;  $\tilde{N}(\infty, \alpha/d) = (\alpha/d)/[(\alpha/d) - 1]$  if  $\alpha/d > 1$ ;  $\lim_{\alpha/d \rightarrow \infty} \tilde{N} = 1$ , thus recovering precisely the traditional intensive and extensive thermodynamical quantities;  $\tilde{N}(N, 1) = \ln N$  (from [176]).





**Fig. 3.10** The so-called *extensive systems* ( $\alpha/d > 1$  for the classical ones) typically involve *absolutely convergent series*, whereas the so-called *nonextensive systems* ( $0 \leq \alpha/d < 1$  for the classical ones) typically involve *divergent series*. The marginal systems ( $\alpha/d = 1$  here) typically involve *conditionally convergent series*, which therefore depend on the boundary conditions, i.e., typically on the external shape of the system. Capacitors constitute a notorious example of the  $\alpha/d = 1$  case. The model usually referred to in the literature as the *Hamiltonian-Mean-Field* (HMF) one lies on the  $\alpha = 0$  axis ( $\forall d > 0$ ). The model usually referred to as the  $d$ -dimensional  $\alpha$ - $XY$  model [177] lies on the vertical axis at abscissa  $d$  ( $\forall \alpha \geq 0$ ).

$$\begin{aligned} G(N, T, p, H) = & U(N, T, p, H) - TS(N, T, p, H) + pV(N, T, p, H) \\ & - HM(N, T, p, H), \end{aligned} \quad (3.70)$$

where  $(T, p, H)$  correspond, respectively, to the temperature, pressure, and external magnetic field,  $U$  is the internal energy,  $S$  is the entropy,  $V$  is the volume, and  $M$  the magnetization.

If the interactions are short-ranged (i.e., if  $\alpha/d > 1$ ), we can divide this equation by  $N$  and then take the  $N \rightarrow \infty$  limit. We obtain

$$g(T, p, H) = u(T, p, H) - Ts(T, p, H) + pv(T, p, H) - Hm(T, p, H), \quad (3.71)$$

where  $g(T, p, H) \equiv \lim_{N \rightarrow \infty} G(N, T, p, H)/N$ , and analogously for the other variables of the equation.

If the interactions are instead long-ranged (i.e., if  $0 \leq \alpha/d \leq 1$ ), all these quantities *diverge*, hence thermodynamically speaking they are nonsense. Consequently, the generically correct procedure, i.e.,  $\forall \alpha/d \geq 0$ , must conform to the following lines:

$$\begin{aligned} \lim_{N \rightarrow \infty} \frac{G(N, T, p, H)}{NN^*} = & \lim_{N \rightarrow \infty} \frac{U(N, T, p, H)}{NN^*} - \lim_{N \rightarrow \infty} \frac{T}{N^*} \frac{S(N, T, p, H)}{N} \\ & + \lim_{N \rightarrow \infty} \frac{p}{N^*} \frac{V(N, T, p, H)}{N} - \lim_{N \rightarrow \infty} \frac{H}{N^*} \frac{M(N, T, p, H)}{N} \end{aligned} \quad (3.72)$$

hence

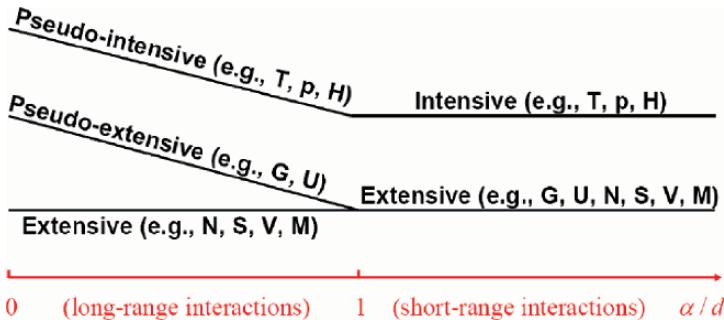
$$g(T^*, p^*, H^*) = u(T^*, p^*, H^*) - T^*s(T^*, p^*, H^*) + p^*v(T^*, p^*, H^*) \\ - H^*m(T^*, p^*, H^*), \quad (3.73)$$

where the definitions of  $T^*$  and all the other variables are self-explanatory (e.g.,  $T^* \equiv T/N^*$ ). In other words, in order to have *finite* thermodynamic equations of states, we must in general express them in the  $(T^*, p^*, H^*)$  variables. If  $\alpha/d > 1$ , this procedure recovers the usual equations of states, and the usual *extensive* ( $G, U, S, V, M$ ) and *intensive* ( $T, p, H$ ) thermodynamic variables. But, if  $0 \leq \alpha/d \leq 1$ , the situation is more complex, and we realize that *three*, instead of the traditional *two*, classes of thermodynamic variables emerge. We may call them *extensive* ( $S, V, M, N$ ), *pseudo-extensive* ( $G, U$ ), and *pseudo-intensive* ( $T, p, H$ ) variables. All the energy-type thermodynamical variables ( $G, F, U$ ) give rise to pseudo-extensive ones, whereas those which appear in the usual Legendre thermodynamical pairs give rise to pseudo-intensive ones ( $T, p, H, \mu$ ) and extensive ones ( $S, V, M, N$ ) (See Figs. 3.10 and 3.11).

The possibly long-range interactions within Hamiltonian (3.65) refer to the *dynamical variables themselves*. There is another important class of Hamiltonians, where the possibly long-range interactions refer to the *coupling constants between localized dynamical variables*. Such is, for instance, the case of the following classical Hamiltonian:

$$\mathcal{H} = K + V = \sum_{i=1}^N \frac{L_i^2}{2I} - \sum_{i \neq j} \frac{J_x s_i^x s_j^x + J_y s_i^y s_j^y + J_z s_i^z s_j^z}{r_{ij}^\alpha} \quad (\alpha \geq 0), \quad (3.74)$$

where  $\{L_i\}$  are the angular momenta,  $I$  the moment of inertia,  $\{(s_i^x, s_i^y, s_i^z)\}$  are the components of classical rotators,  $(J_x, J_y, J_z)$  are coupling constants, and  $r_{ij}$  runs over all distances between sites  $i$  and  $j$  of a  $d$ -dimensional lattice. For example, for



**Fig. 3.11** For long-range interactions ( $0 \leq \alpha/d \leq 1$ ) we have *three* classes of *thermodynamic variables*, namely the *pseudo-intensive* (scaling with  $N^*$ ), *pseudo-extensive* (scaling with  $NN^*$ ), and *extensive* (scaling with  $N$ ) ones. For short-range interactions ( $\alpha/d > 1$ ) the pseudo-intensive variables become *intensive* (independent from  $N$ ), and the pseudo-extensive variables merge with the extensive ones, all being now *extensive* (scaling with  $N$ ), thus recovering the traditional *two* textbook classes of thermodynamical variables.

a simple hypercubic lattice with unit crystalline parameter we have  $r_{ij} = 1, 2, 3, \dots$  if  $d = 1$ ,  $r_{ij} = 1, \sqrt{2}, 2, \dots$  if  $d = 2$ ,  $r_{ij} = 1, \sqrt{2}, \sqrt{3}, 2, \dots$  if  $d = 3$ , and so on. For such a case, we have that

$$N^* \equiv \sum_{i=2}^N r_{li}^{-\alpha}, \quad (3.75)$$

which has in fact the same asymptotic behaviors as indicated in Eq. (3.69). In other words, here again  $\alpha/d > 1$  corresponds to short-range interactions, and  $0 \leq \alpha/d \leq 1$  corresponds to long-range ones.

For example, the  $\alpha/d = 0$  particular case corresponds to the usual mean field approach. Indeed, in this case we have  $N^* = N - 1 \sim N$ , which is equivalent to the usual rescaling of the microscopic coupling constant through division by  $N$  (see also [177]). In fact, to accommodate with the common use of dividing by  $N$  (instead of  $N - 1$ ) for the  $\alpha/d = 0$  case, it is sometimes practical to use, as done in Fig. 3.9,

$$\tilde{N} \equiv N^* + 1 = \frac{N^{1-\alpha/d} - (\alpha/d)}{1 - \alpha/d}. \quad (3.76)$$

For short-range interactions,  $N^* \rightarrow \text{constant}$ , consequently we recover the usual *extensivity* of Gibbs, Helmholtz, and internal thermodynamical energies, entropy, volume, and magnetization, as well as the *intensivity* of temperature, pressure, and magnetic field. But for long-range interactions,  $N^*$  diverges with  $N$ , therefore the situation is quite more subtle. Indeed, in order to have *nontrivial equations of states* we must express the *nonextensive* Gibbs, Helmholtz, and internal thermodynamical energies, as well as the *extensive* entropy, volume and magnetization in terms of the rescaled variables  $(T^*, p^*, H^*)$ . In general, i.e.,  $\forall(\alpha/d)$ , we see that the variables that are intensive when the interactions are short-ranged remain a *single class* (although scaling with  $N^*$ ) in the presence of long-ranged interactions. But, in what concerns the variables that are extensive when the interactions are short-ranged, the situation is more complex. Indeed, they split into *two classes*. One of them contains all types of thermodynamical energies ( $G, F, U$ ), which scale with  $NN^*$ . The other one contains all those variables ( $S, V, M$ ) that appear *in pairs* in the thermodynamical energies. These variables remain extensive, in the sense that they scale with  $N$ .<sup>5</sup>

By no means this implies that thermodynamical equilibrium between two systems occurs in general when they share the same values of say  $(T^*, p^*, H^*)$ . It only means that, in order to have *finite* mathematical functions for their *equations of states*, the variables  $(T^*, p^*, H^*)$  must be used. Although this has to be verified, thermodynamical equilibrium might still be directly related to sharing the usual variables  $(T, p, H)$ .

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<sup>5</sup> Consequently, for  $0 \leq \alpha/d < 1$ , we expect  $U(N, T) \sim N^{2-\alpha/d} u(T/N^{1-\alpha/d})$ ,  $S(N, T) \sim N s(T/N^{1-\alpha/d})$ , the specific heat  $C(N, T) \sim N c(T/N^{1-\alpha/d})$ , etc.

The correctness of the present generalized thermodynamical scaling has already been specifically checked in many physical systems, such as a ferrofluid-like model [869], Lennard-Jones-like fluids [870], magnetic systems [174, 175, 177, 871, 872], anomalous diffusion [873], percolation [878, 879]. It has been also argued analytically [807].

In addition to this, if a phase transition occurs in the system at a temperature  $T_c$ , it is expected to happen for a *finite* value of  $T_c/\tilde{N}$ . This implies that (i) in the limit  $\alpha/d \rightarrow 1 + 0$ ,  $T_c \propto 1/(\alpha/d - 1)$ , thus recovering a result known since long (for instance for the  $n$ -vector ferromagnet, including the Ising one); (ii) for  $0 \leq \alpha/d < 1$ ,  $T_c \propto N^{1-\alpha/d}$ . In the latter context, let us mention that, for the  $\alpha = 0$  models (i.e., mean-field-like models), it is largely spread in the literature to divide by  $N$  (in general, by  $N^{1-\alpha/d}$  if  $0 \leq \alpha/d < 1$ ) the interaction term of the Hamiltonian in order to make it extensive *by force*. Although mathematically admissible (see [177] for an isomorphism involving rescaling of time  $t$ ), this obviously is physically quite bizarre. Indeed it implies a microscopic coupling constant which depends on  $N$ . What we have described here turns out to be the thermodynamically proper and unified way of eliminating the mathematical difficulties emerging in the models whenever long-range interactions are present.<sup>6</sup>

Notice also that it belongs to the essence of thermodynamics the following property. If we know, for a large system  $\Sigma$ , quantities such as  $U(\Sigma)$ ,  $S(\Sigma)$ ,  $F(\Sigma)$ , etc, we should be able to easily calculate the same quantities for say an even larger such system  $(\lambda\Sigma)$ , with  $N(\lambda\Sigma) = \lambda N(\Sigma)$  ( $\lambda > 1$ ). It is indeed so in the present case. For example, for  $N \gg 1$  we have

$$\frac{U(\lambda\Sigma)}{U(\Sigma)} = \lambda \frac{(\lambda N)^{1-\alpha/d} - 1}{N^{1-\alpha/d} - 1} \sim \begin{cases} \lambda & \text{if } \alpha/d \geq 1; \\ \lambda^{2-\alpha/d} & \text{if } 0 < \alpha/d < 1. \end{cases} \quad (3.77)$$

We see therefore that, for short-range interactions, the result depends on no microscopic detail at all, thus confirming the concept usually emphasized in textbooks of thermodynamics. This is, however, not true for long-range interactions, where we can see that, although in a mathematically very simple manner, the result *does* depend on the microscopic ratio  $\alpha/d$ .

It is clear that all these notions are quite subtle and yet a subject of active research. Nevertheless, they constitute a strong indication that, no matter the range of the interactions,  $S_{BG}$  should be generalized *preserving its extensivity*, i.e., as introduced on macroscopic grounds by Clausius. What we present in the next subsections is consistent with this expectation.

<sup>6</sup> Let us illustrate this point on a  $d$ -dimensional  $n$ -vector ferromagnet whose microscopic coupling constant decays with distance as  $J/r_{ij}^\alpha$  ( $J > 0$ ,  $0 \leq \alpha/d < 1$ ). The critical temperature is given by  $T_c = \mu J N^{1-\alpha/d}/[(1 - \alpha/d)k_B]$ , where the pure number  $\mu \simeq 1$ . This is the thermodynamically correct result. What is instead customary to do in the literature is to (unphysically) replace  $J$  by  $J/N^{1-\alpha/d}$ , thus obtaining  $T_c = \mu J/[(1 - \alpha/d)k_B]$ , which remains *finite* for  $N \rightarrow \infty$ .

### 3.3.2 The $q$ -Product

In relation with the pseudo-additive property (3.44) of  $S_q$ , it has been recently introduced (independently and virtually simultaneously) [182, 183] a generalization of the product, which is called  *$q$ -product*. It is defined as follows:

$$x \otimes_q y \equiv \left[ x^{1-q} + y^{1-q} - 1 \right]_+^{\frac{1}{1-q}} \quad (x \geq 0, y \geq 0),^7 \quad (3.78)$$

or, equivalently,

$$x \otimes_q y \equiv e_q^{\ln_q x + \ln_q y} \quad (3.79)$$

Let us list some of its main properties:

(i) It recovers the *standard product* as a particular instance, namely,

$$x \otimes_1 y = xy; \quad (3.80)$$

(ii) It is *commutative*, i.e.,

$$x \otimes_q y = y \otimes_q x; \quad (3.81)$$

(iii) It is *additive under  $q$ -logarithm* (hereafter referred to as *extensive*), i.e.,

$$\ln_q(x \otimes_q y) = \ln_q x + \ln_q y, \quad (3.82)$$

whereas we remind that

$$\ln_q(x y) = \ln_q x + \ln_q y + (1 - q)(\ln_q x)(\ln_q y). \quad (3.83)$$

Consistently

$$e_q^x \otimes_q e_q^y = e_q^{x+y}, \quad (3.84)$$

whereas

$$e_q^x e_q^y = e_q^{x+y+(1-q)xy}; \quad (3.85)$$

(iv) It has a  $(2 - q)$ -*duality/inverse* property, i.e.,

<sup>7</sup> It is in fact easy to get rid of the requirement of non-negativity of  $x$  and  $y$  through the following extended definition:  $x \otimes_q y \equiv \text{sign}(x)\text{sign}(y)\left[|x|^{1-q} + |y|^{1-q} - 1\right]_+^{\frac{1}{1-q}}$ . The correct  $q = 1$  limit is obtained by using  $\text{sign}(x)|x| = x$  (and similarly for  $y$ ).

$$1/(x \otimes_q y) = (1/x) \otimes_{2-q} (1/y); \quad (3.86)$$

(v) It is *associative*, i.e.,

$$x \otimes_q (y \otimes_q z) = (x \otimes_q y) \otimes_q z = x \otimes_q y \otimes_q z = (x^{1-q} + y^{1-q} + z^{1-q} - 2)^{1/(1-q)}; \quad (3.87)$$

(vi) It admits *unity*, i.e.,

$$x \otimes_q 1 = x; \quad (3.88)$$

(vii) It admits *zero* under certain conditions, more precisely,

$$x \otimes_q 0 = \begin{cases} 0 & \text{if } (q \geq 1 \text{ and } x \geq 0) \text{ or if } (q < 1 \text{ and } 0 \leq x \leq 1), \\ (x^{1-q} - 1)^{\frac{1}{1-q}} & \text{if } q < 1 \text{ and } x > 1 \end{cases} \quad (3.89)$$

For a special range of  $q$ , e.g.,  $q = 1/2$ , the argument of the  $q$ -product can attain negative values, specifically at points for which  $|x|^{1-q} + |y|^{1-q} - 1 < 0$ . In these cases, and consistently with the cut-off for the  $q$ -exponential, we have set  $x \otimes_q y = 0$ . With regard to the  $q$ -product domain, and restricting our analysis of Eq. (3.78) to  $x, y > 0$ , we observe that for  $q \rightarrow -\infty$  the region  $\{0 \leq x \leq 1, 0 \leq y \leq 1\}$  leads to a vanishing  $q$ -product. As the value of  $q$  increases, the area of the vanishing region decreases, and when  $q = 0$  we have the limiting line given by  $x + y = 1$ , for which  $x \otimes_0 y = 0$ . Only for  $q = 1$ , the *whole set* of real values of  $x$  and  $y$  has a defined value for the  $q$ -product. For  $q > 1$ , definition (3.78) yields a curve,  $|x|^{1-q} + |y|^{1-q} = 1$ , at which the  $q$ -product diverges. This undefined region increases as  $q$  goes to infinity. At the  $q \rightarrow \infty$  limit, the  $q$ -product is only defined in  $\{x > 1, y \leq 1\} \cup \{0 \leq x \leq 1, 0 \leq y \leq 1\} \cup \{x \leq 1, y > 1\}$ . This entire scenario is depicted on the panels of Fig. 3.12. The profiles presented by  $x \otimes_\infty y$  and  $x \otimes_{-\infty} y$  illustrate the above features. To illustrate the  $q$ -product in another simple form, we show, in Fig. 3.13, a representation of  $x \otimes_q x$  for typical values of  $q$ .

(viii) It satisfies

$$(x^q \otimes_{1/q} y^q)^{1/q} = x \otimes_{2-q} y, \quad (3.90)$$

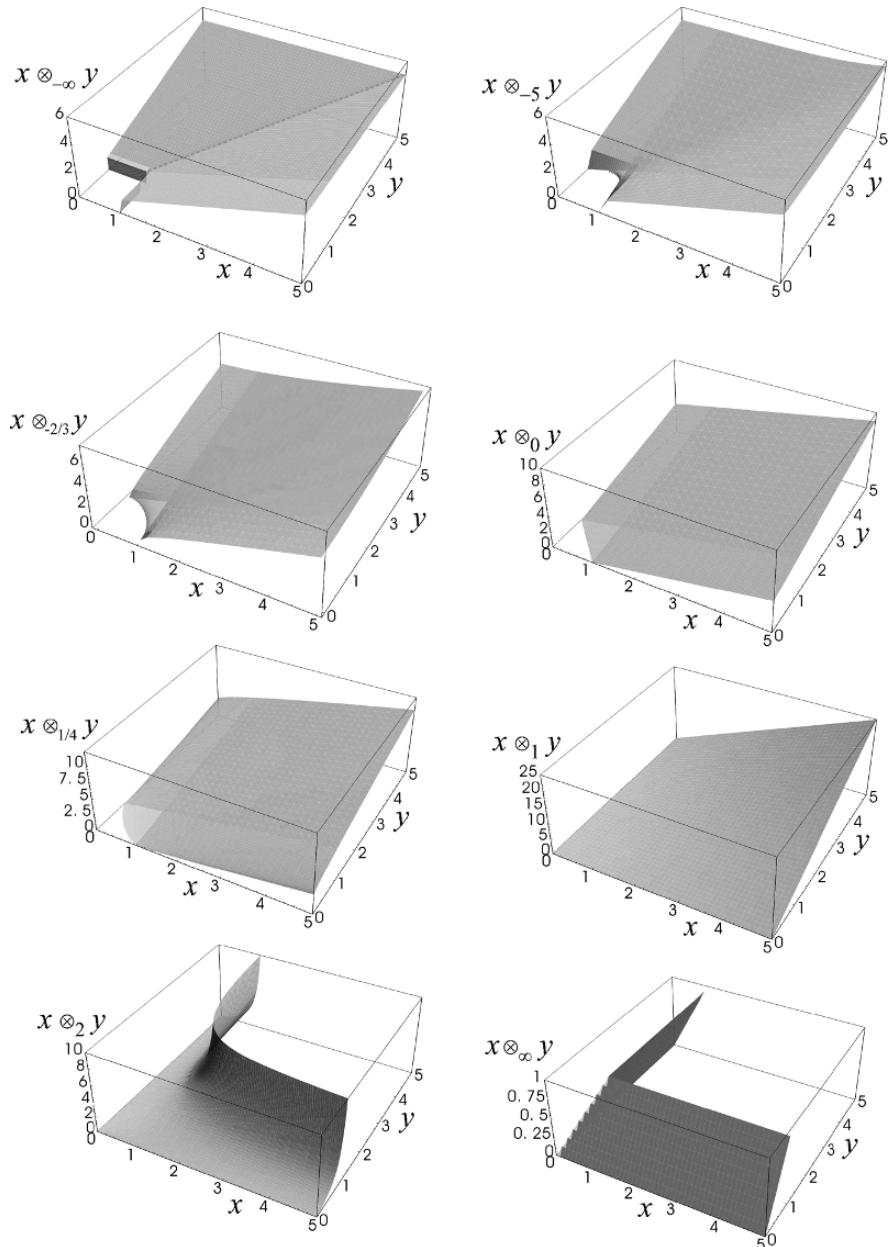
or, equivalently,

$$x \otimes_{1/q} y = (x^{1/q} \otimes_{2-q} y^{1/q})^q; \quad (3.91)$$

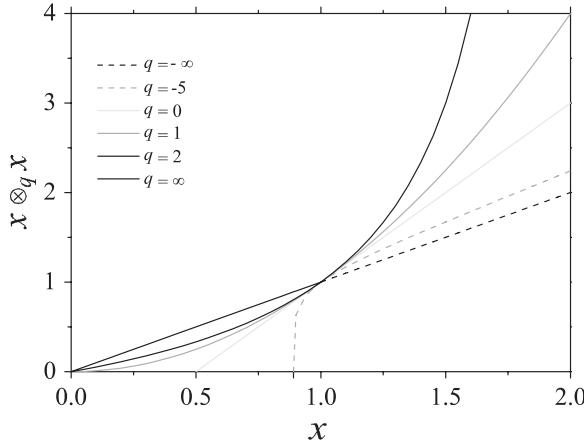
(ix) By  $q$ -multiplying  $n$  equal factors we can define the  $n$ th  $q$ -power as follows:

$$x^{\otimes_q^n} \equiv x \otimes_q x \otimes_q \dots \otimes_q x = [nx^{1-q} - (n-1)]^{1/(1-q)}, \quad (3.92)$$

which immediately suggests the following analytical extension



**Fig. 3.12** Representation of the  $q$ -product, Eq. (3.78), for  $q = -\infty, -5, -2/3, 0, 1/4, 1, 2, \infty$ . As it is visible, the squared region  $\{0 \leq x \leq 1, 0 \leq y \leq 1\}$  is gradually integrated into the nontrivial domain as  $q$  increases up to  $q = 1$ . From this value on, a new prohibited region appears, but this time coming from large values of  $(|x|, |y|)$ . This region reaches its maximum when  $q = \infty$ . In this case, the domain is composed by a horizontal and vertical strip of width 1.



**Fig. 3.13** Representation of the  $q$ -product,  $x \otimes_q x$  for  $q = -\infty, -5, 0, 1, 2, \infty$ . Excluding  $q = 1$ , there is a special value  $x^* = 2^{1/(q-1)}$ , for which  $q < 1$  represents the lower bound [in figure  $x^*(q = -5) = 2^{-1/6} \simeq 0.89089$  and  $x^*(q = 0) = 1/2$ ], and for  $q > 1$  the upper bound [in figure  $x^*(q = 2) = 2$ ]. For  $q = \pm\infty$ ,  $x \otimes_q x$  lies on the diagonal of bisection, but following the lower and upper limits mentioned above.

$$x^{\otimes_q^y} \equiv [yx^{1-q} - (y-1)]^{1/(1-q)}, \quad (3.93)$$

where both  $x$  and  $y$  can be real numbers (with  $y(x^{1-q} - 1) \geq -1$ ). From this, an interesting, *extensive*-like property follows, namely

$$\ln_q(x^{\otimes_q^y}) = y \ln_q x. \quad (3.94)$$

It will gradually become clear that the peculiar mathematical structure associated with the  $q$ -product appears to be at the “heart” of the *nonadditive* entropy  $S_q$  (which is nevertheless *extensive* for a special class of correlations) and its associated statistical mechanics (see also [185]).

### 3.3.3 The $q$ -Sum

Analogously to the  $q$ -product we can define the  $q$ -sum

$$x \oplus_q y \equiv x + y + (1 - q)xy. \quad (3.95)$$

It has the following main properties:

- (i) It recovers the *standard sum* as a particular instance, i.e.,

$$x \oplus_1 y = x + y; \quad (3.96)$$

(ii) It is *commutative*, i.e.,

$$x \oplus_q y = y \oplus_q x; \quad (3.97)$$

(iii) It is *multiplicative under  $q$ -exponential*, i.e.,

$$e_q^{x \oplus_q y} = e_q^x e_q^y; \quad (3.98)$$

(iv) It is *associative*, i.e.,

$$\begin{aligned} x \oplus_q (y \oplus_q z) &= (x \oplus_q y) \oplus_q z = x \oplus_q y \oplus_q z \\ &= x + y + z + (1 - q)(xy + yz + zx) + (1 - q)^2 xyz; \end{aligned} \quad (3.99)$$

(v) It admits *zero*, i.e.,

$$x \oplus_q 0 = x; \quad (3.100)$$

(vi) By  $q$ -summing  $n$  equal terms we obtain:

$$x^{\oplus_q^n} \equiv x \oplus_q x \oplus_q \dots \otimes_q x = nx \left[ \sum_{i=0}^{n-2} (1 - q)^i x^i \right] + (1 - q)^{n-1} x^n \quad (n = 2, 3, \dots); \quad (3.101)$$

(vii) It satisfies the following generalization of the *distributive* property of standard sum and product, i.e., of  $a(x + y) = ax + ay$ :

$$a(x \oplus_q y) = (ax) \oplus_{\frac{q+a-1}{a}} (ay). \quad (3.102)$$

Interesting *cross* properties emerge from the  $q$ -generalizations of the product and of the sum, for instance

$$\ln_q(x y) = \ln_q x \oplus_q \ln_q y, \quad (3.103)$$

$$\ln_q(x \otimes_q y) = \ln_q x + \ln_q y, \quad (3.104)$$

and, consistently,<sup>8</sup>

$$e_q^{x+y} = e_q^x \otimes_q e_q^y, \quad (3.105)$$

$$e_q^{x \oplus_q y} = e_q^x e_q^y. \quad (3.106)$$

---

<sup>8</sup> While both the  $q$ -sum and the  $q$ -product are mathematically interesting structures, they play a quite different role within the deep structure of the nonextensive theory. The  $q$ -product reflects an essential property, namely the extensivity of the entropy in the presence of special global correlations. The  $q$ -sum instead only reflects how the entropies would compose if the subsystems were independent, even if we know that in such a case we only actually need  $q = 1$ .

Let us make, at this point, a mathematical digression. If, to the relation  $\ln(xy) = \ln x + \ln y$ , we add relations (3.103) and (3.104), we feel tempted to find out whether a further generalized logarithmic function exists which would elegantly unify all of them in the form

$$\ln_{q,q'}(x \otimes_q y) = \ln_{q,q'} x \oplus_{q'} \ln_{q,q'} y. \quad (3.107)$$

It turns out that it *does* exist, and is given by [187]

$$\ln_{q,q'} x \equiv \ln_{q'} e^{\ln_q x} = \frac{1}{1-q'} \left[ \exp \left( \frac{1-q'}{1-q} (x^{1-q} - 1) \right) - 1 \right]. \quad (3.108)$$

The relations  $\ln_{q,1} x = \ln_{1,q} x = \ln_q x$  are easily recovered by evaluating Eq. (3.108) in the limits  $q \rightarrow 1$  and  $q' \rightarrow 1$ . From Eq. (3.108), the inverse function  $e_{q,q'}^x$  can be easily obtained as well.

Finally, let us end by mentioning some related *open* problems. Does a generalized sum  $x \oplus^{(q)} y$  exist such as a  $q$ -generalized distributivity like the following holds?

$$x \otimes_q (y \oplus^{(q)} z) = (x \otimes_q y) \oplus^{(q)} (x \otimes_q z). \quad (3.109)$$

Could it be  $\oplus^{(q)} = \oplus_{f(q)}$ ,  $f$  being some specific function?

Analogously, does a generalized product  $x \otimes^{(q)} y$  exist such as a  $q$ -generalized distributivity like the following holds?

$$x \otimes^{(q)} (y \oplus_q z) = (x \otimes^{(q)} y) \oplus_q (x \otimes^{(q)} z). \quad (3.110)$$

Could it be  $\otimes^{(q)} = \otimes_{g(q)}$ ,  $g$  being some specific function?

These questions are presently open. However, preliminary results suggest that no equality (3.109) can generically exist with a generalized sum that would be associative.

### 3.3.4 Extensivity of $S_q$ – Effective Number of States

Suppose we are composing the discrete states of two subsystems  $A$  and  $B$ , whose total numbers of states are, respectively,  $W_A \geq 1$  and  $W_B \geq 1$ . To be more specific,  $W_A (W_B)$  is the total number of states of  $A$  ( $B$ ) whose associated probability is *not zero*. The total number of states of the system  $A + B$  is then

$$W_{A+B} = W_A W_B. \quad (3.111)$$

Let us now denote by  $W_{A+B}^{eff}$  the *effective number of states* of the system  $A + B$ , where by *effective* we mean the number of states whose *joint* probability is *not zero*. It will in general be

$$W_{A+B}^{eff} \leq W_{A+B}. \quad (3.112)$$

If  $A$  and  $B$  are independent, then the equality holds. The opposite is not true: correlation might exist between  $A$  and  $B$  and, nevertheless, the equality be satisfied. It is not, however, this kind of (weak) correlation that we are interested here. Our focus is on a *special* type of (strong) correlation, which *necessarily* decreases the number of joint states whose probability differs from zero. More specifically, we focus on a correlation such that

$$W_{A+B}^{eff} = W_A \otimes_q W_B = (W_A^{1-q} + W_B^{1-q} - 1)^{1/(1-q)} \quad (q \leq 1). \quad (3.113)$$

We can verify that  $W_{A+B}^{eff}/W_{A+B}$  generically decreases from unity to zero when  $q$  decreases from unity to  $-\infty$ .

Let us generalize the above to  $N$  subsystems  $A_1, A_2, \dots, A_N$  (they typically are the elements of the system) whose numbers of states (with nonzero probabilities) are, respectively,  $W_{A_1}, W_{A_2}, \dots, W_{A_N}$ . We then have

$$W_{A_1+A_2+\dots+A_N} = \prod_{r=1}^N W_{A_r}, \quad (3.114)$$

and

$$W_{A_1+A_2+\dots+A_N}^{eff} = W_{A_1} \otimes_q W_{A_2} \otimes_q \dots \otimes_q W_{A_N} = \left[ \left( \sum_{r=1}^N W_{A_r} \right) - (N-1) \right]. \quad (3.115)$$

It will generically be  $W_{A_1+A_2+\dots+A_N}^{eff} \leq W_{A_1+A_2+\dots+A_N}$  for  $q \leq 1$ , the equality generically holds for and only for  $q = 1$ .

A frequent and important case is that in which the  $N$  subsystems are all equal (hence  $W_{A_r} = W_{A_1} \equiv W_1, \forall r$ ). In such a case, we have

$$W_{A_1+A_2+\dots+A_N}^{eff} = [NW_1^{1-q} - (N-1)]^{1/(1-q)} \leq W_1^N \quad (q \leq 1), \quad (3.116)$$

where the notation  $W_{A_1+A_2+\dots+A_N}^{eff}$  is self-explanatory. This equality immediately yields the following *very suggestive* result:

$$\ln_q [W_{A_1+A_2+\dots+A_N}^{eff}] = N \ln_q W_1. \quad (3.117)$$

If  $q = 1$ ,  $W_{A_1+A_2+\dots+A_N}^{eff} = W(N) = W_1^N$ , and this result recovers the well-known additivity of  $S_{BG}$ , i.e.,  $S_{BG}(N) = NS_{BG}(1)$  for the case of equal probabilities. Indeed, in the  $q = 1$  case, the hypothesis of *simultaneously having equal probabilities* in each of the  $N$  equal subsystems as well as in the total system is *admissible*: the probability of each state of any single subsystem is  $1/W_1$ , and the probability of each state of the entire system is  $1/W = 1/W_1^N$ .

The situation is more complex for  $q \neq 1$ , and here we focus on  $q < 1$ . Indeed, it appears (as we shall verify in the next Subsection) that, in such cases, a few or many of the states of the entire system become *forbidden* (in the sense that their corresponding probabilities vanish), either for finite  $N$  or in the limit  $N \rightarrow \infty$ . This is precisely why  $W^{eff}(N) < W(N) = W_1^N$ . So, if we assume that all states of each subsystem are *equally probable* (with probability  $1/W_1$ ), then the states of the entire system are *not*. Reciprocally, if we assume that the *allowed* states of the entire system are *equally probable* (with probability  $1/W^{eff}(N) > 1/W(N) = 1/W_1^N$ ), then the states of each of the subsystems are *not*. We see here the seed of nonergodicity, hence the failure of the *BG* statistical mechanical basic hypothesis for systems of this sort.

Let us first consider the possibility in which the states of *each subsystem* are equally probable. Then  $k \ln_q W_1$  is the entropy  $S_q(1)$  associated with *one* subsystem. In other words Eq. (3.94) implies

$$k \ln_q [W^{eff}(N)] = N S_q(1). \quad (3.118)$$

Let us then consider the other possibility, namely that in which it is the allowed states of the *entire system* that are equally probable. Then  $k \ln_q W^{eff}(N)$  is the entropy  $S_q(N)$  associated with the entire system. In other words Eq. (3.94) implies

$$S_q(N) = N k \ln_q W_1. \quad (3.119)$$

We may say that we are now very close to answer a crucial question: *Can  $S_q$  for  $q \neq 1$  generically be strictly or asymptotically proportional to  $N$  in the presence of these strong correlations, i.e., can it be extensive?* The examples that we present next exhibit that the answer is yes. By *generically* we refer to the most common case, in which neither the states of each subsystem are equally probable, nor the allowed states of the entire system are equally probable. This is what we address in the next Section.

But before that, let us summarize the knowledge that we acquired in the present Subsection. We assume, for simplicity, that the  $W^{eff}(N)$  joint states of a system are equally probable. See [190]

(i) If  $W^{eff}(N) \sim A\mu^N$  ( $N \rightarrow \infty$ ) with  $A > 0$  and  $\mu > 1$ , the entropy which is *extensive* is  $S_{BG}(N) = \ln W^{eff}(N)$ , i.e.,  $\lim_{N \rightarrow \infty} S_{BG}(N)/N = \ln \mu \in (0, \infty)$ . The nonadditive entropy  $S_q$  for  $q \neq 1$  is, in contrast, *nonextensive*. It is primarily systems like this that are addressed within the *BG* scenario.

(ii) If  $W^{eff}(N) \sim BN^\rho$  ( $N \rightarrow \infty$ ) with  $B > 0$  and  $\rho > 0$ , the entropy which is *extensive* is  $S_q(N) = \ln_q W^{eff}(N) \propto N^{\rho(1-q)}$  with

$$q = 1 - \frac{1}{\rho}, \quad (3.120)$$

i.e.,  $\lim_{N \rightarrow \infty} S_{1-(1/\rho)}(N)/N = B^{1-q}/(1-q)$  is *finite*. For any other value of  $q$  (including  $q = 1$ !),  $S_q$  is *nonextensive* (e.g.,  $S_{BG} \sim \rho \ln N$ ). It is primarily systems

like this that are addressed within the nonextensive scenario.<sup>9</sup> This remark may be considered as some sort of *golden* reason for the present generalization of *BG* statistical mechanics!<sup>10</sup>

(iii) If  $W^{eff}(N) \sim Cv^{N^\gamma}$  ( $N \rightarrow \infty$ ) with  $C > 0$  and  $v > 1$  and  $0 < \gamma < 1$ , neither  $S_{BG}(N)$  nor  $S_q(N)$  ( $q \neq 1$ ) can be extensive. This type of more complex situation would demand a special approach, which is out of the present scope.<sup>11</sup>

### 3.3.5 Extensivity of $S_q$ – Binary Systems

We wish to address here an issue of central importance in statistical mechanics and thermodynamics, namely the extensivity of the entropy [191, 197–200]. Let us start with the simple case of a system composed of  $N$  distinguishable subsystems, each of them characterized by a binary random variable.

#### 3.3.5.1 $N$ Binary Subsystems

If  $N = 1$ , we shall note  $p_1^A$  and  $p_2^A$  the probabilities of states 1 and 2, respectively. Of course, they satisfy  $p_1^A + p_2^A = 1$ .

If  $N = 2$ , we shall note  $p_{11}^{A+B}$ ,  $p_{12}^{A+B}$ ,  $p_{21}^{A+B}$ , and  $p_{22}^{A+B}$  the corresponding joint probabilities. Of course, they satisfy  $p_{11}^{A+B} + p_{12}^{A+B} + p_{21}^{A+B} + p_{22}^{A+B} = 1$  (see Table 3.2).

**Table 3.2** Two binary subsystems *A* and *B*: joint probabilities  $p_{11}^{A+B}$ ,  $p_{12}^{A+B}$ ,  $p_{21}^{A+B}$ , and  $p_{22}^{A+B}$ , and marginal probabilities  $p_1^{(A+B)}$ ,  $p_2^{(A+B)}$ ,  $p_1^{(A+B)}$ , and  $p_2^{(A+B)}$

$A \setminus B$	1	2	
1	$p_{11}^{A+B}$	$p_{12}^{A+B}$	$p_1^{A+(B)} \equiv p_{11}^{A+B} + p_{12}^{A+B}$
2	$p_{21}^{A+B}$	$p_{22}^{A+B}$	$p_2^{A+(B)} \equiv p_{21}^{A+B} + p_{22}^{A+B}$
	$p_1^{(A+B)} \equiv p_{11}^{A+B} + p_{21}^{A+B}$	$p_2^{(A+B)} \equiv p_{12}^{A+B} + p_{22}^{A+B}$	1

<sup>9</sup> In our present examples,  $N$  typically is the *total* number of elements. But, as we shall see later in some applications related to quantum entanglement, the system whose entropy we are interested in might be *part* of a substantially larger system. In such a case, the expression *block entropy* is commonly used in the literature.

<sup>10</sup> Cases (i) and (ii) can be unified through the form  $W^{eff}(N) \sim A \left(1 + \frac{\ln \mu}{\rho} N\right)^\rho = Ae_{1-1/\rho}^{(\ln \mu)N}$  ( $A > 0$ ,  $\mu > 1$ , and  $1/\rho \geq 0$ ). If  $1/\rho = 0$  we obtain  $W^{eff}(N) \sim A\mu^N$ , i.e., case (i). If  $1/\rho > 0$  we obtain  $W^{eff}(N) \sim BN^\rho$  with  $B \equiv A \left(\frac{\ln \mu}{\rho}\right)^\rho$ , i.e., case (ii).

<sup>11</sup> We might consider the following entropic functional:  $S_\gamma = \sum_{i=1}^W p_i \ln^{1/\gamma}(1/p_i)$  ( $S_1 = S_{BG}$ ), whose equal-probability expression is given by  $S_\gamma = \ln^{1/\gamma} W$ . If we use as  $W$  the expression  $W^{eff}(N) \sim Cv^{N^\gamma}$ , we immediately verify that  $S_\gamma(N) \sim (\ln^{1/\gamma} v) N$ , hence *extensive*. It can be straightforwardly verified that  $S_\gamma(\{p_i\})$  is nonnegative, expandible, concave, and nonadditive.

**Table 3.3** Three binary subsystems: joint probabilities  $p_{ijk}^{A+B+C}$  ( $i, j, k = 1, 2$ ). The quantities without (within) square brackets [] correspond to state 1 (state 2) of subsystem  $C$ . The marginal probabilities where we have summed over the states of  $B$  are defined as indicated in the Table. The marginal probabilities where we have summed over the states of  $A$  are defined as follows:  $p_{11}^{(A)+B+C} \equiv p_{111}^{A+B+C} + p_{211}^{A+B+C}$ ,  $p_{21}^{(A)+B+C} \equiv p_{121}^{A+B+C} + p_{221}^{A+B+C}$ ,  $p_{12}^{(A)+B+C} \equiv p_{112}^{A+B+C} + p_{212}^{A+B+C}$  and  $p_{22}^{(A)+B+C} \equiv p_{122}^{A+B+C} + p_{222}^{A+B+C}$ . The marginal probabilities where we have summed over the states of both  $A$  and  $B$  are defined as follows:  $p_1^{(A)+(B)+C} \equiv p_{111}^{A+B+C} + p_{121}^{A+B+C} + p_{211}^{A+B+C} + p_{221}^{A+B+C}$  and  $p_2^{(A)+(B)+C} \equiv p_{112}^{A+B+C} + p_{122}^{A+B+C} + p_{212}^{A+B+C} + p_{222}^{A+B+C}$ . Of course,  $p_1^{(A)+(B)+C} + p_2^{(A)+(B)+C} = 1$

$A \setminus B$	1	2	
1	$p_{111}^{A+B+C}$	$p_{121}^{A+B+C}$	$p_{11}^{A+(B)+C} \equiv p_{111}^{A+B+C} + p_{121}^{A+B+C}$
	$[p_{112}^{A+B+C}]$	$[p_{122}^{A+B+C}]$	$[p_{12}^{A+(B)+C}] \equiv p_{112}^{A+B+C} + p_{122}^{A+B+C}$
	$p_{211}^{A+B+C}$	$p_{221}^{A+B+C}$	$p_{21}^{A+(B)+C} \equiv p_{211}^{A+B+C} + p_{221}^{A+B+C}$
2	$[p_{212}^{A+B+C}]$	$[p_{222}^{A+B+C}]$	$[p_{22}^{A+(B)+C}] \equiv p_{212}^{A+B+C} + p_{222}^{A+B+C}$
	$p_{11}^{(A)+B+C}$	$p_{21}^{(A)+B+C}$	$p_1^{(A)+(B)+C}$
	$[p_{12}^{(A)+B+C}]$	$[p_{22}^{(A)+B+C}]$	$[p_2^{(A)+(B)+C}]$

If  $N = 3$ , we shall note  $p_{111}^{A+B+C}$ ,  $p_{112}^{A+B+C}$ ,  $p_{121}^{A+B+C}$ , ..., and  $p_{222}^{A+B+C}$  the corresponding joint probabilities. Of course, they satisfy  $p_{111}^{A+B+C} + \dots + p_{222}^{A+B+C} = 1$  (see Table 3.3).

The joint probabilities corresponding to the general case are noted  $p_{11\dots 1}^{A_1+A_2+\dots+A_N}$ ,  $p_{11\dots 2}^{A_1+A_2+\dots+A_N}$ , ..., and  $p_{22\dots 2}^{A_1+A_2+\dots+A_N}$ . They satisfy

$$\sum_{i_1, i_2, \dots, i_N=1,2} p_{i_1 i_2 \dots i_N}^{A_1+A_2+\dots+A_N} = 1 \quad (N = 1, 2, 3, \dots), \quad (3.121)$$

and can be represented as a  $2 \times 2 \times \dots \times 2$  hypercube, which is associated with  $2^N$  states. There are  $N$  sets of marginal probabilities where we have summed over one subsystem. They are noted  $p_{i_2 \dots i_N}^{(A_1)+A_2+\dots+A_N}$ ,  $p_{i_1 i_3 \dots i_N}^{A_1+(A_2)+\dots+A_N}$ , ..., and  $p_{i_1 i_2 \dots i_{N-1}}^{A_1+A_2+\dots+A_N}$ . There are  $N(N - 1)/2$  sets of marginal probabilities where we have summed over two subsystems and so on.

For future use, let us right away introduce the notation corresponding to the most general case of  $N$  distinguishable discrete subsystems. Subsystem  $A_r$  is assumed to have  $W_r$  states ( $r = 1, 2, \dots, N$ ). The joint probabilities for the whole system are  $\{p_{i_1 i_2 \dots i_N}^{A_1+A_2+\dots+A_N}\}$ , such that

$$\sum_{i_1=1}^{W_1} \sum_{i_2=1}^{W_2} \dots \sum_{i_N=1}^{W_N} p_{i_1 i_2 \dots i_N}^{A_1+A_2+\dots+A_N} = 1 \quad (N = 1, 2, 3, \dots). \quad (3.122)$$

These probabilities can be represented in a  $W_1 \times W_2 \times \dots \times W_N$  hypercube. The marginal probabilities are obtained by summing over the states of at least one

subsystem. For example,  $p_{i_1 i_2 \dots i_N}^{(A_1) + (A_2) + \dots + (A_N)} \equiv \sum_{i_1=1}^{W_1} p_{i_1 i_2 \dots i_N}^{A_1 + A_2 + \dots + A_N}$ ,  $p_{i_1 i_2 \dots i_N}^{(A_1) + (A_2) + \dots + (A_N)} \equiv \sum_{i_1=1}^{W_1} \sum_{i_2=1}^{W_2} p_{i_1 i_2 \dots i_N}^{A_1 + A_2 + \dots + A_N}$ , and so on. The binary case that we introduced above corresponds of course to the particular case  $W_r = 2 (\forall r)$ . Let us go now back to it.

Let us assume the simple case in which all  $N$  binary subsystems are equal. Tables 3.2 and 3.3 then become Tables 3.5 and 3.6 respectively.

The general case of  $N$  equal subsystems has the joint probabilities  $\{r_{Nn}\}$  ( $n = 0, 1, 2, \dots, N$ ), which satisfy

$$\sum_{n=0}^N \frac{N!}{(N-n)! n!} r_{Nn} = 1 \quad (N = 1, 2, 3, \dots). \quad (3.123)$$

The probability  $r_{Nn}$  equals all the  $\frac{N!}{(N-n)! n!}$  joint probabilities  $\{p_{i_1 i_2 \dots i_N}^{A_1 + A_2 + \dots + A_N}\}$  that are associated with  $(N-n)$  subsystems in state 1 and  $n$  subsystems in state 2, in whatever order.<sup>12</sup>

The instance of the  $N$  subsystems being equal admits a representation which is much simpler than the hypercubic one used up to now. They admit a “triangular” representation: see Table 3.4.

A particular case of this probabilistic triangle is indicated in Table 3.7. The set of all the *left* members of the pairs constitute the so-called *Pascal triangle*, where each element equals the sum of its “North-West” and “North-East” neighbors. The set of all the *right* members of the pairs constitute the so-called *Leibnitz triangle* [844], where each element equals the sum of its “South-West” and “South-East” neighbors. In other words, Leibnitz triangle satisfies the rule

$$r_{N,n} + r_{N,n+1} = r_{N-1,n} \quad (\forall n, \forall N). \quad (3.124)$$

**Table 3.4** Merging of the Pascal triangle (*left* member of each pair) with the probabilities  $\{r_{Nn}\}$  (*right* member of each pair) associated with  $N$  equal subsystems

$(N = 0)$	$(1, 1)$
$(N = 1)$	$(1, r_{10}) (1, r_{11})$
$(N = 2)$	$(1, r_{20}) (2, r_{21}) (1, r_{22})$
$(N = 3)$	$(1, r_{30}) (3, r_{31}) (3, r_{32}) (1, r_{33})$
$(N = 4)$	$(1, r_{40}) (4, r_{41}) (6, r_{42}) (4, r_{43}) (1, r_{44})$

<sup>12</sup> If we consider the outcomes 1 and 2 in a specific order, we can think of them as being a time series. In such a case, for say  $N = 3$ , the probabilities  $p_{112}$ ,  $p_{121}$ , and  $p_{211}$ , might not coincide due to memory effects. If they did, that would be a case in which we have no memory of their order of appearance. Within this interpretation, the case we are addressing above would correspond to having memory of how many 1s and 2s we have, but *not* having memory of their order. If we have no memory at all, that would correspond to *equal probabilities*, i.e.,  $r_{Nn} = 1/2^N, \forall n$ . Normalization of these probabilities is in this case preserved through  $\sum_{n=0}^N \frac{N!}{(N-n)! n!} = 2^N$ .

**Table 3.5** Two equal binary subsystems  $A$  and  $B$ . *Joint* probabilities  $r_{20}$ ,  $r_{21}$ , and  $r_{22}$ , with  $r_{20} + 2r_{21} + r_{22} = 1$

$A \setminus B$	1	2	
1	$r_{20} \equiv p_{11}^{A+B}$	$r_{21} \equiv p_{12}^{A+B} = p_{21}^{A+B}$	$r_{20} + r_{21}$
2	$r_{21}$	$r_{22} \equiv p_{22}^{A+B}$	$r_{21} + r_{22}$
	$r_{20} + r_{21}$	$r_{21} + r_{22}$	1

From now on we shall refer to this rule as “Leibnitz triangle rule”, or simply “Leibnitz rule”.<sup>13</sup> It should be clear that the Leibnitz triangle satisfies Leibnitz rule, but infinitely many different probabilistic triangles also satisfy it. As we shall see, this rule will turn out to play an important role in the discussion of the nature and applicability of the entropy  $S_g$ .

Let us answer this crucial question: *What is the probabilistic meaning of Leibnitz rule?* If we compare the triangle representation (Table 3.4) with the hypercubic representation (e.g., Tables 3.5 and 3.6), we immediately verify that the Leibnitz rule means that *the marginal probabilities of the  $N$ -system coincide with the joint probabilities of the  $(N - 1)$ -system*. Generally speaking, if we calculate the marginal probabilities of the  $N$ -system where we have summed over the states of  $M$  subsystems, we precisely obtain the joint probabilities of the  $(N - M)$ -subsystem. This is a remarkable property which implies in a specific form of *scale-invariance*. This invariance is in fact quite close to that emerging within analytical procedures such as the renormalization group, successfully applied in critical phenomena and elsewhere [208–211]. Equation 3.124 will be referred to as *strict scale-invariance*. It can and does happen that this relation is only asymptotically true for large  $N$ , i.e.,

$$\lim_{N \rightarrow \infty} \frac{r_{N,n} + r_{N,n+1}}{r_{N-1,n}} = 1 \quad (\forall n). \quad (3.125)$$

In this case, we talk of *asymptotic scale-invariance*.

Leibnitz rule is in fact stronger than it might look at first sight. If we give, *for all  $N$* , the value of the probability  $r_{Nn}$  for a *single* value of  $n$ , Leibnitz rule completely determines the entire set  $\{r_{Nn}\} \forall(N, n)$ . A simple choice might be to give  $r_{N0}, \forall N$ .

<sup>13</sup> This rule should not be confused with Kolmogorov’s *consistency conditions* characterizing a *stochastic process* [297, 298]. Indeed, Kolmogorov conditions refer to the various marginal probabilities that are associated with a given set of  $N$  random variables (e.g., observing the probabilities associated with  $N'$  elements belonging to one and the same physical system with  $N$  elements, where  $N' < N$ ), whereas the Leibnitz rule relates the marginal probabilities of a system with  $N$  variables with the joint probabilities of a *different* system with  $N'$  variables, where  $N' < N$ . Whereas Kolmogorov conditions are very generic, the Leibnitz rule is extremely restrictive. Another famous rule associated with Leibnitz is the so-called “Leibnitz chain rule” for derivation of a function of a function. These two rules are in principle unrelated. However, they both have a recurrent structure. Is this just a coincidence, or does it provide a hint on the manner through which Leibnitz liked to think mathematics?

**Table 3.6** Three equal binary subsystems. *Joint* probabilities  $r_{30}, r_{31}, r_{32}$ , and  $r_{33}$ , with  $r_{30} + 3r_{31} + 3r_{32} + r_{33} = 1$ . The quantities without (within) square brackets [ ] correspond to state 1 (state 2) of subsystem C

$A \setminus B$	1	2	
1	$r_{30} \equiv p_{111}^{A+B+C}$ [ $r_{31}$ ]	$r_{31} \equiv p_{121}^{A+B+C} = p_{211}^{A+B+C} = p_{112}^{A+B+C}$ [ $r_{32} \equiv p_{122}^{A+B+C} = p_{212}^{A+B+C} = p_{221}^{A+B+C}$ ]	$r_{30} + r_{31}$ [ $r_{31} + r_{32}$ ]
	$r_{31}$ [ $r_{32}$ ] $r_{30} + r_{31}$ [ $r_{31} + r_{32}$ ]	$r_{32}$ [ $r_{33} \equiv p_{222}^{A+B+C}$ ] $r_{31} + r_{32}$ [ $r_{32} + r_{33}$ ]	$r_{31} + r_{32}$ [ $r_{32} + r_{33}$ ] $r_{30} + 2r_{31} + r_{32}$ [ $r_{31} + 2r_{32} + r_{33}$ ]
2			

For example, if we assume

$$r_{N0} = \frac{1}{N+1} \quad (N = 1, 2, 3, \dots), \quad (3.126)$$

we straightforwardly obtain

$$r_{Nn} = \frac{1}{N+1} \frac{(N-n)! n!}{N!} \quad (n = 0, 1, 2, \dots, N; N = 1, 2, 3, \dots), \quad (3.127)$$

which precisely recovers the *Leibnitz triangle* itself, as exhibited in Table 3.7.

A second example is to assume

$$r_{N0} = p^N \quad (0 \leq p \leq 1; N = 1, 2, 3, \dots). \quad (3.128)$$

It then follows that

$$r_{Nn} = p^{N-n} (1-p)^n \quad (n = 0, 1, 2, \dots, N; N = 1, 2, 3, \dots), \quad (3.129)$$

which recovers the basic case of  $N$  *independent* variables, with probabilities  $p$  and  $(1-p)$ , respectively, for the two states of each individual variable. In particular, for  $p = 1/2$ , we obtain  $r_{Nn} = 1/2^N$ ,  $\forall n$ , i.e., *equal probabilities*.<sup>14</sup>

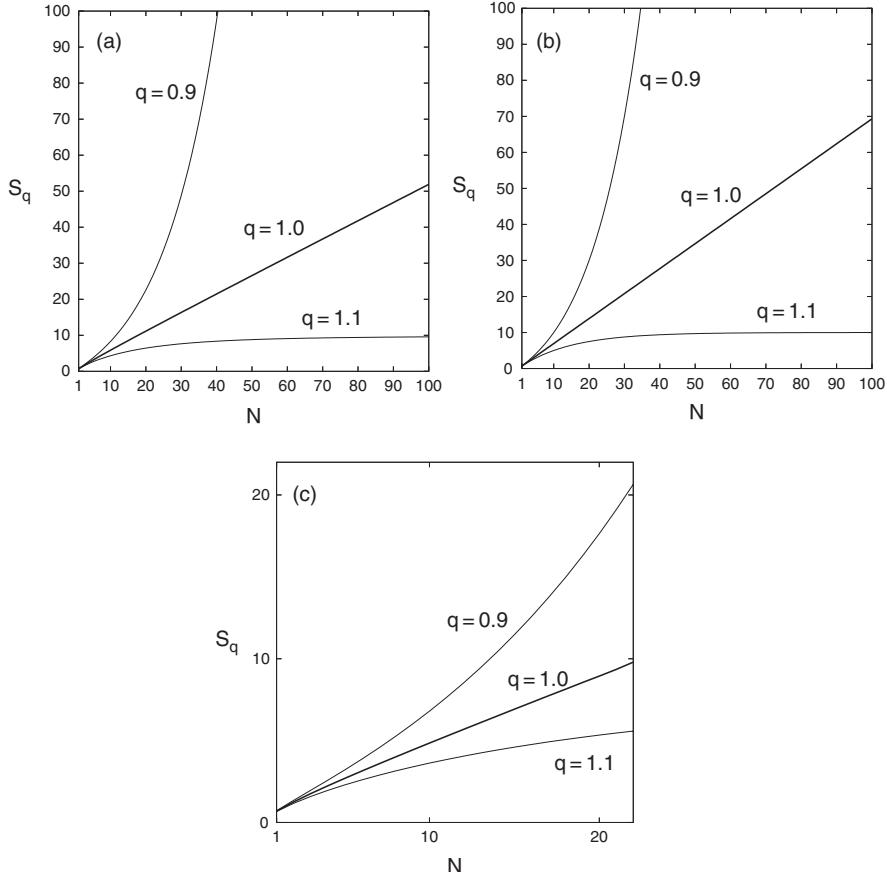
A third example is to assume [199]

$$r_{N0} = p^{N^\alpha} \quad (0 \leq p \leq 1; \alpha \geq 0; N = 1, 2, 3, \dots). \quad (3.130)$$

**Table 3.7** Merging of the Pascal triangle (the set of all *left* members) with the Leibnitz triangle [844] (the set of all *right* members) associated with  $N$  equal subsystems

$(N=0)$	$(1, 1)$
$(N=1)$	$(1, \frac{1}{2}) (1, \frac{1}{2})$
$(N=2)$	$(1, \frac{1}{3}) (2, \frac{1}{6}) (1, \frac{1}{3})$
$(N=3)$	$(1, \frac{1}{4}) (3, \frac{1}{12}) (3, \frac{1}{12}) (1, \frac{1}{4})$
$(N=4)$	$(1, \frac{1}{5}) (4, \frac{1}{20}) (6, \frac{1}{30}) (4, \frac{1}{20}) (1, \frac{1}{5})$

<sup>14</sup> Notice that, in the case of independent variables,  $r_{N0}$  decays *exponentially* with  $N$ , whereas, in the Leibnitz triangle, it decays much more slowly, as the  $1/N$  *power-law*.



**Fig. 3.14**  $S_q(N)$  for (a) the Leibnitz triangle, (b)  $p = 1/2$  independent subsystems, and (c)  $r_{N,0} = (1/2)^{N^{1/2}}$ . Only for  $q = 1$  we have a finite value for  $\lim_{N \rightarrow \infty} S_q(N)/N$ ; it vanishes (diverges) for  $q > 1$  ( $q < 1$ ). From [199].

**Table 3.8** Restricted uniform distribution model with  $d = 1$  (top) and  $d = 2$  (bottom). Notice that the number of triangle elements with nonzero probabilities grows like  $N$ , whereas that of zero probability grows like  $N^2$

$(N = 0)$	$(1, 1)$
$(N = 1)$	$(1, 1/2) (1, 1/2)$
$(N = 2)$	$(1, 1/3) (2, 1/3) (1, 0)$
$(N = 3)$	$(1, 1/4) (3, 1/4) (3, 0) (1, 0)$
$(N = 4)$	$(1, 1/5) (4, 1/5) (6, 0) (4, 0) (1, 0)$
$(N = 0)$	$(1, 1)$
$(N = 1)$	$(1, 1/2) (1, 1/2)$
$(N = 2)$	$(1, 1/4) (2, 1/4) (1, 1/4)$
$(N = 3)$	$(1, 1/7) (3, 1/7) (3, 1/7) (1, 0)$
$(N = 4)$	$(1, 1/11) (4, 1/11) (6, 1/11) (4, 0) (1, 0)$

We shall refer to this choice as the *stretched exponential* model. If  $\alpha = 1$ , it recovers the previous case, i.e., the *independent* model. If  $\alpha = 0$  and  $0 < p < 1$ , we have that all probabilities vanish for fixed  $N$ , excepting  $r_{N0} = p$  and  $r_{NN} = 1 - p$ .

All these models, with the unique exception of the independent model, involve correlations. These correlations might however be *not* strong enough in order to require an entropy different from  $S_{BG}$  if we seek for extensivity. Let us be more precise. The entropy of the  $N$ -system is given by

$$S_q(N) = \frac{1 - \sum_{n=0}^N \frac{N!}{(N-n)! n!} [r_{Nn}]^q}{q-1} \quad \left( S_1(N) = - \sum_{n=0}^N \frac{N!}{(N-n)! n!} r_{Nn} \ln r_{Nn} \right). \quad (3.131)$$

The question we want to answer is the following: *Is there a value of  $q$  such that  $S_q(N)$  is extensive, i.e., such that  $\lim_{N \rightarrow \infty} S_q(N)/N$  is finite?*

The answer is trivial for the independent model. The special value of  $q$  is simply unity. Indeed, in that case, we straightforwardly obtain

$$S_{BG}(N) = N S_{BG}(1) = -N[p \ln p + (1-p) \ln(1-p)]. \quad (3.132)$$

In this simple case, the *BG* entropy is not only extensive but even additive.

Numerical calculation has shown that the answer still is  $q = 1$  for the Leibnitz triangle, and for the stretched model with  $p > 0$  and  $\alpha > 0$ . All these examples are illustrated in Fig. 3.14.

**Table 3.9** Anomalous probability sets:  $d = 1$  (*top*) and  $d = 2$  (*bottom*). The left number within parentheses indicates the multiplicity (i.e., Pascal triangle). The right number indicates the corresponding probability. The probabilities, noted  $r_{N,n}$ , asymptotically satisfy the Leibnitz rule, i.e.,  $\lim_{N \rightarrow \infty} \frac{r_{N,n} + r_{N,n+1}}{r_{N-1,n}} = 1$  ( $\forall n$ ). In other words, the system is, in this sense, *asymptotically scale-invariant*. Notice that the number of triangle elements with nonzero probabilities grows like  $N^2$ , whereas that of zero probability grows like  $N^2$

( $N = 0$ )	(1, 1)
( $N = 1$ )	(1, 1/2) (1, 1/2)
( $N = 2$ )	(1, 1/2) (2, 1/4) (1, 0)
( $N = 3$ )	(1, 1/2) (3, 1/6) (3, 0) (1, 0)
( $N = 4$ )	(1, 1/2) (4, 1/8) (6, 0) (4, 0) (1, 0)
( $N = 0$ )	(1, 1)
( $N = 1$ )	(1, 1/2) (1, 1/2)
( $N = 2$ )	(1, 1/3) (2, 1/6) (1, 1/3)
( $N = 3$ )	(1, 3/8) (3, 5/48) (3, 5/48) (1, 0)
( $N = 4$ )	(1, 2/5) (4, 3/40) (6, 3/60) (4, 0) (1, 0)

*Is it possible to have special correlations that make  $S_q$  to be extensive only for  $q \neq 1$ ?* The answer is yes. Let us illustrate this on two examples [199]. The first of them is neither strictly nor asymptotically scale-invariant. The second one is asymptotically invariant. To construct both of them we start from the Leibnitz triangle, and then impose that most of the possible states have zero probability. Their initial

probabilities are redistributed into a small number of all the other possible states, in such a way that norm is preserved. Notice in both Tables 3.8 and 3.9 that only a “left” strip of width  $d + 1$  has nonvanishing probabilities. All the other probabilities are strictly zero. To complete the description of these models we need to indicate the values of the nonvanishing probabilities.

The first model (Table 3.8), hereafter referred to as the *restricted uniform* one, has, for a fixed value of  $N$ , all nonvanishing  $r_{Nn}$  equal. This is to say

$$\begin{aligned} r_{N,n}^{(d)} &= 1/2^N && (\text{if } N \leq d), \\ r_{N,n}^{(d)} &= \frac{1}{W^{eff}(N, d)} && (\text{if } N > d \text{ and } n \leq d), \\ r_{N,n}^{(d)} &= 0 && (\text{if } N > d \text{ and } n > d), \end{aligned} \quad (3.133)$$

with

$$W^{eff}(N, d) = \sum_{n=0}^d \frac{N!}{(N-n)! n!}, \quad (3.134)$$

where *eff* stands for *effective*. For example,  $W^{eff}(N, 0) = 1$ ,  $W^{eff}(N, 1) = N + 1$ ,  $W^{eff}(N, 2) = \frac{1}{2}N(N+1)+1$ ,  $W^{eff}(N, 3) = \frac{1}{6}N(N^2+5)+1$ , and so on. For fixed  $d$  and  $N \rightarrow \infty$ , we have that

$$W^{eff}(N, d) \sim \frac{N^d}{d!} \propto N^d. \quad (3.135)$$

The entropy is given by

$$S_q(N) = \ln_q W^{eff}(N, d). \quad (3.136)$$

Therefore, by using Eq. (3.120), we obtain that  $S_q(N)$  is extensive if and only if

$$q = 1 - \frac{1}{d}. \quad (3.137)$$

If  $q > 1 - \frac{1}{d}$  ( $q < 1 - \frac{1}{d}$ ) we have that  $\lim_{N \rightarrow \infty} S_q(N)/N$  vanishes (diverges). But this limit converges to a *finite* value for the special value of  $q$ . More precisely,

$$\lim_{N \rightarrow \infty} \frac{S_{1-1/d}(N)}{N} = \frac{d}{(d!)^{1/d}}. \quad (3.138)$$

Let us address now the second model (Table 3.9). The probabilities are given by

$$r_{N,n}^{(d,\epsilon)} = \begin{cases} \frac{1}{N+1} \frac{(N-n)! n!}{N!} + l_{N,n}^{(d,\epsilon)} s_N^{(d)} & (n \leq d) \\ 0 & (n > d) \end{cases}, \quad (3.139)$$

where the *excess probability*  $s_N^{(d)}$  and the *distribution ratio*  $l_{N,n}^{(d,\epsilon)}$  (with  $0 < \epsilon < 1$ ) are defined through

$$s_N^{(d)} \equiv \sum_{n=d+1}^N \frac{1}{N+1} \frac{(N-n)! n!}{N!} = \frac{N-d}{N+1}, \quad (3.140)$$

$$l_{N,n}^{(d,\epsilon)} \equiv \begin{cases} (1-\epsilon) \epsilon^n \frac{(N-n)! n!}{N!} & (0 \leq n < d) \\ \epsilon^d & (n = d). \end{cases} \quad (3.141)$$

The entropy is given by

$$S_q(N) = \frac{1 - \sum_{n=0}^d \frac{N!}{(N-n)! n!} [r_{N,n}^{(d,\epsilon)}]^q}{q-1}. \quad (3.142)$$

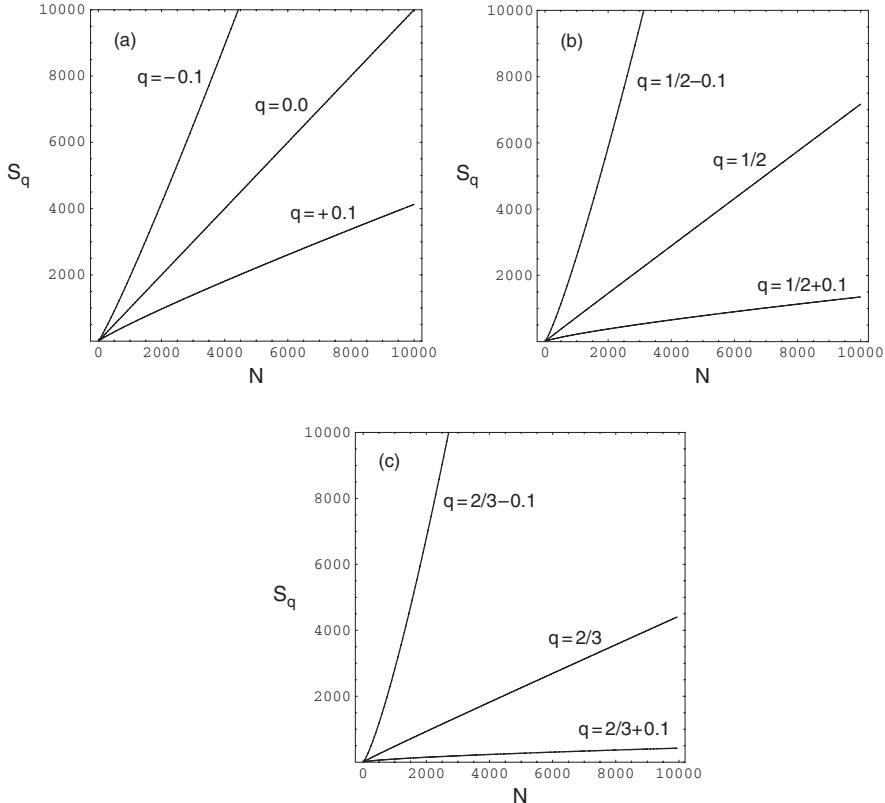
In Fig. 3.15 we have shown typical examples. As the previous example, the entropy is extensive if and only if  $q$  is given by Eq. (3.137).

Summarizing this Subsection, we have seen that, if the correlations are either strictly or asymptotically nonexistent,  $S_{BG}$  is extensive whereas  $S_q$  for  $q \neq 1$  is nonextensive. In contrast, when we have correlations so global that a large region of phase-space is unoccupied, then  $S_q$  is extensive for a special value of  $q$  which differs from unity, whereas it is nonextensive for all other values of  $q$ , including  $q = 1$ . We have presented some models that basically satisfy Leibnitz rule. However, some of them yield  $q = 1$ , whereas others yield  $q \neq 1$ . The full understanding of these facts still eludes us. We shall come back onto the subject when addressing the  $q$ -generalization of the Central Limit Theorem (CLT).

### 3.3.6 Extensivity of $S_q$ – Physical Realizations

In the two previous Subsections we have presented abstract realizations of the extensivity of  $S_q$  for  $q \neq 1$ . Let us exhibit now physical realizations of the same property in Hamiltonian many-body systems. We shall focus on the block entropy of quantum systems at temperature  $T = 0$  [201, 202]. One of them has a fermionic nature, the other one has a bosonic one. Both systems have  $N$  elements on a  $d$ -dimensional regular lattice, with  $N \rightarrow \infty$ , and we focus on a block of  $L$  contiguous elements within the  $N$ , with  $L \gg 1$ .

The system is assumed at  $T = 0$ , hence it is in its ground state (assumed non degenerate due to the presence of a vanishing external field within the easy magnetization plane). Since it is in a *pure state*, its density matrix  $\rho_N$  satisfies  $Tr\rho_N^2 = 1$ . Consequently, the entropy  $S_q(N) = 0, \forall q > 0$ . If we focus, however, on a block of  $L$  elements with  $L < N$ , and define  $\rho_L \equiv Tr_{N-L}\rho_N$  ( $Tr_{N-L}$  denotes that we are



**Fig. 3.15**  $S_q(N)$  for anomalous systems: **(a)**  $d = 1$ , **(b)**  $d = 2$ , and **(c)**  $d = 3$ . Only for  $q = 1 - (1/d)$  we have a *finite* value for  $\lim_{N \rightarrow \infty} S_q(N)/N$ ; it *vanishes* (*diverges*) for  $q > 1 + (1/d)$  ( $q < 1 + (1/d)$ ). From [199].

tracing over all but  $L$  of the  $N$  elements), we will have (in the case of our quantum systems)  $\text{Tr}\rho_L^2 < 1$ , i.e., a *mixed state*. Therefore, the block entropy  $S_q(L, N) > 0$ . This fact is due to the nontrivial entanglement associated with quantum nonlocality. Our goal is to calculate for what value of the index  $q$  (noted  $q_{ent}$  if such value exists, where *ent* stands for *entropy*) the block entropy  $S_{q_{ent}}(L) \equiv \lim_{N \rightarrow \infty} S_{q_{ent}}(L, N)$  is extensive. In other words,  $S_{q_{ent}}(L) \sim s_{q_{ent}} L$  ( $L \rightarrow \infty$ , *after* we have taken  $N \rightarrow \infty$ ), with the slope  $s_{q_{ent}} \in (0, \infty)$ .

Our first system [201] consists in the well-known linear chain of spin 1/2 XY ferromagnet with transverse magnetic field  $\lambda$ . The Hamiltonian is given by

$$\mathcal{H} = - \sum_{j=1}^{N-1} [(1 + \gamma) \hat{\sigma}_j^x \hat{\sigma}_{j+1}^x + (1 - \gamma) \hat{\sigma}_j^y \hat{\sigma}_{j+1}^y] - 2\lambda \sum_{j=1}^N \hat{\sigma}_j^z, \quad (3.143)$$

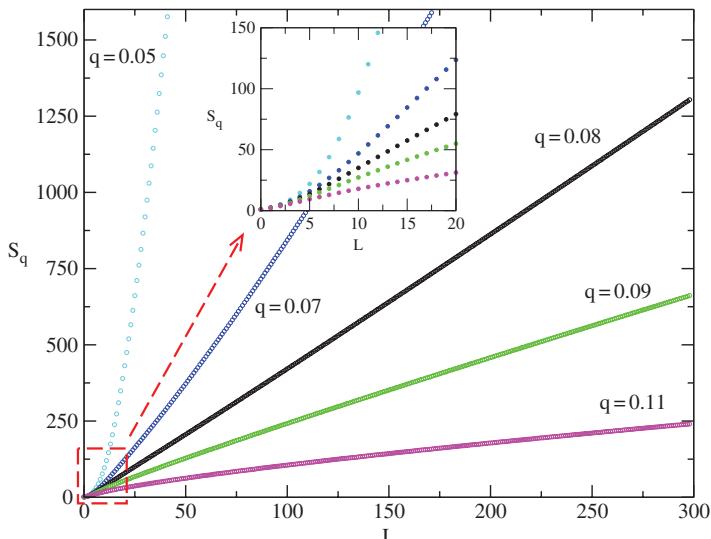
where we assume periodic boundary conditions, i.e., we have a ring with  $N$  spins, and  $(\sigma_j^x, \sigma_j^y, \sigma_j^z)$  are the Pauli matrices. For  $|\gamma| = 1$  we have the *Ising ferromagnet*, for  $0 < |\gamma| < 1$  we have the *anisotropic XY ferromagnet*, and for  $\gamma = 0$  we have the *isotropic XY ferromagnet* (or, simply, the *XY ferromagnet*). This model, being one-dimensional, has no phase transition at  $T > 0$ . But it does have a second order one at  $T = 0$ . More precisely, it is critical at  $\lambda = 1$  if  $\gamma \neq 0$ , and at  $0 \leq \lambda \leq 1$  if  $\gamma = 0$ .

See [201] for the details of the numerical and analytical calculations. The results are presented in Figs. 3.16, 3.17, 3.18, and 3.19. The numbers are consistent with the main present relation, namely  $q_{ent}$  as a function of the *central charge*  $c$ . This concept is since long known in quantum field theory (see [204] and references therein). The central charge characterizes the critical universality class of vast sets of systems (more precisely, various critical exponents are shared between the systems that have the same value of  $c$ ).

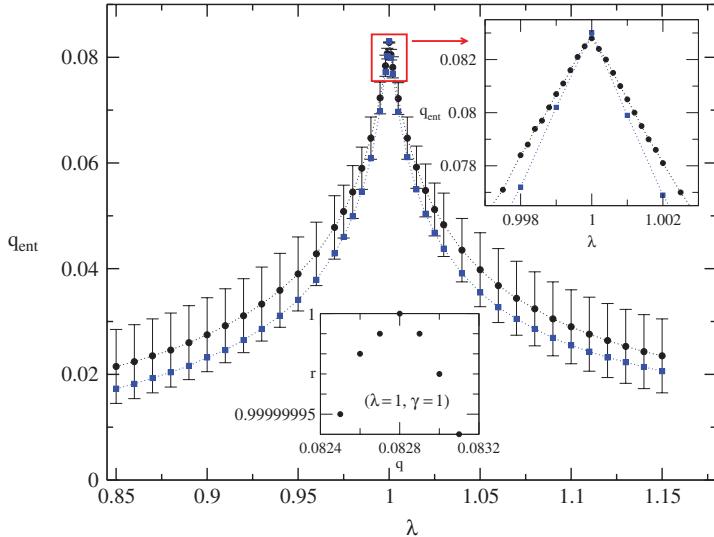
Reference [205] enables us to analytically confirm, at the critical point, the numerical results exhibited in the above figures. The continuum limit of a (1+1)-dimensional critical system is a conformal field theory with central charge  $c$ . In this quite different context, the authors re-derive the result

$$S_1(L) \sim (c/3) \ln L \quad (3.144)$$

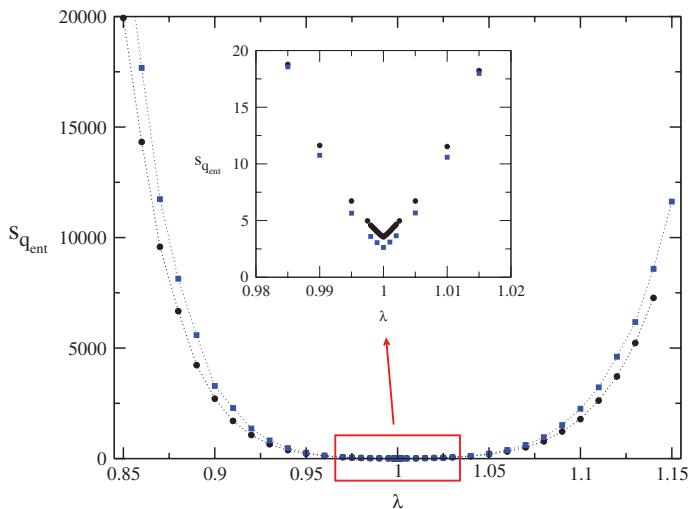
for a finite block of length  $L$  in an infinite critical system. To obtain this (clearly *nonextensive*) expression of the von Neumann entropy  $S_1(L)$ , they first find an analytical expression, namely  $\text{Tr} \hat{\rho}_L^q \sim L^{-c/6(q-1/q)}$ . Here, this expression is used quite



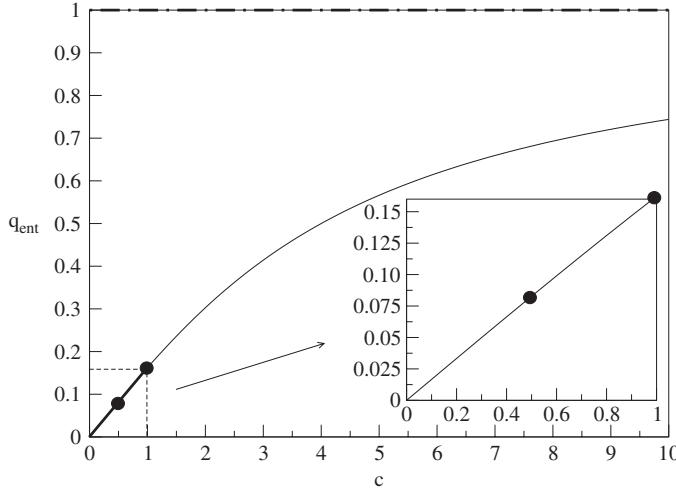
**Fig. 3.16** Block  $q$ -entropy  $S_q(\hat{\rho}_L)$  as a function of the block size  $L$  in a critical Ising chain ( $\gamma = 1$ ,  $\lambda = 1$ ), for typical values of  $q$ . Only for  $q = q_{ent} \simeq 0.0828$ ,  $s_q$  is finite (i.e.,  $S_q$  is extensive); for  $q < q_{ent}$  ( $q > q_{ent}$ ) it diverges (vanishes).



**Fig. 3.17** The  $\lambda$ -dependence of the index  $q_{ent}$  in the Ising ( $\gamma = 1$ , circle) and XY ( $\gamma = 0.75$ , square) chains. At bottom: Determination of  $q_{ent}$  through numerical maximization of the linear correlation coefficient  $r$  of  $S_q(\hat{\rho}_L)$ . The error bars for the Ising chain are obtained considering the variation of  $q_{ent}$  when using the range  $100 \leq L \leq 400$  in the search of  $S_q(\hat{\rho}_L)$  linear behavior. Actually, at the present numerical level, we cannot exclude finite-size effects of criticality.



**Fig. 3.18** The  $\lambda$ -dependence of the  $q$ -entropic density  $s_{q_{ent}}$  in the Ising ( $\gamma = 1$ , circle) and XY ( $\gamma = 0.75$ , square) models. For  $\lambda = 1$ , the slopes are (3.56) and (2.63), for  $\gamma = 1$  and  $\gamma = 0.75$ , respectively.



**Fig. 3.19**  $q_{ent}$  vs.  $c$  with the  $q$ -entropy,  $S_q(\hat{\rho}_L)$ , being *extensive*, i.e.,  $\lim_{L \rightarrow \infty} S_{\frac{\sqrt{9+c^2}-3}{c}}(\hat{\rho}_L)/L < \infty$ . When  $c$  increases from 0 to infinity,  $q_{ent}$  increases from 0 to unity (von Neumann entropy); for  $c = 4$ ,  $q = 1/2$  and for  $c \gg 1$ , see Ref. [203]. Inset: for the critical quantum Ising and XY models  $c = 1/2$  and  $q_{ent} = \sqrt{37} - 6 \simeq 0.0828$ , while for the critical isotropic XX model  $c = 1$  and  $q_{ent} = \sqrt{10} - 3 \simeq 0.16$ .

differently. We impose the *extensivity* of  $S_q(L)$  finding the value of  $q$  for which  $-c/6(q_{ent} - 1/q_{ent}) = 1$ , i.e.,

$$q_{ent} = \frac{\sqrt{9+c^2}-3}{c}. \quad (3.145)$$

Consequently,  $\lim_{L \rightarrow \infty} S_{\frac{\sqrt{9+c^2}-3}{c}}(L)/L < \infty$ . When  $c$  increases from 0 to infinity (see Fig. 3.19),  $q_{ent}$  increases from 0 to unity (von Neumann entropy). For  $c = 4$  (dimension of physical space-time),  $q = 1/2$ ;  $c = 26$  corresponds to a 26-dimensional bosonic string theory, see [203]. It is well-known that for critical quantum Ising and anisotropic XY models the central charge is equal to  $c = 1/2$  (indeed they are in the same universality class and can be mapped to a free (nonlocal) fermionic field theory). For these models, at  $\lambda = 1$ , the value of  $q$  for which  $S_q(L)$  is *extensive* is given by  $q_{ent} = \sqrt{37} - 6 \simeq 0.0828$ , in perfect agreement with our numerical results in Fig. 3.17. The critical isotropic XX model ( $\gamma = 0$  and  $|\lambda| \leq 1$ ) is, instead, in another universality class, the central charge is  $c = 1$  (free bosonic field theory) and  $S_q(L)$  is *extensive* for  $q_{ent} = \sqrt{10} - 3 \simeq 0.16$ , as found numerically also. We finally notice that, in the  $c \rightarrow \infty$  limit,  $q_{ent} \rightarrow 1$ . The physical interpretation of this fact is not clearly understood. However, since  $c$  in some sense plays the role of a dimension (see [203]), this limit could correspond to some sort of mean field approximation. If so, it is along a line such as this one that a mathematical justification could emerge for the widely spread use of BG concepts in the discussion of mean-field theories of

spin-glasses (within the replica-trick and related approaches). Indeed, BG statistical mechanics is essentially based on the *ergodic* hypothesis. It is firmly known that glassy systems (e.g., spin-glasses) precisely *violate ergodicity*, thus leading to an intriguing and fundamental question. Consequently, a mathematical justification for the use of BG entropy and energy distribution for such complex mean-field systems would be more than welcome.

The Hamiltonian (3.143) can be generalized into the following quantum Heisenberg one:

$$\mathcal{H} = - \sum_{j=1}^{N-1} [(1+\gamma)\hat{\sigma}_j^x\hat{\sigma}_{j+1}^x + (1-\gamma)\hat{\sigma}_j^y\hat{\sigma}_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z] - 2\lambda \sum_{j=1}^N \hat{\sigma}_j^z, \quad (3.146)$$

For  $\Delta = 1$  and  $\lambda = 0$  there also occurs a critical phenomenon. Its associated value of  $c$  also is 1, hence  $q_{ent} = \sqrt{10} - 3 \simeq 0.16$ . If we include in this Hamiltonian say second-neighbor coupling (or, in fact, any short-range coupling which does not alter the ferromagnetic order parameter), the value of  $c$ , hence that of  $q_{ent}$ , remains the same. Not so with the slope  $s_{q_{ent}}$ , which depends on the details and not only on the symmetry which is being broken at criticality.

Let us address now our second system, the bosonic one [202]. It is the bidimensional system of infinite coupled harmonic oscillators studied in Ref. [206], with Hamiltonian

$$\begin{aligned} \mathcal{H} = & \frac{1}{2} \sum_{x,y} \left( \Pi_{x,y}^2 + \omega_0^2 \Phi_{x,y}^2 \right. \\ & \left. + (\Phi_{x,y} - \Phi_{x+1,y})^2 + (\Phi_{x,y} - \Phi_{x,y+1})^2 \right) \end{aligned} \quad (3.147)$$

where  $\Phi_{x,y}$ ,  $\Pi_{x,y}$ , and  $\omega_0$  are coordinate, momentum, and self-frequency of the oscillator at site  $\mathbf{r} = (x, y)$ . The system has the dispersion relation

$$E(\mathbf{k}) = \sqrt{\omega_0^2 + 4 \sin^2 k_x/2 + 4 \sin^2 k_y/2}, \quad (3.148)$$

hence, a *gap*  $\omega_0$  at  $\mathbf{k} = \mathbf{0}$ . Applying the canonical transformation  $b_i = \sqrt{\frac{\omega}{2}}(\Phi_i + \frac{i}{\omega}\Pi_i)$  with  $\omega = \sqrt{\omega_0^2 + 4}$ , the Hamiltonian (3.147) is mapped into the quadratic canonical form

$$\mathcal{H} = \sum_{ij} \left[ a_i^\dagger A_{ij} a_j + \frac{1}{2}(a_i^\dagger B_{ij} a_j^\dagger + h.c.) \right], \quad (3.149)$$

where  $a_i$  are bosonic operators. It is found [206] that, for typical values of  $\omega_0$ ,

$$S_1(L) \propto L \quad (L \gg 1) \quad (3.150)$$

for square blocks of area  $L^2$ , i.e., the von Neumann entropy is nonextensive. This is so no matter how close the gap energy is to zero. In contrast, when we consider  $q \neq 1$ , it is found [202]

$$S_{q_{ent}}(L) \sim s_{q_{ent}}(\omega_0)L^2, \quad (3.151)$$

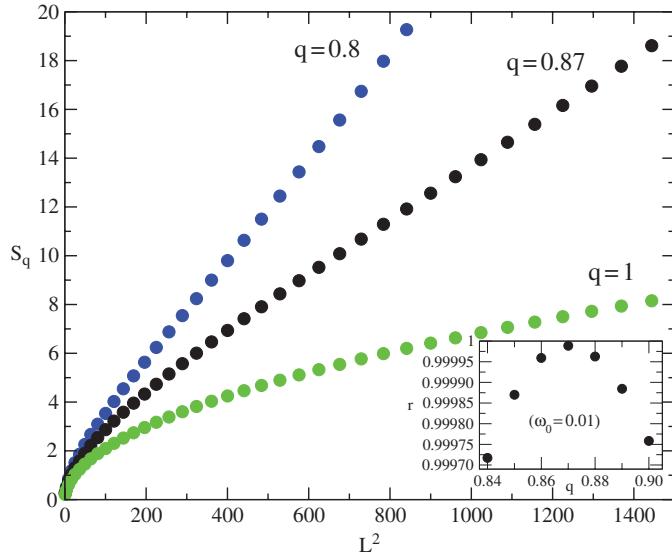
i.e., an extensive entropy (see Figs. 3.20 and 3.21). Equation (3.150) can be seen as the  $d = 2$  case of the so-called *areas law*, namely

$$S_1(L) \propto L^{d-1} \quad (d > 1; L \rightarrow \infty). \quad (3.152)$$

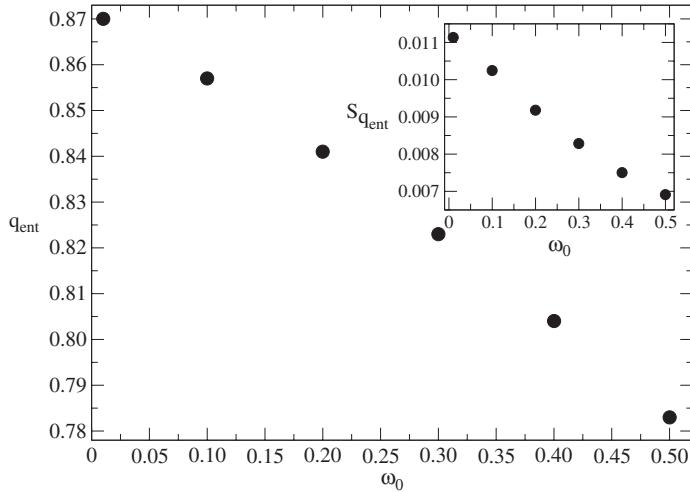
The  $d = 3$  case recovers the celebrated scaling for black holes, namely  $S_1(L) \propto L^2$ . Equations such as (3.144) and (3.152) can be unified as follows

$$S_1(L) \propto \frac{L^{d-1} - 1}{d - 1} \equiv \ln_{2-d} L \quad (d \geq 1; L \rightarrow \infty), \quad (3.153)$$

i.e., the Boltzmann–Gibbs–von Neumann entropy is nonextensive. Given the above results for fermionic and bosonic systems, a conjecture is very plausible, namely that, for such systems, a value of  $q < 1$  exists such that



**Fig. 3.20** Block  $q$ -entropy  $S_q(\hat{\rho}_L)$  as a function of the square block area  $L^2$  in a bosonic  $d = 2$  array of infinite coupled harmonic oscillators at  $T = 0$ , for typical values of  $q$ . Only for  $q = q_{ent} \simeq 0.87$ ,  $s_q$  is finite (i.e.,  $S_q$  is extensive); for  $q < q_{ent}$  ( $q > q_{ent}$ ) it diverges (vanishes). Inset: determination of  $q_{ent}$  through numerical maximization of the linear correlation coefficient  $r$  of  $S_q(\hat{\rho}_L)$  when using the range  $400 \leq L^2 \leq 1600$ .



**Fig. 3.21** The  $\omega_0$ -dependence of the index  $q_{ent}$  in a bosonic  $d = 2$  array of infinite coupled harmonic oscillators at  $T = 0$ . Inset: the  $\omega_0$ -dependence of the  $q$ -entropic density  $s_{q_{ent}}$ .

$$S_{q_{ent}}(L) \propto L^d \quad (d \geq 1; L \rightarrow \infty), \quad (3.154)$$

i.e., the thermodynamic extensivity of the entropy is recovered. The index  $q_{ent}$  is expected to depend on some generic parameters (symmetries, gaps, etc), but also on the dimension  $d$ . In particular, since the exponent  $(d - 1)$  in Eq. (3.153) and the exponent  $d$  in Eq. (3.154) become closer and closer in the limit  $d \rightarrow \infty$ , we expect  $\lim_{d \rightarrow \infty} q_{ent}(d) = 1$ . As mentioned before, it is along lines such as this one that a transparent justification could be found for the current use of BG statistical mechanics in systems like spin-glasses in the mean-field approximation (replica trick).

### 3.4 $q$ -Generalization of the Kullback–Leibler Relative Entropy

The Kullback–Leiber entropy introduced in Section 2.2 can be straightforwardly  $q$ -generalized [88, 92]. The continuous version becomes

$$I_q(p, p^{(0)}) \equiv - \int dx p(x) \ln_q \left[ \frac{p^{(0)}}{p(x)} \right] = \int dx p(x) \frac{[p(x)/p^{(0)}(x)]^{q-1} - 1}{q-1}. \quad (3.155)$$

With  $r > 0$  we have that

$$\begin{aligned} \frac{r^{q-1} - 1}{q - 1} &\geq 1 - \frac{1}{r} \quad \text{if } q > 0, \\ &= 1 - \frac{1}{r} \quad \text{if } q = 0, \\ &\leq 1 - \frac{1}{r} \quad \text{if } q < 0. \end{aligned} \tag{3.156}$$

Consequently, for say  $q > 0$ , we have that

$$\frac{[p(x)/p^{(0)}(x)]^{q-1} - 1}{q - 1} \geq 1 - \frac{p^{(0)}(x)}{p(x)}, \tag{3.157}$$

hence

$$\int dx p(x) \frac{[p(x)/p^{(0)}(x)]^{q-1} - 1}{q - 1} \geq \int dx p(x) \left[ 1 - \frac{p^{(0)}(x)}{p(x)} \right] = 1 - 1 = 0. \tag{3.158}$$

Therefore, we have

$$\begin{aligned} I_q(p, p^{(0)}) &\geq 0 \quad \text{if } q > 0, \\ &= 0 \quad \text{if } q = 0, \\ &\leq 0 \quad \text{if } q < 0. \end{aligned} \tag{3.159}$$

It satisfies therefore the same basic property as the standard Kullback–Leibler entropy, and can be used for the same purposes, while we have now the extra freedom of choosing  $q$  adequately for the specific system which we are analyzing.

By performing the transformation  $q - \frac{1}{2} \leftrightarrow \frac{1}{2} - q$  into the definition (3.155), we can easily prove the following property:

$$\frac{I_q(p, p^{(0)})}{q} = \frac{I_{1-q}(p^{(0)}, p)}{1 - q}. \tag{3.160}$$

Consequently, as a family of entropy-based testing, it is enough to consider  $q \geq 1/2$ , for which  $I_q(p, p^{(0)}) \geq 0$  (the equality holding whenever  $p(x) = p^{(0)}(x)$  almost everywhere). Also, as a corollary we have that only  $I_{1/2}(p, p^{(0)})$  is generally symmetric with regard to permutation between  $p$  and  $p^{(0)}$ , i.e.,

$$I_{1/2}(p, p^{(0)}) = I_{1/2}(p^{(0)}, p). \tag{3.161}$$

Moreover, the property  $I_{1/2}(p, p^{(0)}) \geq 0$  implies

$$\int dx \sqrt{p(x) p^{(0)}(x)} \leq 1. \tag{3.162}$$

This expression can be interpreted as the continuous version of the scalar product between two unitary vectors, namely  $\sqrt{p(x)}$  and  $\sqrt{p^{(0)}(x)}$ , and is directly related to the so-called *Fisher genetic distance* [89].

Let us also  $q$ -generalize Eq. (2.37). By choosing as  $p^{(0)}(x)$  the uniform distribution on a compact support of length  $W$ , we easily establish the desired generalization,<sup>15</sup> i.e.,

$$I_q(p, 1/W) = W^{q-1}[\ln_q W - S_q(p)]. \quad (3.163)$$

As in the  $q = 1$  case, for  $q > 0$ , the *minimization* of the  $q$ - generalized Kulback–Leibler entropy  $I_q$  may be used instead of the *maximization* of the entropy  $S_q$ . More properties can be found in [92].

Let us finally mention an elegant property, referred to as the *triangle pseudo-equality* [95, 96]. Through some algebra, it is possible to prove

$$I_q(p, p') = I_q(p, p'') + I_q(p'', p') + (q - 1)I_q(p, p'')I_q(p'', p'). \quad (3.164)$$

A simple corollary follows, namely

$$\begin{aligned} I_q(p, p') &\geq I_q(p, p'') + I_q(p'', p') && \text{if } q > 1, \\ &= I_q(p, p'') + I_q(p'', p') && \text{if } q = 1, \\ &\leq I_q(p, p'') + I_q(p'', p') && \text{if } q < 1. \end{aligned} \quad (3.165)$$

The name *triangle pseudo-equality* for Eq. (3.164) obviously comes from the  $q = 1$  case, where we do have a strict equality.

Let us now adapt our present main result, i.e., Eq. (3.159), to the problem of independence of random variables. Let us consider the two-dimensional random variable  $(x, y)$ , and its corresponding distribution function  $p(x, y)$ , with  $\int dx dy p(x, y) = 1$ . The marginal distribution functions are then given by  $h_1(x) \equiv \int dy p(x, y)$  and  $h_2(y) \equiv \int dx p(x, y)$ . The discrimination criterion for independence concerns the comparison of  $p(x, y)$  with  $p^{(0)}(x, y) \equiv h_1(x)h_2(y)$ . The one-dimensional random variables  $x$  and  $y$  are independent if and only if  $p(x, y) = p^{(0)}(x, y)$  (almost everywhere). The criterion (3.159) then becomes

$$\int dx dy p(x, y) \frac{\left[ \frac{p(x, y)}{h_1(x)h_2(y)} \right]^{q-1} - 1}{q - 1} \geq 0 \quad (q \geq 1/2). \quad (3.166)$$

In the limit  $q \rightarrow 1$ , this criterion recovers the usual one, namely [90]

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<sup>15</sup> This formula appears misprinted in Eq. (3.15) of the original paper [88]. This erratum was kindly communicated to me by R. Piasecki.

$$\int dx dy p(x, y) \ln p(x, y) - \int dx h_1(x) \ln h_1(x) - \int dy h_2(y) \ln h_2(y) \geq 0. \quad (3.167)$$

For  $q = 1/2$ , we obtain a particularly simple criterion, namely

$$\int dx dy p(x, y) \sqrt{p(x, y) h_1(x) h_2(y)} \leq 1. \quad (3.168)$$

For  $q = 2$ , we obtain

$$\int dx dy \frac{[p(x, y)]^2}{h_1(x) h_2(y)} \geq 1. \quad (3.169)$$

This can be considered as a satisfactory quadratic-like criterion, as opposed to the quantity introduced in [91]. We refer to the quantity frequently used in economics [91], namely, for  $h_1 = h_2 \equiv h$ ,

$$\int dx dy [p(x, y)]^2 - \left\{ \int dx [h(x)]^2 \right\}^2. \quad (3.170)$$

This quantity has not a definite sign. In fact, if  $x$  and  $y$  are independent, this quantity vanishes. But, if it vanishes,  $x$  and  $y$  are *not* necessarily independent. In other words, its zero is *not* a necessary and sufficient condition for independence, and therefore it does *not* constitute an optimal criterion. It could be advantageously replaced, in applications such as financial analysis, by the present criterion (3.169).

The generalization of criterion (3.166) for an arbitrary number  $d$  of variables (with  $d \geq 2$ ) is straightforward, namely

$$I_q(p(x_1, x_2, \dots, x_d), p^{(0)}(x_1, x_2, \dots, x_d)) \geq 0 \quad (q \geq 1/2), \quad (3.171)$$

where

$$\begin{aligned} p^{(0)}(x_1, x_2, \dots, x_d) &\equiv \left[ \int dx_2 dx_3 \dots dx_d p(x_1, x_2, \dots, x_d) \right] \\ &\times \left[ \int dx_1 dx_3 \dots dx_d p(x_1, x_2, \dots, x_d) \right] \\ &\times \dots \\ &\times \left[ \int dx_1 dx_2 \dots dx_{d-1} p(x_1, x_2, \dots, x_d) \right]. \end{aligned} \quad (3.172)$$

Depending on the specific purpose, one might even prefer to use the symmetrized version of the criterion, i.e.,

$$\frac{1}{2} \left[ I_q(p(x_1, x_2, \dots, x_d), p^{(0)}(x_1, x_2, \dots, x_d)) + I_q(p^{(0)}(x_1, x_2, \dots, x_d), p(x_1, x_2, \dots, x_d)) \right] \geq 0 \quad (q \geq 1/2). \quad (3.173)$$

The equalities in (3.171) and (3.173) hold if and only if *all* the variables  $x_1, x_2, \dots, x_d$  are independent among them (almost everywhere).

Before closing this Section, let us mention that the discrete version of definition (3.155) naturally is

$$I_q(p, p^{(0)}) \equiv \sum_{i=1}^W p_i \frac{[p_i/p_i^{(0)}]^{q-1} - 1}{q-1}. \quad (3.174)$$

## 3.5 Constraints and Entropy Optimization

As we did with the *BG* entropy, let us work out here the most simple entropic optimization cases.

### 3.5.1 Imposing the Mean Value of the Variable

In addition to

$$\int_0^\infty dx \, p(x) = 1, \quad (3.175)$$

we might know the following mean value of the variable (referred to as the *q-mean value*):

$$\langle x \rangle_q \equiv \int_0^\infty dx \, x \, P(x) = X_q^{(1)}, \quad (3.176)$$

where the *escort distribution*  $P(x)$  is defined through [212]

$$P(x) \equiv \frac{[p(x)]^q}{\int_0^\infty dx' [p(x')]^q}. \quad (3.177)$$

We immediately verify that also  $P(x)$  is normalized, i.e.,

$$\int_0^\infty dx \, P(x) = 1. \quad (3.178)$$

The reasons for which we use  $P(x)$  instead of  $p(x)$  to express the constraint (3.176) are somewhat subtle and will be discussed later on. At the present stage, we

just assume that, for whatever reason, what we know is the mean value of  $x$  with the escort distribution. We wish now to optimize  $S_q$  with the constraints (3.178) and (3.176), or, equivalently, with the constraints (3.175) and (3.176).

In order to use the Lagrange method to find the optimizing distribution, we define

$$\Phi[p] \equiv \frac{1 - \int_0^\infty dx [p(x)]^q}{q - 1} - \alpha \int_0^\infty dx p(x) - \beta_q^{(1)} \frac{\int_0^\infty dx x [p(x)]^q}{\int_0^\infty dx [p(x)]^q}, \quad (3.179)$$

where  $\alpha$  and  $\beta_q^{(1)}$  are the Lagrange parameters. We then impose  $\partial\Phi[p]/\partial p = 0$ , and straightforwardly obtain

$$p_{opt}(x) = \frac{e_q^{-\beta_q^{(1)}(x-X_q^{(1)})}}{\int_0^\infty dx' e_q^{-\beta_q^{(1)}(x'-X_q^{(1)})}}, \quad (3.180)$$

where  $opt$  stands for *optimal*, and where we have used condition (3.175) to eliminate the Lagrange parameter  $\alpha$ . Notice that the fact that Lagrange parameter  $\alpha$  can be factorized, and therefore eliminated, constitutes a quite remarkable mathematical property.

### 3.5.2 Imposing the Mean Value of the Squared Variable

Another simple and quite frequent case is when we know that  $\langle x \rangle_q = 0$ . In such case, in addition to

$$\int_{-\infty}^\infty dx p(x) = 1, \quad (3.181)$$

we might know the  $q$ -mean value of the squared variable, i.e.,

$$\langle x^2 \rangle_q \equiv \int_{-\infty}^\infty dx x^2 P(x) = X_q^{(2)} > 0. \quad (3.182)$$

In order to use, as before, the Lagrange method to find the optimizing distribution, we define

$$\Phi[p] \equiv \frac{1 - \int_{-\infty}^\infty dx [p(x)]^q}{q - 1} - \alpha \int_{-\infty}^\infty dx p(x) - \beta_q^{(2)} \frac{\int_{-\infty}^\infty dx x^2 [p(x)]^q}{\int_{-\infty}^\infty dx [p(x)]^q}. \quad (3.183)$$

We then impose  $\partial\Phi[p]/\partial p = 0$ , and straightforwardly obtain

$$p_{opt}(x) = \frac{e_q^{-\beta_q^{(2)}(x^2-X_q^{(2)})}}{\int_{-\infty}^\infty dx' e_q^{-\beta_q^{(2)}(x'^2-X_q^{(2)})}}, \quad (3.184)$$

where we have used condition (3.181) to eliminate the Lagrange parameter  $\alpha$ . This distribution can be straightforwardly rewritten as

$$p_{opt}(x) = \frac{e_q^{-\beta_q^{(2)\gamma} x^2}}{\int_{-\infty}^{\infty} dx' e_q^{-\beta_q^{(2)\gamma} x'^2}}, \quad (3.185)$$

with

$$\beta_q^{(2)\gamma} \equiv \frac{\beta_q^{(2)}}{1 + (1 - q) \beta_q^{(2)} X_q^{(2)}}. \quad (3.186)$$

We thus see that, in the same way Gaussians are deeply connected to  $S_{BG}$ , the present distributions, frequently referred to as *q-Gaussians*, are connected to the  $S_q$  entropy.

### 3.5.3 Others

A quite general situation would be to impose, in addition to

$$\int dx p(x) = 1, \quad (3.187)$$

the constraint

$$\langle f(x) \rangle_q \equiv \int dx f(x) P(x) = F_q, \quad (3.188)$$

where  $f(x)$  is some known function and  $F_q$  a known number. We obtain

$$p_{opt}(x) = \frac{e_q^{-\beta_q(f(x)-F_q)}}{\int dx' e_q^{-\beta_q(f(x')-F_q)}}. \quad (3.189)$$

As for the  $BG$  case, it is clear that, by appropriately choosing  $f(x)$ , we can force  $p_{opt}(x)$  to be virtually *any* distribution we wish. For example, by choosing  $f(x) = |x|^\gamma$  ( $\gamma \in \mathbb{R}$ ), we obtain a generic *stretched q-exponential*  $p_{opt}(x) \propto e_q^{-\beta|x|^\gamma}$ .

## 3.6 Nonextensive Statistical Mechanics and Thermodynamics

We arrive now to the central goal of the present introduction to *nonextensive statistical mechanics*. This theory was first introduced in 1988 [39] as a possible generalization of Boltzmann–Gibbs statistical mechanics. The idea first emerged in my mind in 1985 during a meeting in Mexico City. The inspiration was related to the

geometrical theory of multifractals and its systematic use of powers of probabilities. It is from that theory that the notation  $q$  was adopted, although, as we shall soon see, these two  $q$ 's are *not* the same. In fact, to avoid confusion, we shall from now on denote by  $q_M$  the multifractal index, where  $M$  stands precisely for *multifractal*. Although different, the indices  $q$  and  $q_M$  ultimately turned out to have some relation. For example, in a class of systems that we discuss in Chapter 5, we may see  $q$  (more precisely the index that will be noted  $q_{sen}$ ) as a special value of  $q_M$  where some discontinuities occur.<sup>16</sup>

The present theory – nowadays known as *nonextensive statistical mechanics* – constitutes a generalization of, and *by no means an alternative to*, the standard *BG* thermostatics. It just attempts to enlarge the domain of applicability of the frame of the standard theory by extending the mathematical form of its entropy. More precisely, by generalizing the entropic functional which connects the microscopic world (i.e., the probabilities of the microscopic possibilities) with some of its macroscopic manifestations. The theory has substantially evolved during the last two decades, and naturally it is still evolving at the rhythm at which new insights emerge that enable a deeper understanding of its nature, its powers, and its limitations. Successive collections of mini-reviews are available in the literature: see [62, 64–76].

The theory starts by postulating the use of the *nonadditive entropy*  $S_q$ <sup>17</sup> as indicated (in its discrete form) in Eq. (3.18), with the norm constraint (1.2), i.e.,

$$\sum_{i=1}^W p_i = 1. \quad (3.190)$$

If the system is *isolated*, no other constraint exists, and this physical situation is referred to as the *microcanonical ensemble*. All nonvanishing probabilities are equal and equal to  $1/W$ . Indeed, this uniform distribution is the one which extremizes  $S_q$ . The entropy is then given by expression (3.16).

<sup>16</sup>  $q_M$  is a *running* index which takes values from  $-\infty$  to  $\infty$  and is useful to characterize the various scalings occurring in multifractal structures, whereas  $q$  is a *fixed* index which characterizes a particular physical system (or, more exactly, its universality class of nonextensivity). The so-called “Thermodynamics of chaotic systems” (see, for instance, [212]) addresses a convenient discussion of multifractal geometry and some of its aspects are isomorphic to *BG* statistical mechanics. Within this theory, one takes Legendre transforms on the index  $q_M$ . In contrast, within “Nonextensive thermodynamics,”  $q$  is fixed once for ever for a given system and its Legendre transforms concern by no means  $q$ , but precisely the same variables that are normally used in classical thermodynamics. Its mathematics is, in variance with that of “Thermodynamics of chaotic systems,” *not* isomorphic to the *BG* one, but rather contains it as a particular case.

<sup>17</sup> Let us emphasize that, although the index  $q$  is in principle chosen so that the *nonadditive entropy*  $S_q$  is *extensive*, the theory is referred to as *nonextensive statistical mechanics*. This is due, on one hand, to historical reasons, and, on the other hand, to the fact that this thermostatics primarily focuses on systems whose total energy is typically *nonextensive*. The systems to which this theory is, in one way or another, applicable are generically referred to as *nonextensive systems*.

If we want to formulate instead the statistical mechanics of the *canonical ensemble*, i.e., of a system *in longstanding contact with a large thermostat at fixed temperature*, we need to add one more constraint (or even more than one, in fact, for more complex systems), namely that associated with the energy. The expression of this constraint is less trivial than it seems at first sight! Indeed, it has been written in different forms since the first proposal of the theory. Let us describe here these successive forms since the underlying epistemological process is undoubtedly quite instructive.

The *first form* was that adopted in 1988 [39], namely the simplest possible one (Eq. (2.63)):

$$\sum_{i=1}^W p_i E_i = U_q^{(1)}. \quad (3.191)$$

The extremization of  $S_q$  with constraints (3.190) and (3.191) yields

$$p_i^{(1)} \propto [1 - (q - 1)\beta^{(1)} E_i]^{1/(q-1)} = e_{2-q}^{-\beta^{(1)} E_i}. \quad (3.192)$$

This expression already exhibits all the important facts of nonextensive statistics, namely the possibility (when  $q < 1$ ) for an *asymptotic power-law behavior at high energies*, and the possibility (when  $q > 1$ ) of a *cutoff*. However, it can be seen that it does *not* allow for a satisfactory connection with thermodynamics, in the sense that no partition function can be defined which would *not* depend on the Lagrange parameter  $\alpha$ , but only on the parameter  $\beta_q^{(1)}$ . Moreover,  $p_i^{(1)}$  is *not* invariant, for fixed  $\beta_q^{(1)}$ , with regard to a changement of zero of energies. Indeed,  $e_q^{a+b} \neq e_q^a e_q^b$  (if  $q \neq 1$ ), and therefore, as it stands, it is not possible to factorize the new zero of energy so that it becomes cancelled between numerator and denominator.

The *second form* for the constraint was first indicated in [39] and developed in 1991 [59]. It is written as follows:

$$\sum_{i=1}^W p_i^q E_i = U_q^{(2)}. \quad (3.193)$$

The extremization of  $S_q$  with constraints (3.190) and (3.193) yields

$$p_i^{(2)} \propto [1 - (1 - q)\beta^{(2)} E_i]^{1/(1-q)} = e_q^{-\beta^{(2)} E_i}. \quad (3.194)$$

It can be seen that this result allows for a simple factorization of the Lagrange parameter  $\alpha$ , hence a partition function emerges which, as in *BG* statistics, only depends on  $\beta_q^{(2)}$ . Consistently, a smooth connection with classical thermodynamics becomes possible. However,  $p_i^{(2)}$  is still *not* invariant, for fixed  $\beta_q^{(2)}$ , with regard to a changement of zero of energies. Even more disturbing, the type of average used in Eq. (3.193) violates the (a priori reasonable) result that the average of a constant

precisely coincides with that constant. For similar reasons, if we consider  $E_{ij}^{A+B} = E_i^A + E_j^B$  with  $p_{ij}^{A+B} = p_i^A p_j^B$ ,<sup>18</sup> we do *not* generically obtain  $U_q^{(2)}(A+B) = U_q^{(2)}(A) + U_q^{(2)}(B)$ . These features led finally to a new formulation of the energy constraint.

The *third form* for the constraint was introduced in 1998 [60]. It is written as follows:

$$\langle E_i \rangle_q \equiv \sum_{i=1}^W P_i E_i = U_q^{(3)}, \quad (3.195)$$

where we have used the escort distribution

$$P_i \equiv \frac{p_i^q}{\sum_{j=1}^W p_j^q}. \quad (3.196)$$

The extremization of  $S_q$  with constraints (3.190) and (3.195) yields

$$p_i^{(3)} = \frac{[1 - (1-q)\beta_q^{(3)}(E_i - U_q^{(3)})]^{1/(1-q)}}{\bar{Z}_q} = \frac{e_q^{-\beta_q^{(3)}(E_i - U_q^{(3)})}}{\bar{Z}_q}, \quad (3.197)$$

with

$$\beta_q^{(3)} \equiv \frac{\beta^{(3)}}{\sum_{j=1}^W [p_j^{(3)}]^q}, \quad (3.198)$$

and

$$\bar{Z}_q \equiv \sum_i^W e_q^{-\beta_q^{(3)}(E_i - U_q^{(3)})}, \quad (3.199)$$

$\beta^{(3)}$  being the Lagrange parameter associated with constraint (3.195). This formulation simultaneously solves *all* the difficulties mentioned above, namely (i) the  $\alpha$  Lagrange parameter factorizes, hence we can define a partition function depending only on  $\beta_q^{(3)}$ , hence we can make a simple junction with thermodynamics; (ii) the average of a constant coincides with that constant; (iii) if we consider  $E_{ij}^{A+B} = E_i^A + E_j^B$  with  $p_{ij}^{A+B} = p_i^A p_j^B$ , we generically obtain  $U_q^{(3)}(A+B) = U_q^{(3)}(A) + U_q^{(3)}(B)$ ; and (iv) since the difference  $E_i - U_q^{(3)}$  does *not* depend on the choice of zero for energies, the probability  $p_i^{(3)}$  is *invariant*, for fixed  $\beta_q^{(3)}$ , with regard to the changement of that zero.

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<sup>18</sup> Notice however that  $E_{ij}^{A+B} = E_i^A + E_j^B$  and  $p_{ij}^{A+B} = p_i^A p_j^B$  are, of course, inconsistent with Eq. (3.194), unless  $q = 1$ .

Because of all these remarkable properties, *the third form is the most commonly used nowadays*. Before enlarging its discussion and presenting its connection with thermodynamics, let us finish the brief review of this instructive evolution of ideas. A few years later, it was noticed [77] that the constraint (3.195) can be rewritten in the following compact manner:

$$\sum_{i=1}^W p_i^q (E_i - U_q) = 0. \quad (3.200)$$

This approach led to the so-called “optimal Lagrange multipliers,” a twist which has some interesting properties. A question obviously arrives: *Which one is the correct one, if any of these?* The answer is quite simple: *basically all of them!*. Indeed, as it was first outlined in [60], and discussed in detail recently [323], they can be transformed one into the other through simple operations redefining the  $q$  s and the  $\beta_q$  s. Further comments can be found in [322, 324–326].

To avoid confusion, and also because of its convenient properties, we shall stick onto the third form [60]. Consistently, we shall from now on use the simplified notation  $(p_i^{(3)}, U_q^{(3)}, \beta^{(3)}, \beta_q^{(3)}) \equiv (p_i, U_q, \beta, \beta_q)$ . Let us rewrite Eqs. (3.197), (3.198), and (3.199) with this simplified notation:

$$p_i = \frac{[1 - (1 - q)\beta_q(E_i - U_q)]^{1/(1-q)}}{\bar{Z}_q} = \frac{e_q^{-\beta_q(E_i - U_q)}}{\bar{Z}_q}, \quad (3.201)$$

with

$$\beta_q \equiv \frac{\beta}{\sum_{j=1}^W p_j^q}, \quad (3.202)$$

and

$$\bar{Z}_q \equiv \sum_i^W e_q^{-\beta_q(E_i - U_q)}. \quad (3.203)$$

Notice that, from the definition of  $S_q$ ,

$$\sum_{j=1}^W p_j^q = 1 + (1 - q)S_q/k, \quad (3.204)$$

and also that

$$\sum_{j=1}^W p_j^q = (\bar{Z}_q)^{1-q}. \quad (3.205)$$

Equation (3.205) can be established from Eq. (3.204) by using

$$S_q = k \ln_q \bar{Z}_q , \quad (3.206)$$

which is proved a few lines further on.

The (meta)equilibrium or stationary state distribution (3.201) can be rewritten as follows:

$$p_i = \frac{e_q^{-\beta'_q E_i}}{Z'_q} , \quad (3.207)$$

with

$$Z'_q \equiv \sum_{j=1}^W e_q^{-\beta'_q E_j} , \quad (3.208)$$

and

$$\beta'_q \equiv \frac{\beta_q}{1 + (1 - q)\beta_q U_q} . \quad (3.209)$$

This form is particularly convenient for many applications where comparison with experimental, observational, or computational data is involved.<sup>19</sup>

The connection to thermodynamics is established in what follows. It can be proved that

$$\frac{1}{T} = \frac{\partial S_q}{\partial U_q} , \quad (3.210)$$

with  $T \equiv 1/(k\beta)$ , where, for clarity,  $k$  has been restored into the expressions. Also we prove, for the free energy,

$$F_q \equiv U_q - T S_q = -\frac{1}{\beta} \ln_q Z_q , \quad (3.211)$$

<sup>19</sup> We may rewrite in fact the distribution (3.201) with regard to *any* referential energy that we wish, say  $E_0$ . It just becomes  $p_i = [1 - (1 - q)\beta_q^{(0)}(E_i - E_0)]^{1/(1-q)}/Z_q^{(0)}$  with  $\beta_q^{(0)} \equiv \beta_q/[1 + (1 - q)\beta_q(U_q - E_0)]$  and  $Z_q^{(0)} \equiv \sum_{j=1}^W [1 - (1 - q)\beta_q^{(0)}(E_j - E_0)]^{1/(1-q)}$ . If we choose  $E_0 = U_q$  we get back Eq. (3.201); if we choose  $E_0 = 0$  we recover Eq. (3.207). The preference of a particular referential energy  $E_0$  is dictated by convenience for specific applications. Notice also that these expressions, e.g., Eq. (3.201) are *self-referential* in the sense that Eq. (3.202) is itself expressed in terms of the set  $\{p_i\}$ . This implies of course in a slight operational complication. There are however in the literature several procedures that conveniently overcome this difficulty. One of those procedures is indicated in [60].

where

$$\ln_q Z_q = \ln_q \bar{Z}_q - \beta U_q . \quad (3.212)$$

This relation takes into account the trivial fact that, in contrast with what is usually done in BG statistics, the energies  $\{E_i\}$  are here referred to  $U_q$  in Eq. (3.195). From Eqs. (3.211) and (3.212), we immediately obtain the anticipated relation (3.206). It can also be proved

$$U_q = -\frac{\partial}{\partial \beta} \ln_q Z_q , \quad (3.213)$$

as well as relations such as

$$C_q \equiv T \frac{\partial S_q}{\partial T} = \frac{\partial U_q}{\partial T} = -T \frac{\partial^2 F_q}{\partial T^2} . \quad (3.214)$$

In fact the entire Legendre transformation structure of thermodynamics is  $q$ -invariant, which no doubt is remarkable and welcome.

Let us stress an important fact. The temperatures  $T \equiv 1/(k\beta)$  and  $T_q \equiv 1/(k\beta_q)$  do *not* depend on the choice of the zero of energies, and are therefore susceptible of physical interpretation (even if they do not necessarily coincide). Not so the temperature  $T'_q \equiv 1/(k\beta'_q)$ .

In addition to the Legendre structure, various other important theorems and properties are  $q$ -*invariant*. Let us briefly mention some of them.

(i) *H-theorem (macroscopic time irreversibility)*. Under a variety of irreversible equations such as the master equation, Fokker–Planck equation, and others, it has been proved (see, for instance, [213–215]) that

$$q \frac{dS_q}{dt} \geq 0 \quad (\forall q) , \quad (3.215)$$

the equality corresponding to (meta)equilibrium. In other words, the arrow time involved in the second principle of thermodynamics basically holds in the usual way. It is appropriate to remind at this point that, for  $q > 0$  ( $q < 0$ ), the entropy tends to attain its maximum (minimum) since it is a concave (convex) functional, as already shown.

(ii) The *Clausius relation* is verified  $\forall q$ , and the second principle of thermodynamics remains the same [337].

(iii) *Ehrenfest theorem (correspondence principle between quantum and classical mechanics)*. It can be shown [216] that

$$\frac{d\langle \hat{O} \rangle_q}{dt} = \frac{i}{\hbar} \langle [\hat{\mathcal{H}}, \hat{O}] \rangle_q \quad (\forall q) , \quad (3.216)$$

where  $\hat{O}$  is any observable of the system.

(iv) *Factorization of the likelihood function (thermodynamically independent systems)*. This property generalizes [218–220] the celebrated one introduced by Einstein in 1910 [20] (*reversal of Boltzmann formula*). The likelihood function satisfies

$$W_q(\{p_i\}) \propto e_q^{S_q(\{p_i\})}. \quad (3.217)$$

If  $A$  and  $B$  are two probabilistically independent systems, it can be immediately verified that

$$W_q(A + B) = W_q(A) W_q(B) \quad (\forall q), \quad (3.218)$$

where we have used  $e_q^{S_q(A)+S_q(B)+(1-q)S_q(A)S_q(B)} = e_q^{S_q(A)} e_q^{S_q(B)}$ .

(v) *Onsager reciprocity theorem (microscopic time reversibility)*. It has been shown [221–223] that the reciprocal linear coefficients satisfy

$$L_{jk} = L_{kj} \quad (\forall q). \quad (3.219)$$

(vi) *Kramers and Kronig relation (causality)*. Its validity has been proved [222] for all values of  $q$ .

(vii) *Pesin-like identity (relation between sensitivity to the initial conditions and the entropy production per unit time)*. It has been conjectured [127] that the  $q$ -generalized entropy production per unit time (Kolmogorov-Sinai-like entropy rate)  $K_q$  and the  $q$ -generalized Lyapunov coefficient  $\lambda_q$  are related through

$$K_q = \begin{cases} \lambda_q & \text{if } \lambda_q > 0, \\ 0 & \text{otherwise.} \end{cases} \quad (3.220)$$

The actual validity of this relation has been analytically proved and/or numerically verified for various classes de models [128, 129, 131–133, 139–142, 146, 147, 150, 153, 358]. We come back onto this identity later on. Indeed, as we shall see, Eq. (3.220) is in fact one among an infinite countable family of such relations.

Properties (i) and (iii–vi) essentially reflect something quite basic. In the theory that we are presenting here, we have generalized *nothing* concerning mechanics, either classical, quantum, or whatsoever. What we have generalized is the *concept of information* upon mechanics. Consistently, the properties whose essential origin lies in mechanics should be expected to be  $q$ -invariant, and we verify that indeed they are.

Some physical interpretations of nonextensive statistics are already available in the literature [327–329]. We come back onto this question later on, in particular in connection with the Beck–Cohen superstatistics.

Let us mention also that various procedures that are currently used in *BG* statistical mechanics have been  $q$ -generalized. These include the variational method [224–226], the Green-function methods [222, 225, 320, 330–333], the Darwin–Fowler

steepest descent method [227, 334], the Khinchin large-numbers-law method [229, 335], and the counting in the microcanonical ensemble [230, 231, 336].

In the continuous (classic) limit, Eqs. (3.201), (3.202), and (3.203) take the form

$$p(\mathbf{p}, \mathbf{x}) = \frac{e_q^{-\beta_q [\mathcal{H}(\mathbf{p}, \mathbf{x}) - U_q]}}{\bar{Z}_q}, \quad (3.221)$$

with

$$\beta_q \equiv \frac{\beta}{\int d\mathbf{p} d\mathbf{x} [p(\mathbf{p}, \mathbf{x})]^q}, \quad (3.222)$$

and

$$\bar{Z}_q \equiv \int d\mathbf{p} d\mathbf{x} e_q^{-\beta_q [\mathcal{H}(\mathbf{p}, \mathbf{x}) - U_q]}, \quad (3.223)$$

$\mathcal{H}(\mathbf{p}, \mathbf{x})$  being the Hamiltonian of the system.

In the generic quantum case, Eqs. (3.201), (3.202), and (3.203) take the form

$$\hat{\rho} = \frac{e_q^{-\beta_q (\hat{\mathcal{H}} - U_q)}}{\bar{Z}_q}, \quad (3.224)$$

with

$$\beta_q \equiv \frac{\beta}{Tr \hat{\rho}^q}, \quad (3.225)$$

and

$$\bar{Z}_q \equiv Tr e_q^{-\beta_q (\hat{\mathcal{H}} - U_q)}, \quad (3.226)$$

$\hat{\mathcal{H}}$  being the Hamiltonian of the system.

### 3.7 About the Escort Distribution and the $q$ -Expectation Values

We have seen that the escort distributions play a central role in nonextensive statistical mechanics. Let us start by analyzing their generic properties. We shall focus on the discrete version, i.e.,

$$P_i \equiv \frac{p_i^q}{\sum_{j=1}^W p_j^q} \quad \left( \sum_{i=1}^W p_i = 1; q \in \mathbb{R} \right). \quad (3.227)$$

We will note this transformation as follows:

$$\mathbf{P} \equiv T_q[\mathbf{p}], \quad (3.228)$$

with the notation  $\mathbf{p} \equiv (p_1, p_2, \dots, p_W)$  and  $\mathbf{P} \equiv (P_1, P_2, \dots, P_W)$ . With the notation

$$(T_q * T_{q'})[\mathbf{p}] \equiv T_q[T_{q'}[\mathbf{p}]]. \quad (3.229)$$

We can easily verify the following properties:

(i) *Unit*. The unit is given by  $T_1$ . Indeed

$$\mathbf{p} \equiv T_1[\mathbf{p}]. \quad (3.230)$$

(ii) *Inverse*. The inverse of  $T_q$  is given by  $T_{1/q}$ . Indeed,

$$T_{1/q} * T_q = T_q * T_{1/q} = T_1. \quad (3.231)$$

(iii) *Commutativity*. This transformation is commutative. Indeed

$$T_q * T_{q'} = T_{q'} * T_q. \quad (3.232)$$

(iv) *Associativity*. This transformation is associative. Indeed

$$T_q * (T_{q'} * T_{q''}) = (T_q * T_{q'}) * T_{q''} \equiv T_q * T_{q'} * T_{q''}. \quad (3.233)$$

(v) *Closure*. Indeed

$$T_q * T_{q'} = T_{qq'}. \quad (3.234)$$

In other words, the set of transformations  $\{T_q\}$  constitutes an Abelian continuous group.

Two more properties deserve to be stated.

(vi) *Certainty is a fixed point* of the transformation. Indeed, if one of the possible states has probability  $p$  equal to unity, hence all the others have probability zero, the same happens with  $P$ .

(vii) *Equal probabilities is a fixed point* of the transformation. Indeed, if  $p_i = 1/W (\forall i)$ , then (and only then)  $P_i = 1/W (\forall i)$ .

We have seen in the previous Subsection that the most convenient manner<sup>20</sup> for performing the optimization of the entropy is to express the constraints as

<sup>20</sup> We have said “the most convenient manner,” and not “the manner,” because, as we have already seen in the previous Subsection, the calculation can be done through various equivalent paths. For example, optimizing  $S_q$  with fixed  $\langle O \rangle_q$  is equivalent to optimizing  $S_{2-q}$  with fixed  $\langle O \rangle_1 \equiv \langle O \rangle$  [325]. Both optimizations yield one and the same result, in this case,  $p_i \propto e_q^{-\bar{\beta} O_i}$ , where  $\bar{\beta}$  is univocally determined by using the constraint (3.235). This freedom is kind of reminiscent of the freedom one has in quantum mechanics, where we can equivalently include the time-dependence

$q$ -expectation values, i.e., through the escort distributions. So, if we have an observable  $O$  whose possible values are  $\{O_i\}$ , the associated constraint is to be written as

$$\langle O \rangle_q \equiv \sum_{i=1}^W P_i O_i = O_q , \quad (3.235)$$

where  $O_q$  is a *known finite quantity*.

Regretfully, it is not yet totally transparent what is the geometrical/probabilistic reason which makes it convenient to express the constraints as  $q$ -expectation values. We do know, however, a set of properties that surely are directly related to this elusive reason. Let us next list some of them that are particularly suggestive.

(i) The derivative of  $e_q^x$  is *not* the same function (unless  $q = 1$ ), but  $(e_q^x)^q$ . This simple property makes naturally appear  $P_i$  instead of  $p_i$  in the steepest descent method developed in [227].

(ii) The conditional entropy (3.41) naturally appears as a  $q$ -expectation value, without involving *any* optimizing operation.

(iii) The norm constraint involves the quantity  $\sum_{i=1}^W p_i$  with  $p_i \propto 1/[1 + (q - 1)\bar{\beta}E_i]^{1/(q-1)}$ . A case, which frequently appears, concerns  $W \rightarrow \infty$ , with  $E_i$  increasingly large with increasing  $i$ . In such a case, we have that  $p_i \propto 1/E_i^{1/(q-1)}$  for *high* values of  $E_i$ . Therefore,  $q$  must be such that  $\sum_{i=i_0}^{\infty} E_i^{-1/(q-1)}$  is *finite*, where  $i_0$  is some value of the index  $i$ . Equivalently, in the continuous limit,  $q$  must be such that

$$\int_{constant}^{\infty} dE g(E) E^{-1/(q-1)} < \infty , \quad (3.236)$$

where  $g(E)$  is the density of states. A typical case is  $g(E) \propto E^\delta$  in the  $E \rightarrow \infty$  limit. In such a case, the theory is mathematically well posed if  $1/(q - 1) - \delta > 1$ , i.e., if

$$q < \frac{2 + \delta}{1 + \delta} . \quad (3.237)$$

For the simplest case, namely for  $\delta = 0$ , this implies  $q < 2$ .

Let us make the same analysis for the constraint  $U_q = [\sum_{i=1}^W p_i^q E_i]/[\sum_{j=1}^W p_j^q]$ . Under the same circumstances analyzed just above, we must have the finiteness of  $\int_{constant}^{\infty} dE g(E) E^{-q/(q-1)}$ . But this equals  $\int_{constant}^{\infty} dE g(E) E^{-1/(q-1)}$ . Consequently, remarkably enough, we arrive to the *same* condition (3.236)! In other words, the *entire theory* is valid up to an *unique* value of  $q$ , namely that which guarantees condition (3.236). This nice property disappears if we impose the constraint

either in the eigenvectors (Schroedinger representation) or in the operators (Dirac representation), or even partially in both (Heisenberg representation).

using the standard expectation value. If we do that, the energy mean value diverges for a value of  $q$  *different (smaller in fact)* than that at which the norm diverges.

(iv) An interesting analysis was recently done [259,260] which exhibited that the relative entropy  $I_q(p, p^{(0)})$  that we introduced in Section 3.4 is directly associated with differences of free energies calculated with the  $q$ -expectation values (i.e., ordinary expectation values but using  $\{P_i\}$  instead of  $\{p_i\}$ ), whereas some different specific relative entropy is directly associated with differences of free energies calculated with the ordinary expectation values (i.e., just using  $\{p_i\}$ ). Then they show that  $I_q(p, p^{(0)})$  satisfies three important properties that the other relative entropy violates. The first of these properties is to be *jointly convex* with regard to either  $p$  or  $p^{(0)}$ . The second of these properties is to be *composable*. And the third of these properties is to satisfy the Shore–Johnson axioms [261] for the principle of minimal relative entropy to be *consistent as a rule of statistical inference*. It is then concluded in [259] that these arguments select the  $q$ -expectation values, and exclude the ordinary expectation values whenever we wish to use the entropy  $S_q$ . These arguments clearly are quite strong. Some further clarification would however be welcome. Indeed, stated in this strong sense, there would be contradiction with the arguments presented in [60, 323], which lead to the conclusion that the various existing formulations of the optimization problem using  $S_q$  are mathematically equivalent, in the sense that they can be transformed one into the other (as long as all the involved quantities are finite, of course).

(v) It has been shown in various systems that the theory based on  $q$ -expectation values exhibits thermodynamic stability (see, for instance, [318, 319, 321, 496]).

(vi) The Beck–Cohen superstatistics [384] (see Chapter 6) is a theory which generalizes nonextensive statistics, in the sense that its stationary state distribution contains the  $q$ -exponential one as a particular case. In order to go one step further along the same line, i.e., for this approach to become a statistical mechanics with a possible connection to thermodynamics, it also needs to have a corresponding entropy. This step was accomplished in [263, 264, 396] by generalizing the entropy  $S_q$ . But it became clear in this extension that generalizing the entropy was not enough: the mathematical form of the energy constraint had to be generalized as well. To be more precise, in order to make some contact with the macroscopic level, the only solution that was found was to simultaneously generalize the entropy *and* the form of the constraint. This fact suggests of course that, from an information-theoretical standpoint, it is kind of natural to generalize not only the entropic functional but *also* the expression of the constraints.

(vii) Let us anticipate that, in the context of the  $q$ -generalization of the central limit theorem that we present later on, a natural generalization emerges for the Fourier transform. This is given, for  $q \geq 1$ , by

$$F_q[p](\xi) \equiv \int_{-\infty}^{\infty} dx e_q^{i x \xi [p(x)]^{q-1}} p(x), \quad (3.238)$$

where  $p(x)$  can be a distribution of probabilities. We immediately verify that

$$F_q[p](0) = 1, \quad (3.239)$$

and

$$\left[ \frac{dF_q[p](\xi)}{d\xi} \right]_{\xi=0} = i \int_{-\infty}^{\infty} dx x [p(x)]^q. \quad (3.240)$$

As we see, it is the numerator of the  $q$ -mean value, and *not* that of the standard mean value, which emerges naturally. As we shall see in due time, Eqs. (3.239) and (3.240) are the two first elements of an infinite set of finite values which, within some restrictions, appear to uniquely determine the distribution  $p(x)$  itself.

(viii) Last but not least, let us rephrase property (iii) in very elementary terms. We assume that we have the simple case of a stationary-state  $q$ -exponential distribution  $p(x) \propto e_q^{-\beta x}$  ( $x \geq 0$ ). The characterization of a distribution such as this one involves *two* important numbers, namely the *decay exponent*  $1/(q - 1)$  of the tail, and the overall *width*  $1/\beta$  of the distribution. It must be so for any value of  $q < 2$  (upper bound for the existence of a norm). We easily verify that the standard mean value of  $x$  diverges in the region  $3/2 \leq q < 2$ , and it is therefore useless for characterizing the width of the distribution. The  $q$ -mean value instead is finite and uniquely determined by the width  $1/\beta$  up to  $q < 2$ . In other words, the *robust* information about the width of the distribution is provided precisely through the escort distribution.

### 3.8 About Universal Constants in Physics

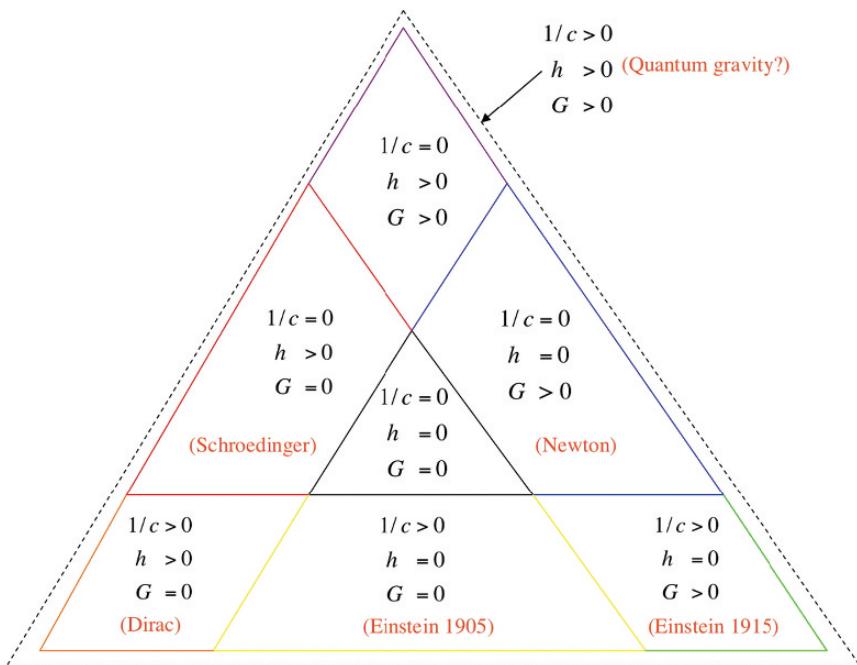
I would mention at this place a point which epistemologically remains kind of mysterious. We shall exhibit and further comment that, *for any value of the entropic index  $q \neq 1$  and all systems*, the stationary-state energy distribution within nonextensive statistical mechanics becomes that of *BG* statistical mechanics in the limit of vanishing inverse Boltzmann constant  $1/k_B$ . The physical interpretation of this property is, in my opinion, quite intriguing and unavoidably reminds the facts such as quantum mechanics becoming Newtonian mechanics in the limit of vanishing  $\hbar$ , special relativity becoming once again Newtonian mechanics in the limit of vanishing  $1/c$ , and general relativity recovering the Newtonian flat space-time in the limit of vanishing  $G$ . While we may say that, for these three mechanical examples, the corresponding physical interpretations are kind of reasonably well understood (see Fig. 3.22), it escapes to equally clear perception what kind of subtle informational meaning could be attributed to  $1/k_B$  going to zero while  $q$  is kept fixed at an arbitrary value. The meaning of the four universal constants  $\hbar$ ,  $c$ ,  $G$ ,  $k_B$  has been addressed by G. Cohen–Tannoudji in terms of *physical horizon* [801] (see also [802]).

If we assume  $k = k_B$  in Eq. (3.21), and cancel it on both sides, we obtain

$$S_q(A + B) = S_q(A) + S_q(B) + \frac{1 - q}{k_B} S_q(A) S_q(B). \quad (3.241)$$

As we see, we go back to the  $BG$  situation if  $(1 - q)/k_B = 0$ . This can occur in two different manners, namely either  $q = 1 (\forall k_B^{-1})$  or  $k_B^{-1} = 0 (\forall q)$ . In this sense, any departure from the  $BG$  entropic composition law is equivalent to a departure from  $k_B^{-1} \neq 0$ .

In thermal equilibrium (as well as in other stationary states)  $k_B$  always appears coupled together with the temperature  $T$  in the form  $k_B T$ . In other words, small values for  $k_B^{-1}$  is equivalent to the high temperature limit. It seems reasonable to think that this connection is not unrelated to the fact that, for small  $(k_B T)^{-1}$ , the  $BG$  canonical and grand-canonical ensembles asymptotically recover the micro-canonical ensemble. The same happens for Bose–Einstein and Fermi–Dirac quantum statistics, in fact for all statistics [101] which unifies the standard quantum ones. Even more, the same happens for all  $q$ -statistics if we take into account the property  $e_q^x \sim 1 + x$ , for  $x \rightarrow 0$  and *all values of  $q$* . In other words, for  $(q - 1)/k_B T \rightarrow 0$ , *all*



**Fig. 3.22** Physical structure at the  $1/k_B = 0$  plane. The full diagram involves 4 universal constants, and would be a tetrahedron. At the center of the tetrahedron we have the case  $c^{-1} = h = G = k_B^{-1} = 0$ , and the overall tetrahedron corresponds to  $1/c > 0, h > 0, G > 0, 1/k_B > 0$  (statistical mechanics of quantum gravity).

the stationary-state statistics that we are focusing on asymptotically exhibit confluence onto a single behavior, namely that corresponding to the *BG* microcanonical ensemble, which corresponds to *even* occupancy of the admissible phase-space. But even occupancy is associated to a Lebesgue measure which essentially factorizes into the Lebesgue measures corresponding to the various degrees of freedom. In other words, it corresponds to independence. The connection ends by recalling that the appropriate entropy for probabilistically independent subsystems precisely is  $S_{BG}$ , i.e.,  $q = 1$ . So, from the entropic viewpoint, the  $k_B^{-1}$  plane represented in Fig. 3.22 equivalently corresponds to  $q = 1$ . Out of this plane, in some subtle sense, we start having information corresponding to nontrivially correlated subsystems.

In this context, it is interesting to focus again on Eq. (3.43). It is precisely the existence of the extra term that enables [262], for special correlations, to recover the Clausius entropy thermodynamical extensivity  $S_q(A + B) \sim S_q(A) + S_q(B)$  for large systems  $A$  and  $B$ .

Let us close this digression about the physical universal constants by focusing on the fact that all known constants used in contemporary physics can be expressed in terms of units of *length*, *time*, *mass*, and *temperature*. Equivalently, each of them can be expressed as a pure number multiplied by some combination of powers of  $c^{-1}$ ,  $h$ ,  $G$ , and  $k_B^{-1}$ . No further reduction below *four* universal constants is possible in contemporary physics. This point is however quite subtle, as can be seen in [308–311]. It is related to the fact that any fundamental discovery tends to reduce the number of units that are necessary to express the physical quantities. For example, in ancient times, there were independent units for *area* and *length*. The situation changed when it became clear that, in Euclidean geometry, an area can be expressed as the square of a length.

Consistently with the above, Planck introduced [312, 831] four natural units for *length*, *mass*, *time*, and *temperature*, namely

$$\text{unit of length} = \sqrt{\frac{hG}{c^3}} = 4.13 \times 10^{-33} \text{ cm} \quad (3.242)$$

$$\text{unit of mass} = \sqrt{\frac{hc}{G}} = 5.56 \times 10^{-5} \text{ g} \quad (3.243)$$

$$\text{unit of time} = \sqrt{\frac{hG}{c^5}} = 1.38 \times 10^{-43} \text{ s} \quad (3.244)$$

$$\text{unit of temperature} = \frac{1}{k_B} \sqrt{\frac{hc^5}{G}} = 3.50 \times 10^{32} \text{ }^\circ\text{K}. \quad (3.245)$$

There is no need to add to this list the elementary electric charge  $e$ . Indeed, it is related to the already-mentioned constants through the *fine-structure constant*  $\alpha \equiv 2\pi e^2/hc = 1/137.035999\dots$

### 3.9 Various Other Entropic Forms

For simplicity, we shall assume  $k = 1$  in all the following definitions.

The *Renyi entropy* is defined as follows [108]:

$$S_q^R \equiv \frac{\ln \sum_{i=1}^W p_i^q}{1-q} = \frac{\ln[1 + (1-q)S_q]}{1-q}. \quad (3.246)$$

The *Curado entropy* is defined as follows [120]:

$$S_b^C \equiv \sum_{i=1}^W (1 - e^{-bp_i}) + e^{-b} - 1 \quad (b \in \mathbb{R}; b > 0). \quad (3.247)$$

The entropy introduced in [383], and which we shall from now on refer to as *exponential entropy*, is defined as follows:

$$S^E = \sum_{i=1}^W p_i \left(1 - e^{\frac{p_i-1}{p_i}}\right). \quad (3.248)$$

The *Anteneodo–Plastino entropy* is defined as follows [121]:

$$S_\eta^{AP} \equiv \sum_{i=1}^W \left[ \Gamma\left(\frac{\eta+1}{\eta}, -\ln p_i\right) - p_i \Gamma\left(\frac{\eta+1}{\eta}\right) \right] \quad (\eta \in \mathbb{R}; \eta > 0), \quad (3.249)$$

where

$$\Gamma(\mu, t) \equiv \int_t^\infty dy y^{\mu-1} e^{-y} = \int_0^{e^{-t}} dx (-\ln x)^{\mu-1} \quad (\mu > 0) \quad (3.250)$$

is the *complementary incomplete Gamma function*, and  $\Gamma(\mu) = \Gamma(\mu, 0)$  is the *Gamma function*.

The *Landsberg–Vedral–Rajagopal–Abe entropy*, or just *normalized  $S_q$  entropy*, is defined as follows [397, 398]:

$$S_q^{LVRA} \equiv S_q^N \equiv \frac{S_q}{\sum_{i=1}^W p_i^q} = \frac{1 - \left[ \sum_{i=1}^W p_i^q \right]^{-1}}{1-q} = \frac{S_q}{1 + (1-q)S_q}. \quad (3.251)$$

The so-called *escort entropy* is defined as follows [60]:

$$S_q^E \equiv \frac{1 - \left[ \sum_{i=1}^W p_i^{1/q} \right]^{-q}}{q-1} = \frac{1 - [1 - \frac{1-q}{q} S_{1/q}]^{-q}}{q-1}. \quad (3.252)$$

The *Kaniadakis entropy*, also called the  $\kappa$ -*entropy*, is defined as follows [399]:

**Table 3.10** Comparative table of selected properties of selected entropies (with  $k = 1$ ):  $S_{BG} = -\sum_{i=1}^W p_i \ln p_i$  [1, 5, 25],  $S_q$  is given by Eq. (3.18) [39], the Renyi entropy  $S_q^R$  is given by Eq. 3.246 [108], the Landsberg–Vedral–Rajagopal–Abe (or *normalized*) entropy  $S_q^{LVRA}$  is given by Eq. (3.251) [397, 398], and the escort entropy  $S_q^E$  is given by Eq. (3.252) [60]. A **NO** appears to make the entropy unacceptable for thermodynamical purposes; not necessarily so a NO. The  $q$ -exponential function ( $q$ -exp) has a cutoff for  $q < 1$ , and an asymptotic power-law for  $q > 1$ . By “special global correlations” we mean such that  $W_{eff}(N) \propto N^\rho$  ( $\rho > 0$ ). The additivity of  $S_{BG}$  and  $S_q^R$  guarantees their extensivity for standard correlations, i.e., those which generically yield  $W_{eff}(N) \propto \mu^N$  ( $\mu > 1$ ). The non-concavity of  $S_q^R$ ,  $S_q^{LVRA}$ , and  $S_q^E$  is illustrated in Fig. 3.7 (for  $S_q^E$  see also [61]). By (–) we mean that it has not been addressed in detail

ENTROPY	$S_{BG}$	$S_q$	$S_q^R$	$S_q^{LVRA}$	$S_q^E$
Additive ( $\forall q \neq 1$ )	YES	NO	YES	NO	NO
$q < 1$ exists such that $S$ is extensive for special global correlations	NO	YES	NO	NO	YES
Concave ( $\forall q > 0$ )	YES	YES	NO	NO	NO
Lesche-stable ( $\forall q > 0$ )	YES	YES	NO	NO	–
$q < 1$ exists such that entropy production per unit time is finite	YES	YES	NO	NO	–
$\hat{S}$ exists, $\forall q \neq 1$ , such that $\hat{S}$ and $S = \langle \hat{S} \rangle$ obey, for independent systems, the same composition law	YES	YES	NO	NO	–
$\hat{S}$ exists, $\forall q \neq 1$ , such that $\hat{S}(\hat{\rho}^{-1})$ has the same functional form as $S(p_i = 1/W)$	YES	YES	NO	NO	–
Same functional form for both $Z_q(\beta F_q)$ and $[Z_q p(\beta E_i)]$ , $\forall q \neq 1$	YES	YES	NO	NO	–
Optimizing distribution, $\forall q \neq 1$	exp	$q$ -exp	$q$ -exp	$q$ -exp	$q$ -exp

$$S_\kappa^K \equiv - \sum_{i=1}^W p_i \ln_\kappa^K p_i , \quad (3.253)$$

with

$$\ln_\kappa^K \equiv \frac{x^\kappa - x^{-\kappa}}{2\kappa} \quad (\ln_0^K x = \ln x) . \quad (3.254)$$

We straightforwardly verify that

$$\lim_{q \rightarrow 1} S_q = \lim_{q \rightarrow 1} S_q^R = \lim_{q \rightarrow 1} S_q^N = \lim_{q \rightarrow 1} S_q^E = \lim_{\eta \rightarrow 1} S_\eta^{AP} = \lim_{\kappa \rightarrow 0} S_\kappa^K = S_{BG} . \quad (3.255)$$

We can also verify that each of  $S_q$ ,  $S_q^R$ , and  $S_q^N$  is a monotonic function of each one of the others. Therefore, under the same constraints, they yield *one and the same extremizing probability distribution*. Indeed, optimization is preserved through monotonicity. Not so, by the way, for concavity, convexity, and other properties. For various comparisons, see Figs. 2.1, 3.6, 3.7, 3.8, and Table 3.10.

Many other extensions of the classical BG entropy are available in the literature that follow along related lines: see for instance [186–189, 383, 396, 400, 401].

**Part II**

**Foundations or Why the Theory Works**

# Chapter 4

## Stochastic Dynamical Foundations of Nonextensive Statistical Mechanics

*Si l'action n'a quelque splendeur de liberté, elle n'a point de grâce ni d'honneur*

Montaigne, *Essais*

### 4.1 Introduction

In this chapter we focus on *mesoscopic*-like nonlinear dynamical systems, in the sense that the time evolution explicitly includes, in addition to deterministic ingredients, *stochastic noise*.

A paradigmatic path in statistical physical systems is as follows. We assume the knowledge of the Hamiltonian of a classical or quantum many-body system. This is referred to as the *microscopic* level or *microscopic* description. If the system is classical, the time evolution is given by Newton's law  $\mathbf{F} = m \mathbf{a}$ , and is therefore completely *deterministic*. The equations of motion of the system are completely determined by the Hamiltonian and the initial conditions. However, it is in general tremendously difficult to solve the corresponding equations. So, as a simpler alternative, Langevin introduced the following *phenomenological* approach. We focus on *one* molecule or element of the system, and its motion is described in terms of the combination of two ingredients. The first ingredient is *deterministic*, coming typically from the existence of a possible external potential acting on the entire system, as well as from the average action of all the other molecules or elements. The second ingredient is *stochastic*, introduced in an *ad hoc* manner into the equations as a *noise*. This noise represents the rapidly fluctuating effects of the rest of the system onto the single molecule we are observing. This level and the associated description are referred to as the *mesoscopic* ones, and the basic equation is of course the *Langevin equation* (as well as the Kramers equation, of similar nature). The time evolution is determined by the initial conditions and the particular stochastic sequence. When we conveniently average over many initial conditions and many stochastic sequences [29], we obtain a probabilistic description of the system. More precisely, we obtain the time evolution of its probability distribution in the phase-space of the system. The basic equation is the so-called *Fokker–Planck equation*, or, for quantum and discrete systems, the *master equation* (whose continuous limit

recovers the Fokker–Planck equation). Finally, at a larger scale, we enter into the thermodynamical description, i.e., the level referred to as the *macroscopic* one. Statistical mechanics bridges from the microscopic level up to the macroscopic one.

For pedagogical reasons, we first discuss the Fokker–Planck-like equations (Sections 4.2, 4.3, and 4.4), and then the Langevin-like equations (Section 4.5). It is only in the next chapter that we focus on the microscopic level, with its deterministic equations.

## 4.2 Normal Diffusion

The basic equation of normal diffusion is the so-called *heat equation*, first introduced by Fourier. It is given, for  $d = 1$ , by

$$\frac{\partial p(x, t)}{\partial t} = D \frac{\partial^2 p(x, t)}{\partial x^2} \quad (D > 0), \quad (4.1)$$

where  $D$  is the *diffusion coefficient*. Let us assume the simplest initial condition, namely

$$p(x, 0) = \delta(x), \quad (4.2)$$

where  $\delta(x)$  is Dirac's delta distribution. The corresponding solution is given by

$$p(x, t) = \frac{1}{\sqrt{2\pi Dt}} e^{-x^2/2Dt} \quad (t \geq 0). \quad (4.3)$$

We can verify that

$$\int_{-\infty}^{\infty} dx p(x, t) = 1 \quad (t \geq 0), \quad (4.4)$$

and that

$$\langle x^2 \rangle \equiv \int_{-\infty}^{\infty} dx x^2 p(x, t) = Dt. \quad (4.5)$$

This corresponds to what is normally referred to as *normal diffusion*. Many types of functions  $\langle x^2 \rangle(t)$  exist (see, for instance, [265, 266]). But a very frequent one is

$$\langle x^2 \rangle \propto t^\mu \quad (\mu \geq 0), \quad (4.6)$$

where  $x$  can be a  $d$ -dimensional quantity (and not necessarily the simple  $d = 1$  case that we are focusing here). Diffusion is said *normal* or *anomalous* for  $\mu = 1$  or  $\mu \neq 1$ , respectively. If  $\mu < 1$  we have *subdiffusion* (*localization* implies  $\mu = 0$ );

if  $\mu > 1$  we have *superdiffusion* (the particular case  $\mu = 2$  is also called *ballistic diffusion*).<sup>1</sup>

### 4.3 Lévy Anomalous Diffusion

Equation (4.1) can be generalized as follows

$$\frac{\partial p(x, t)}{\partial t} = D_\gamma \frac{\partial^\gamma p(x, t)}{\partial |x|^\gamma} \quad (D_\gamma > 0; 0 < \gamma < 2), \quad (4.7)$$

where we have introduced fractional derivatives (see, for instance, [267–270]). The solution corresponding to the initial condition (4.2) is given by [340, 341]

$$p(x, t) = (D_\gamma t)^{1/\gamma} L_\gamma(x/(D_\gamma t)^{1/\gamma}) \quad (t \geq 0), \quad (4.8)$$

where  $L_\gamma(z)$  is the Lévy distribution with index  $\gamma$ . It follows that  $\mu = 2/\gamma$ , hence  $\mu > 1$ . Therefore this case is a superdiffusive one, in a quite strong sense in fact. Indeed, the corresponding variance, i.e.  $\langle z^2 \rangle$ , diverges. An illustration of this can be seen for the Cauchy–Lorentz distribution  $L_1(z) = \frac{1}{\pi(1+z^2)}$ . We remind that  $L_\gamma(z)$  is given by the Fourier transform of  $e^{-z|k|^\gamma}$  (see, for instance, [340] and references therein). Connections between the Lévy distributions and  $S_q$  have been discussed in the literature [338, 339, 342, 344, 345].

### 4.4 Correlated Anomalous Diffusion

Let us consider a different generalization of (4.1), namely [348, 349]

$$\frac{\partial p(x, t)}{\partial t} = D \frac{\partial^2 [p(x, t)]^\nu}{\partial x^2} \quad (\nu \in \mathbb{R}). \quad (4.9)$$

This nonlinear equation is sometimes referred to as the *Porous medium equation* [346, 347], and has already been applied to various physical systems (see, for instance, references in [349]). In order to easily make the junction with nonextensive concepts, let us define

$$q \equiv 2 - \nu, \quad (4.10)$$

and rewrite Eq. (4.9) as follows:

<sup>1</sup> A more general definition is sometimes used. It concerns the frequent cases where  $x$  scales like  $t^{\mu/2}$ . Once again  $\mu > 1$ ,  $\mu = 1$ , and  $\mu < 1$  correspond respectively to superdiffusion, normal diffusion, and subdiffusion. The point is that  $x$  scaling like  $t^{\mu/2}$  is necessary but not sufficient for having a *finite* value of  $\langle x^2 \rangle$  scaling like  $t^\mu$ .

$$\begin{aligned} \frac{\partial p(x, t)}{\partial t} &= D_q \frac{\partial^2 [p(x, t)]^{2-q}}{\partial x^2} \\ &= (2 - q) D_q \frac{\partial}{\partial x} \left\{ [p(x, t)]^{1-q} \frac{\partial p(x, t)}{\partial x} \right\} \\ &\quad (q \in \mathbb{R}; (2 - q)D_q > 0). \end{aligned} \quad (4.11)$$

Its solution for the initial condition (4.2) is given by

$$p_q(x, t) = p_q(x/[D_q t]^{\frac{1}{3-q}}), \quad (4.12)$$

where

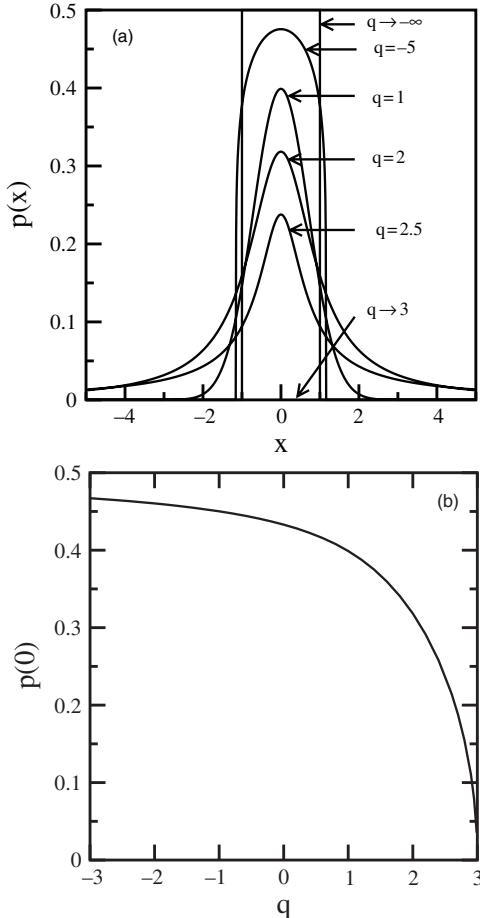
$$p_q(x) = \frac{1}{\sqrt{\pi A_q}} e_q^{-x^2/A_q} = \frac{1}{\sqrt{\pi A_q}} \frac{1}{\left[1 + (q-1)\frac{x^2}{A_q}\right]^{\frac{1}{q-1}}}, \quad (4.13)$$

with

$$A_q = \begin{cases} \frac{\sqrt{q-1}\Gamma(\frac{1}{q-1})}{\Gamma(\frac{3-q}{2(q-1)})} & \text{if } 1 < q < 3, \\ 2 & \text{if } q = 1, \\ \frac{\sqrt{1-q}\Gamma(\frac{5-3q}{2(1-q)})}{\Gamma(\frac{2-q}{1-q})} & \text{if } q < 1. \end{cases} \quad (4.14)$$

See Fig. 4.1. See the text for several remarks.

- i. The upper bound  $q = 3$  arrives from the imposition of normalization. In other words,  $\int_{-\infty}^{\infty} dx p_q(x)$  diverges if  $q \geq 3$ , and converges otherwise.
- ii. If  $1 \leq q < 3$ , these distributions have an infinite support. If  $q < 1$ , they have a compact support; indeed, for  $q < 1$ , they vanish for  $|x| > \sqrt{A_q/(1-q)}$ .
- iii. The variance  $\langle x^2 \rangle \equiv \int_{-\infty}^{\infty} dx x^2 p_q(x)$  of these distributions is *finite* for  $q < 5/3$  and *divergent* for  $5/3 \leq q < 3$ . This implies that, if we convolute them  $N$  times with  $N \rightarrow \infty$ , they approach a Gaussian distribution for  $q < 5/3$  and a Lévy distribution for  $5/3 < q < 3$ . This corresponds to independence between the  $N$  random variables. The situation is completely different if strong correlation exists between them. We focus on this interesting case later on, when  $q$ -generalizing the Central Limit Theorem.
- iv. The  $q$ -variance  $\langle x^2 \rangle_q \equiv \{\int_{-\infty}^{\infty} dx x^2 [p_q(x)]^q\}/\{\int_{-\infty}^{\infty} dx [p_q(x)]^q\}$  of these distributions is *finite* for  $q < 3$ . Indeed,  $\int_{constant > 0}^{\infty} dx x^2 x^{-2q/(q-1)}$  is finite for  $q < 3$ .
- v. These distributions extremize (maximize for  $q > 0$ , and minimize for  $q < 0$ )  $S_q$  under the appropriate constraints (see Section 3.5.2).



**Fig. 4.1** (a) Distributions  $p_q(x)/\sqrt{\beta}$  vs.  $\sqrt{\beta}x$  for typical values of  $q$ , [ $\beta = 1/(3 - q)$ ] (b) Values of  $p_q(0)/\sqrt{\beta}$  as a function of  $q$ .

- vi. If  $q = \frac{3+m}{1+m}$  where  $m$  is a positive integer, these distributions recover the Student's *t-distributions* with  $m$  degrees of freedom.<sup>2</sup> If  $q = \frac{n-6}{n-4}$  where  $n > 4$  is a positive integer, these distributions recover the so-called *r-distributions* [271].
- vii. The relation  $q \leftrightarrow (2 - q)$  existing between the nonlinearity of the Fokker-Planck-like equation and its  $q$ -exponential solution is remarkable.

<sup>2</sup> In the financial literature, these  $q$ -Gaussian distributions with  $q > 1$  emerge quite frequently ( $p(x) \propto 1/(a^2 + x^2)^\eta$  with  $\eta > 0$ ). They are referred to as Student's distributions for *any* real value of  $\eta \equiv 1/(q - 1)$ . Strictly speaking, this is an abusive notation.

- viii.  $x$  scales with  $t^{1/(3-q)}$ . Consequently, if  $\langle x^2 \rangle$  is finite (i.e., if  $q < 5/3$ ), it must be

$$\langle x^2 \rangle \propto t^{\frac{2}{3-q}}. \quad (4.15)$$

By using Eq. (4.6), we obtain

$$\mu = \frac{2}{3-q}. \quad (4.16)$$

Analogously we have that

$$\langle x^2 \rangle_q \propto t^{\frac{2}{3-q}} \quad (q < 3). \quad (4.17)$$

Consequently, we have superdiffusion for  $1 < q < 3$  (ballistic for  $q = 2$ ), and subdiffusion for  $q < 1$  (localization for  $q \rightarrow -\infty$ ).

- ix. We see that  $D_q > 0$  ( $D_q < 0$ ) if  $q < 2$  ( $2 < q < 3$ ). The  $q \rightarrow 2$  limit deserves a special comment. Equation (4.11) can be re-written in the following form [272, 273, 275]:

$$\frac{\partial p(x, t)}{\partial t} = (2-q)D_q \frac{\partial^2}{\partial x^2} \left[ \frac{[p(x, t)]^{2-q} - 1}{2-q} \right]. \quad (4.18)$$

In the limit  $q \rightarrow 2$ , this equation becomes

$$\frac{\partial p(x, t)}{\partial t} = \left\{ \lim_{q \rightarrow 2} [(2-q)D_q] \right\} \frac{\partial^2}{\partial x^2} \ln p(x, t), \quad (4.19)$$

with  $\left\{ \lim_{q \rightarrow 2} [(2-q)D_q] \right\} > 0$ . This equation is known to have as solution the Cauchy–Lorentz distribution (more precisely,  $p_2(x, t)$ ).

In the presence of an external drift, Eq. (4.11) is extended as follows [348, 349]:

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} [F(x)p(x, t)] + D_q \frac{\partial^2[p(x, t)]^{2-q}}{\partial x^2}, \quad (4.20)$$

where  $F(x) = -dV/dx$  is an external force associated with the potential  $V(x)$ . We shall consider the simple case where

$$F(x) = k_1 - k_2 x \quad (k_2 \geq 0); \quad (4.21)$$

$k_2 = 0$  corresponds to the important case of external constant force, and  $k_1 = 0$  corresponds to the Uhlenbeck–Ornstein process. For this simple force, it is possible to find the analytical solution of the equation. It is given by [349]

$$p_q(x, t) = \frac{\{1 - (1-q)\beta(t)[x - x_M(t)]^2\}^{1/(1-q)}}{Z_q(t)}, \quad (4.22)$$

with

$$\frac{\beta(0)}{\beta(t)} = \left[ \frac{Z_q(t)}{Z_q(0)} \right]^2 = \left[ \left(1 - \frac{1}{K_2}\right) e^{-t/\tau} + \frac{1}{K_2} \right]^{\frac{2}{3-q}}, \quad (4.23)$$

where

$$K_2 \equiv \frac{k_2}{2(2-q)D_q \beta(0)[Z_q(0)]^{q-1}}, \quad (4.24)$$

and

$$\tau \equiv \frac{1}{k_2(3-q)}. \quad (4.25)$$

To close this discussion, let us mention that it can be straightforwardly shown that

$$\int dx p_q(x, t) = 1, \forall t \geq 0. \quad (4.26)$$

(x) Lévy distributions asymptotically satisfy

$$L_\gamma(x) \propto \frac{1}{|x|^{1+\gamma}} \quad (|x| \rightarrow \infty; 0 < \gamma < 2), \quad (4.27)$$

whereas  $q$ -Gaussians asymptotically satisfy

$$p_q(x) \propto \frac{1}{|x|^{2/(q-1)}} \quad (|x| \rightarrow \infty; 1 < q < 3). \quad (4.28)$$

If we identify the exponents of these two power laws we obtain

$$\gamma = \begin{cases} 2 & \text{if } q \leq 5/3, \\ \frac{3-q}{q-1} & \text{if } 5/3 < q < 3, \end{cases} \quad (4.29)$$

where we have used the above remark (iii), i.e., that, if  $q < 5/3$ , there is no possible comparison between  $L_\gamma(x)$  and  $p_q(x)$  (see Fig. 4.2).

The above  $d = 1$  connection can be straightforwardly generalized to the isotropic  $d$ -dimensional case. In that case, we have, for  $|\mathbf{x}| \rightarrow \infty$ ,  $L_\gamma(\mathbf{x}) \propto 1/|\mathbf{x}|^{d+\gamma}$  (hence

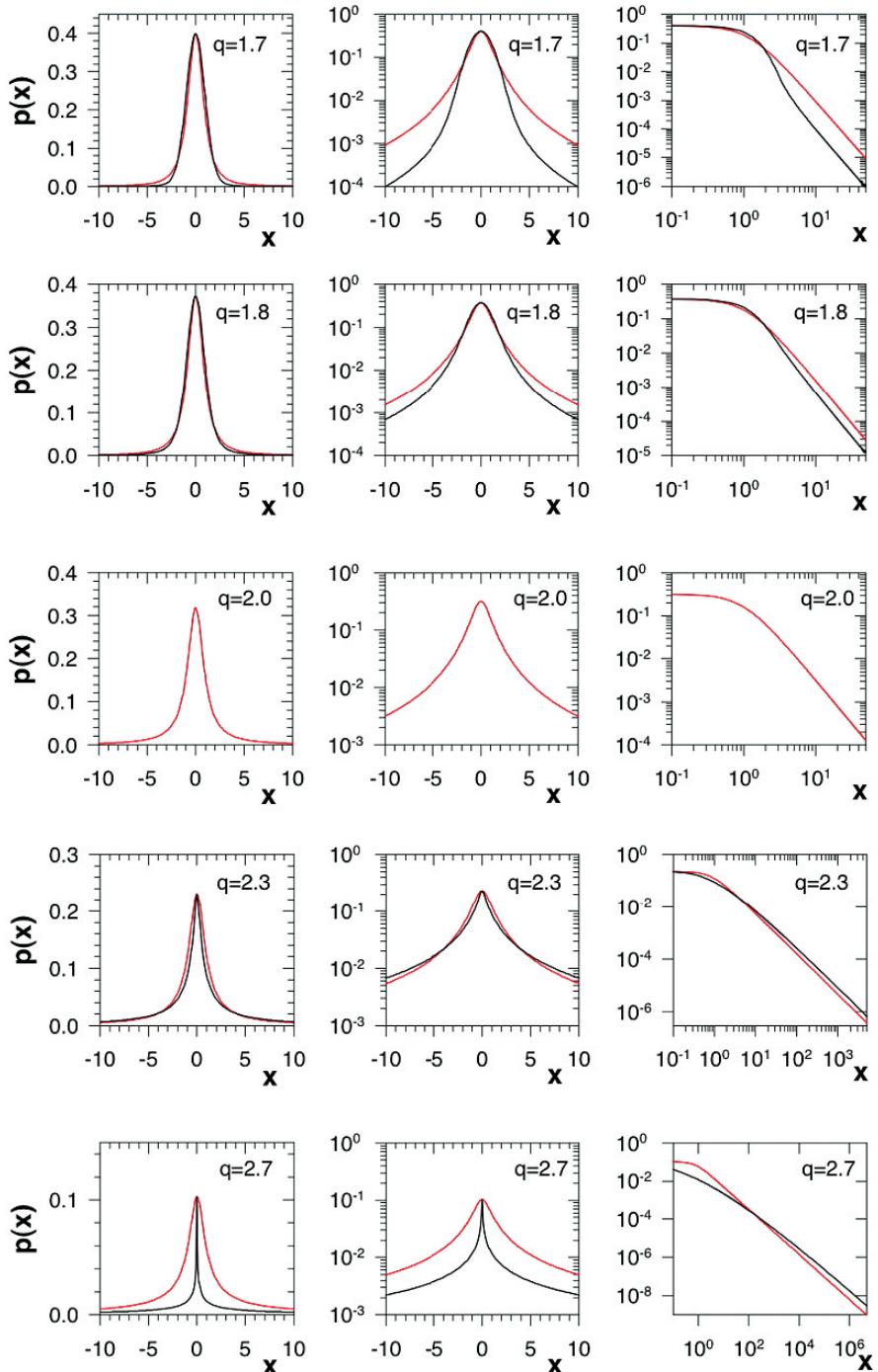


Fig. 4.2 (continued).

$L_\gamma(|\mathbf{x}|) \propto |\mathbf{x}|^{d-1}/|\mathbf{x}|^{d+\gamma} = 1/|\mathbf{x}|^{1+\gamma}$  and  $p_q(\mathbf{x}) \propto 1/|\mathbf{x}|^{2/(q-1)}$ , where  $\mathbf{x}$  is a  $d$ -dimensional variable. By identifying the exponents we obtain

$$\gamma = \begin{cases} 2 & \text{if } q \leq \frac{4+d}{2+d}, \\ \frac{2}{q-1} - d & \text{if } \frac{4+d}{2+d} < q < \frac{2+d}{d}, \end{cases} \quad (4.30)$$

where we have taken into account that  $p_q(\mathbf{x})$  is normalizable only if  $q < \frac{2+d}{d}$ , and that its variance is finite only if  $q < \frac{4+d}{2+d}$ . The particular instance  $\gamma = 1$  corresponds to the distribution of the radial component  $|\mathbf{x}|$  of the  $d$ -dimensional Cauchy–Lorentz distribution (proportional to  $1/(a^2 + |\mathbf{x}|^2)$ ,  $a$  being a constant). The value  $q = (3+d)/(1+d)$  precisely leads to  $\gamma = 1$ . Similarly, when  $q$  approaches  $(2+d)/d$  from below,  $\gamma$  approaches zero from above. The similarities and differences between Lévy distributions and  $q$ -Gaussians are illustrated in Fig. 4.2.

#### 4.4.1 Further Generalizing the Fokker–Planck Equation

Equation (4.1) can of course be generalized even more, as follows:

$$\frac{\partial^\beta p(x, t)}{\partial |t|^\beta} = D_{\beta, \gamma, q} \frac{\partial^\gamma [p(x, t)]^{2-q}}{\partial |x|^\gamma} \quad (0 < \beta \leq 1; 0 < \gamma \leq 2). \quad (4.31)$$

This equation contains Eqs. (4.7) and (4.11) as particular cases. No general solution of Eq. (4.31) is yet known to the best of our knowledge. However, a solution for its  $\beta = 1$  particular case is available [826]. We shall not discuss it here, but we shall make, in what follows, some considerations regarding this case.

## 4.5 Stable Solutions of Fokker–Planck–Like Equations

For  $\beta = 1$ , Eq. (4.31) becomes

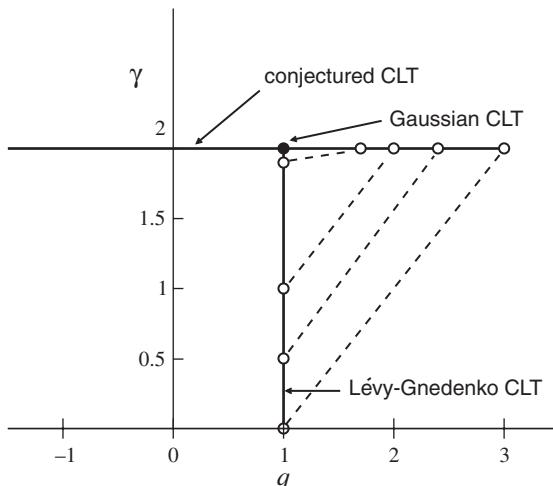
$$\frac{\partial p(x, t)}{\partial t} = D_{\gamma, q} \frac{\partial^\gamma [p(x, t)]^{2-q}}{\partial |x|^\gamma} \quad (0 < \gamma \leq 2; q < 3). \quad (4.32)$$

◀   
**Fig. 4.2** (continued) Lévy distributions  $L_\gamma(x) \equiv \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \cos kx e^{-\alpha|k|^\gamma}$ , with  $0 < \gamma < 2$  and  $\alpha > 0$  (black curves), and  $q$ -Gaussians  $P_q(x) \equiv [1 - (1-q)\beta x^2]^{1/(1-q)}/Z_q$ , with  $5/3 < q < 3$ ,  $\beta > 0$  and  $Z_q = \sqrt{\frac{\pi}{\beta(q-1)}} \Gamma(\frac{3-q}{2(q-1)})/\Gamma(\frac{1}{q-1})$  (red curves). Parameters  $(q, \gamma)$  are related through  $q = \frac{\gamma+3}{\gamma+1}$  so that the tails of both distributions decay with the same power-law exponent. Without loss of generality, we have taken  $\beta = 1$  which corresponds to a simple rescaling;  $\alpha$  was chosen such that  $P_q(0) = L_\gamma(0)$ . Notice that, in log–log representation, Lévy distributions may have an inflection point, whereas this never occurs for  $q$ -Gaussians (from [585]).

This equation has four classes of solutions (see Fig. 4.3) which provide interesting hints.

First of all, the *Gaussian class*, corresponding to  $q = 1$  and  $\gamma = 2$ . Its basic solution is, as already shown, a Gaussian. This corresponds to the *standard Central Limit Theorem (G-CLT)*. This theorem essentially states that, if we add (or arithmetically average)  $N$  random variables, that are probabilistically *independent* and have *finite variance*, then the distribution of the sum approaches, after appropriate centering and rescaling, a *Gaussian* when  $N \rightarrow \infty$ .

Second, the *Lévy class*, or  $\alpha$ -*class* (with  $\alpha \equiv \gamma$ ), corresponding to  $q = 1$  and  $0 < \gamma < 2$ . Its basic solutions are, as already discussed, Lévy distributions (also called  $\alpha$ -*stable distributions*). This corresponds to the *Lévy–Gnedenko Central Limit Theorem (L-CLT)*. This theorem essentially states that, if we add (or arithmetically average)  $N$  random variables, that are probabilistically *independent* and have *infinite variance* (due to fat tails of the power-law class, excepting for possible logarithmic corrections; see, for instance, [340] and references therein), then the



**Fig. 4.3** Localization in the  $(q, \gamma)$ -space of the standard and Lévy–Gnedenko CLTs, as well as of the conjectural  $q$ -generalized CLT (based on [191]). The schematic dashed lines are curves that share the *same* exponent of the power-law behavior that emerges in the limit  $|x| \rightarrow \infty$ . At the  $q = 1$  axis, we have Lévy distributions which asymptotically decay as  $1/|x|^{1+\gamma}$ , and at the  $\gamma = 2$  axis, we have  $q$ -Gaussians which decay as  $1/|x|^{2/(q-1)}$ . The connection is therefore given by  $q = (\gamma + 3)/(\gamma + 1)$  for  $2 > \gamma > 0$ , hence  $5/3 < q < 3$  (see [338, 339, 341–343], based on [344, 345]). For instance, the dashed line which joins the  $(q, \gamma)$  points  $(1, 1)$  and  $(2, 2)$  schematically indicates those solutions of Eq. (4) which asymptotically decay as  $1/x^2$ , and the dashed line joining  $(1, 1/2)$  and  $(7/3, 2)$  indicates those solutions which decay as  $1/|x|^{3/2}$ . The dot slightly to the right of the point  $(5/3, 2)$  is joint to the point slightly below  $(1, 2)$ .

distribution of the sum approaches, after appropriate centering and rescaling, a *Lévy distribution* when  $N \rightarrow \infty$ .

Third, we have the class (from now on referred to as the  *$q$ -Gaussian class*) corresponding to  $\gamma = 2$  and  $q \neq 1$ . Its basic solutions are, as already discussed,  *$q$ -Gaussians*. And these solutions are *stable* in the sense that, if we start with an arbitrary (symmetric) solution  $p(x, 0)$ , it asymptotically approaches a  *$q$ -Gaussian*. This has been numerically verified and analytically proved in [272–274]. As we shall see, a generalized Central Limit Theorem (noted  *$q$ -G-CLT* or just  *$q$ -CLT*) can be established for this situation. It corresponds to the violation of the hypothesis of *independence*. Not a weak violation with correlations that gradually disappear in the  $N \rightarrow \infty$  limit, but a certain class of global correlations which persist up to infinity. This makes sense since Eq. (4.32) is *nonlinear* for  $q \neq 1$ . The possible existence of such a theorem was first suggested in [826], specifically conjectured in [191] and finally proved in [247]. This theorem also demands the finiteness of a certain  *$q$ -variance*. If this  *$q$ -variance* diverges, then we are led to the fourth and last present class.

The fourth class (from now on referred to as the  *$(q, \alpha)$  class*) corresponds to  $\gamma \equiv \alpha < 2$  and  $q \neq 1$ . Its basic solutions are the so-called  *$(q, \alpha)$ -stable distributions* that will be described later on.

The existence of such theorems is of extreme interest. Indeed, they provide a plausible mathematical basis for the ubiquity of distributions such as the  *$q$ -Gaussians* (generically  *$q$ -exponentials*) as actually observed in many natural, artificial, and even social systems (see Chapter 7). A variety of physical situations and interesting questions related with nonlinear Fokker–Planck equations are discussed in [192–196].

## 4.6 Probabilistic Models with Correlations – Numerical and Analytical Approaches

Before addressing the above theorems and their proofs, let us present four interesting models that provide some degree of intuition on the type of correlations that are assumed within the present context. These models will be referred to as the *MTG (Moyano-Tsallis-Gell-Mann) model* [239], the *TMNT (Thistleton-Marsh-Nelson-Tsallis) model* [240], the *RST1 (Rodríguez-Schwammle-Tsallis 1) model* [244], and finally the *RST2 model* [244]. The first three are  $q \leq 1$  models; also, they are strictly scale-invariant. The fourth model is defined for both  $q < 1$  and  $q \geq 1$  cases, and it is asymptotically (but not strictly) scale-invariant. All four models numerically appear to approach, when  $N \rightarrow \infty$ ,  *$q$ -Gaussian* forms. The MTG and TMNT models do *not* do so in fact, as analytically proved in [241]. In contrast, the RST1 model *does* approach a  *$q$ -Gaussian*, as analytically proved in [244]. Also *does* (by construction) the RST2 model.

We first introduce and numerically discuss the MTG and TMNT models, and then we present their analytical solutions [241]. We present next the RST1 and RST2 models and their corresponding results [244].

### 4.6.1 The MTG Model and Its Numerical Approach

Here we follow [239]. The de Moivre–Laplace theorem is the simplest (and historically the earliest) form of the *CLT*. It consists in proving that the  $N \rightarrow \infty$  limit of the binomial distribution is, after centering and rescaling, a Gaussian. More precisely, we consider  $N$  independent and distinguishable binary variables, each of them having two equally probable states. The joint probabilities are then given by

$$r_{Nn} = \frac{1}{2^N} \quad (n = 0, 1, 2, \dots, N; N = 1, 2, \dots). \quad (4.33)$$

This set of probabilities can be reobtained by assuming

$$r_{N0} = \frac{1}{2^N} \quad (N = 1, 2, \dots), \quad (4.34)$$

and the Leibnitz rule, i.e., Eq. (3.124). We remind that this rule guarantees scale-invariance, as seen in Section 3.3.5. To avoid the Gaussian as the  $N \rightarrow \infty$  attractor, we need to introduce persistent correlations. We shall do this by generalizing Eq. (4.34) and re-written in the following form:

$$\frac{1}{r_{N0}} = \frac{1}{1/2} \times \frac{1}{1/2} \times \dots \times \frac{1}{1/2} \quad (\text{N factors}). \quad (4.35)$$

The generalization will consist in introducing the  $q$ -product as follows:

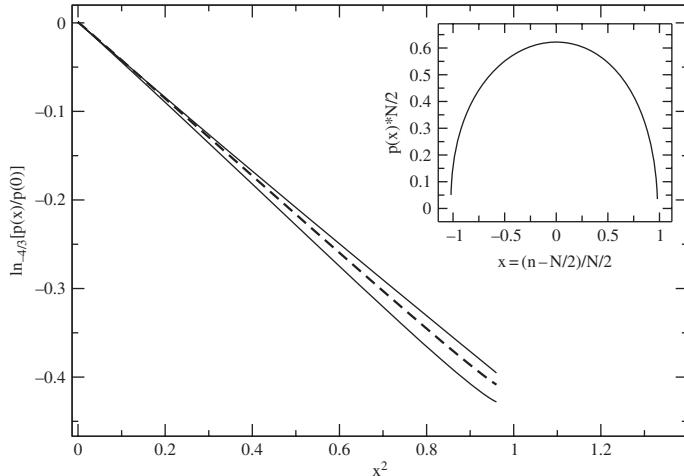
$$\frac{1}{r_{N0}} = \frac{1}{1/2} \otimes_q \frac{1}{1/2} \otimes_q \dots \otimes_q \frac{1}{1/2} = [2^{1-q} N - (N-1)]^{\frac{1}{1-q}} \quad (0 \leq q \leq 1). \quad (4.36)$$

We have generalized the product between the *inverse* probabilities, and not the probabilities themselves, in order to (conveniently) conform to the requirements of the  $q$ -product (see Eq. (3.78)). The Leibnitz rule is maintained, which enables us to calculate the entire set  $\{r_{Nn}\}$  by assuming Eq. (4.36).

If we define  $p(x) \equiv \frac{N!}{(N-n)!n!} r_{Nn}$ , and  $x \equiv \frac{n-(N/2)}{N/2}$ , we obtain the results exhibited in Figs. 4.4 and 4.5. In other words, we verify that, in the limit  $N \rightarrow \infty$ , the numerical results approach

$$p(x) = \begin{cases} p(0) e^{-\beta_+ x^2} & \text{if } x \geq 0, \\ p(0) e^{-\beta_- x^2} & \text{if } x \leq 0, \end{cases} \quad (4.37)$$

where  $\beta_+$  and  $\beta_-$  are slightly different, i.e., the distribution is slightly asymmetric. This specific asymmetry is caused by the fact that we have imposed  $r_{N0}$ , instead of say  $r_{NN}$ , or something similar. By introducing  $\beta \equiv \frac{1}{2}(\beta_+ + \beta_-)$ , we obtain the dashed line of Fig. 4.4, and the results of Fig 4.5. The index  $q_e$  in the  $q_e$ -Gaussian (*apparent – but not exact*, as we shall see! – attractor for  $N \rightarrow \infty$ ) is a function



**Fig. 4.4**  $\ln_{-4/3} \frac{p(x)}{p(0)}$  vs  $x^2$  for  $(q, p) = (3/10, 1/2)$  and  $N = 1000$ . Two branches are observed due to the asymmetry emerging from the fact that we have imposed the  $q$ -product on the left side of the triangle; we could have done otherwise. The mean value of the two branches is indicated in dashed line. It is through this mean line that we have numerically calculated  $q_e(q)$  as indicated in Fig. 4.6. In order to minimize the tiny asymmetry, we have represented a variable  $x$  slightly displaced with regard to  $\frac{n-(N/2)}{N/2}$  so that the center  $x = 0$  precisely coincides with the location of the maximum of  $p(x)$ . INSET: Linear–linear representation of  $p(x)$  (from [239]).

of the index  $q$  in the  $q$ -product (which, together with Leibnitz rule, introduces the scale-invariant correlations into the probability sets). The numbers strongly suggest (see Fig. 4.6)

$$q_e = 2 - \frac{1}{q} \quad (0 \leq q \leq 1). \quad (4.38)$$

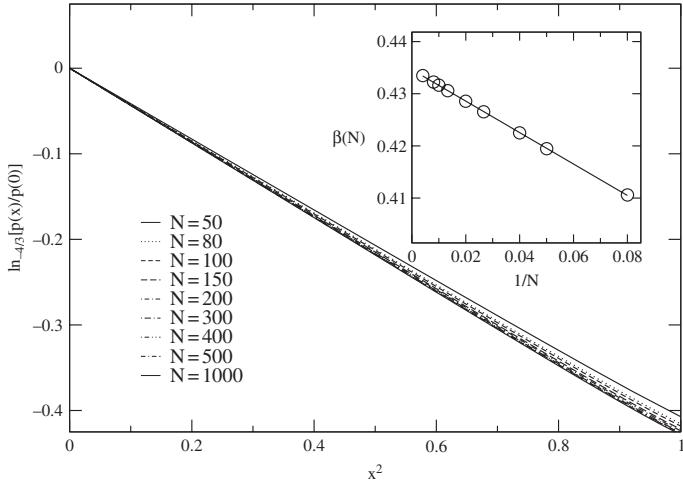
The particular case  $q = q_e = 1$  recovers of course the celebrated de Moivre–Laplace theorem. This transformation is a simple combination of the *multiplicative duality*

$$\mu(q) \equiv 1/q, \quad (4.39)$$

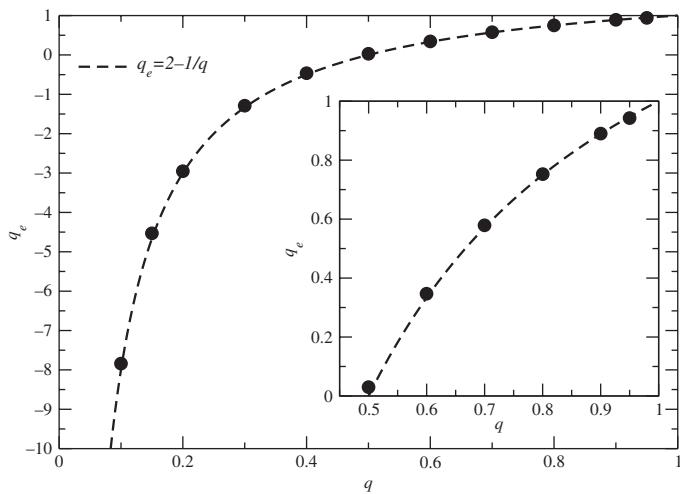
and the *additive duality*

$$v(q) \equiv 2 - q. \quad (4.40)$$

In other words, relation (4.38) can be rewritten as  $q_e = v\mu(q) \equiv v(\mu(q))$ . This relation as well as the two basic dualities appear again and again in the literature of nonextensive statistical mechanics, in very many contexts (see, for instance, [284, 417, 419, 420, 869]).



**Fig. 4.5**  $\ln_{q_e} \frac{p(x)}{p(0)}$  vs  $x^2$  for  $(q, p) = (3/10, 1/2)$  and various system sizes  $N$ . INSET:  $N$ -dependence of the (negative) slopes of the  $\ln_{q_e}$  vs  $x^2$  straight lines. We find that, for  $p = 1/2$  and  $N \gg 1$ ,  $\langle (n - \langle n \rangle)^2 \rangle \sim N^2/\beta(N) \sim a(q)N + b(q)N^2$ . For  $q = 1$  we find  $a(1) = 1$  and  $b(1) = 0$ , consistent with *normal* diffusion as expected. For  $q < 1$  we find  $a(q) > 0$  and  $b(q) > 0$ , thus yielding *ballistic* diffusion. The linear correlation factor of the  $q - \log$  vs.  $x^2$  curves range from 0.999968 up to near 0.999971 when  $N$  increases from 50 to 1000. The very slight lack of linearity that is observed could be expected to vanish in the limit  $N \rightarrow \infty$  (from [239]).



**Fig. 4.6** Relation between the index  $q$  from the  $q$ -product definition, and the index  $q_e$  resulting from the numerically calculated probability distribution. The agreement with the analytical conjecture  $q_e = 2 - \frac{1}{q}$  is remarkable. INSET: Detail for the range  $0 < q_e < 1$  (from [239]).

Transformations (4.39) and (4.40) enable the construction of an interesting algebra.<sup>3</sup> Indeed, the following properties can be easily established:

$$\mu^2 = \mathbf{1}, \quad (4.41)$$

and

$$\nu^2 = \mathbf{1}, \quad (4.42)$$

where  $\mathbf{1}$  represents the *identity*, i.e.,  $\mathbf{1}(q) = q$ ,  $\forall q$ . These properties justify the name *duality*.

We immediately verify that

$$(\mu\nu)^n (\nu\mu)^n = (\nu\mu)^n (\mu\nu)^n = \mathbf{1} \quad (n = 0, 1, 2, \dots). \quad (4.43)$$

Consistently, we may define  $(\mu\nu)^{-n} \equiv (\nu\mu)^n$  and  $(\nu\mu)^{-n} \equiv (\mu\nu)^n$ .

We verify also that, for  $z = 0, \pm 1, \pm 2, \dots$ , and  $\forall q$ ,

$$(\mu\nu)^z(q) = \frac{z - (z - 1)q}{z + 1 - zq}, \quad (4.44)$$

$$\nu(\mu\nu)^z(q) = \frac{z + 2 - (z + 1)q}{z + 1 - zq}, \quad (4.45)$$

$$(\mu\nu)^z \mu(q) = \frac{-z + 1 + zq}{-z + (z + 1)q}. \quad (4.46)$$

These three expressions have the form

$$q^* = \frac{A + Bq}{C + Dq}, \quad (4.47)$$

$q = q^* = 1$  being a fixed point, hence  $A + B = D + C$ . The constants  $A$ ,  $B$ ,  $C$ , and  $D$  generically (but not necessarily) do not vanish. In such a case, these expressions can be rewritten in the form

$$Q^* = f_\lambda(Q), \quad (4.48)$$

with

$$Q^* \equiv \frac{C}{A} q^*, \quad (4.49)$$

---

<sup>3</sup> Private discussions with M. Gell-Mann in the context of a possible understanding of the numerical values determined (for the solar wind) in [361] for the  $q$ -triplet that will be discussed in Section 5.4.4.

$$Q \equiv -\frac{B}{A} q , \quad (4.50)$$

$$\lambda \equiv -\frac{AD}{BC} , \quad (4.51)$$

and

$$f_\lambda(x) \equiv \frac{1-x}{1+\lambda x} . \quad (4.52)$$

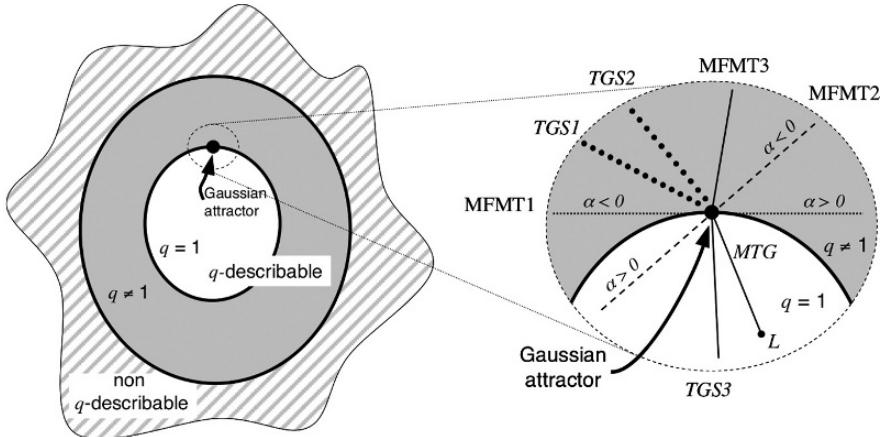
Notice that  $f_\lambda(x)$  satisfies  $f_\lambda(0) = 1$  and  $f_\lambda(1) = 0$ . It has a fixed point located at

$$Q = Q^* = \begin{cases} \frac{1}{\lambda}(\sqrt{1+\lambda} - 1) & \text{if } \lambda > 0 , \\ \frac{1}{2} & \text{if } \lambda = 0 , \\ -\frac{1}{\lambda}(1 - \sqrt{1+\lambda}) & \text{if } -1 \leq \lambda < 0 . \end{cases} \quad (4.53)$$

The function  $f_\lambda(x)$  has also a remarkable dual property, namely  $f(f(x)) = x$ , or, equivalently,  $f(x) = f^{-1}(x)$ . The physical interpretation of this property in the present context is by now unknown. Let us finally mention that, in the complex plane  $q$  and for  $AB - CD \neq 0$ , Eq. (4.47) corresponds to the conformal transformations known as the *Moebius* (or *homographic* or *fractional linear*) *transformations*.

The numerical discussion that we have provided in this subsection is restricted to  $q \leq 1$ , hence to  $q_e$ -Gaussians with  $q_e \leq 1$ . It would be most interesting to find similar arguments for  $q_e > 1$  (in this case, one should of course *avoid* to scale, after centering, the variable  $n$  in such a way that it yields a compact support, as it occurs in Figs. 4.4 and 4.5). Further related analytical and numerical results can be found in [184, 185]. These results provided a preliminary basis that reinforced the conjecture of the existence of the  $q$ -CLT.

Let us remind that, in the  $(q, \gamma)$  plane of Fig. 4.3, we have addressed four classes of CLTs. These various CLTs will be shown to correspond to classes of global correlations or absence of correlations. Two of those theorems violate the traditional hypothesis of independence of the random variables that are being summed or arithmetically averaged. In what concerns the region that simultaneously has  $q > 1$  and  $\gamma < 2$ , the attractors will be shown to be different from  $q$ -Gaussians. However, they all share asymptotic power-law behaviors for large values of  $|x|$  (see the dashed lines in Fig. 4.3). This is so for large  $t$  if we are addressing the corresponding Fokker-Planck-like equation, or large  $N$  if we are addressing the corresponding CLT. The situation is of course expected to be even richer in the  $(q, \gamma, \beta)$  space characterizing Eq. (4.31), or for different types of strong correlations [245] (see Fig. 4.7).



**Fig. 4.7** Schematic connections between various probabilistic models. From [245].

### 4.6.2 The TMNT Model and Its Numerical Approach

Here we follow [240]. This model, in contrast with the *MTG* one, concerns *continuous* random variables. Let us consider  $N$  correlated uniform random variables

$$f(x) = \begin{cases} 1 & \text{if } -1/2 \leq x \leq 1/2, \\ 0 & \text{otherwise.} \end{cases} \quad (4.54)$$

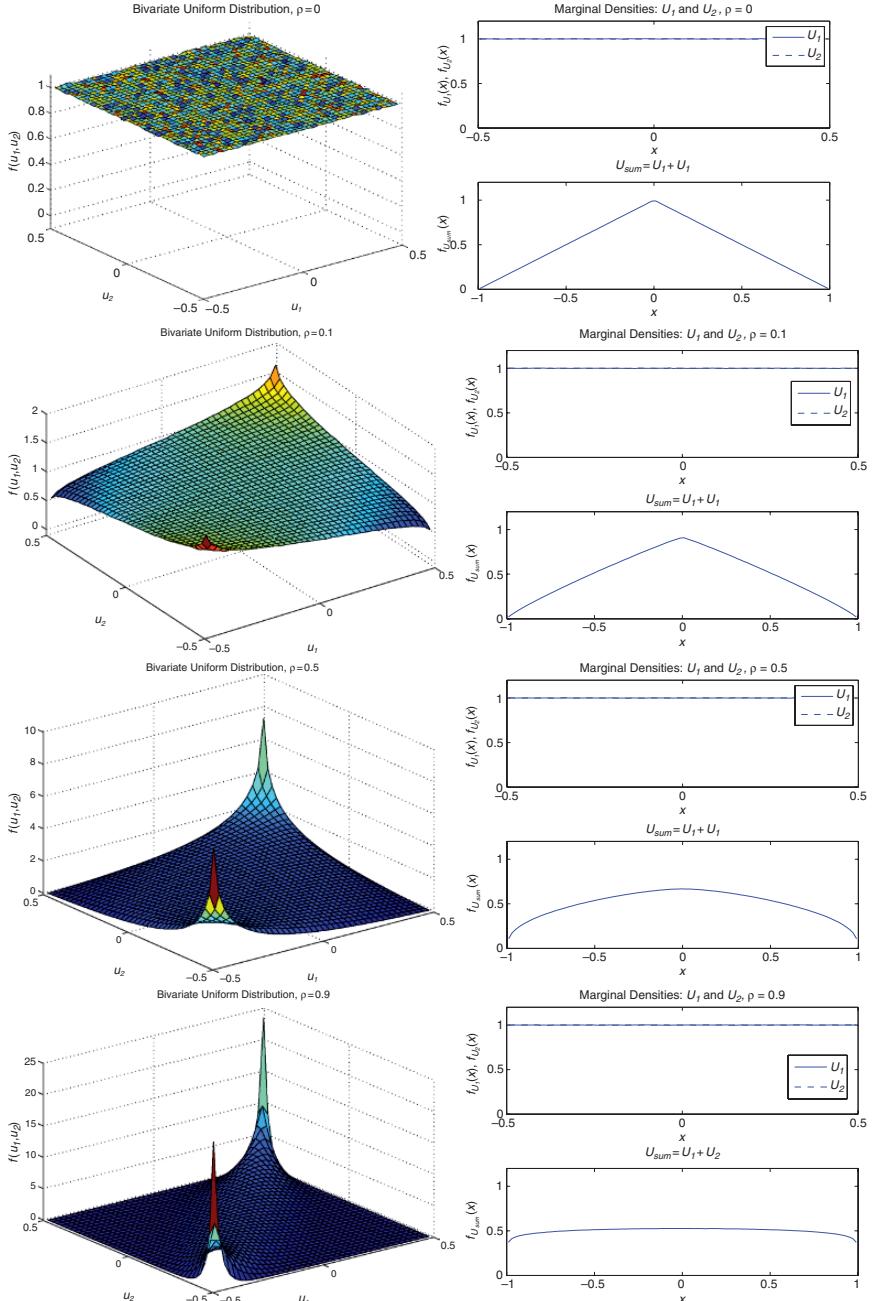
The correlation is introduced through the following multivariate Gaussian  $N \times N$  covariance matrix, using probability integral transform (component by component):

$$\begin{pmatrix} 1 & \rho & \rho & \dots & \rho \\ \rho & 1 & \rho & \dots & \rho \\ \rho & \rho & 1 & \dots & \rho \\ \dots & \dots & \dots & \dots & \dots \\ \rho & \rho & \rho & \dots & 1 \end{pmatrix} \quad (4.55)$$

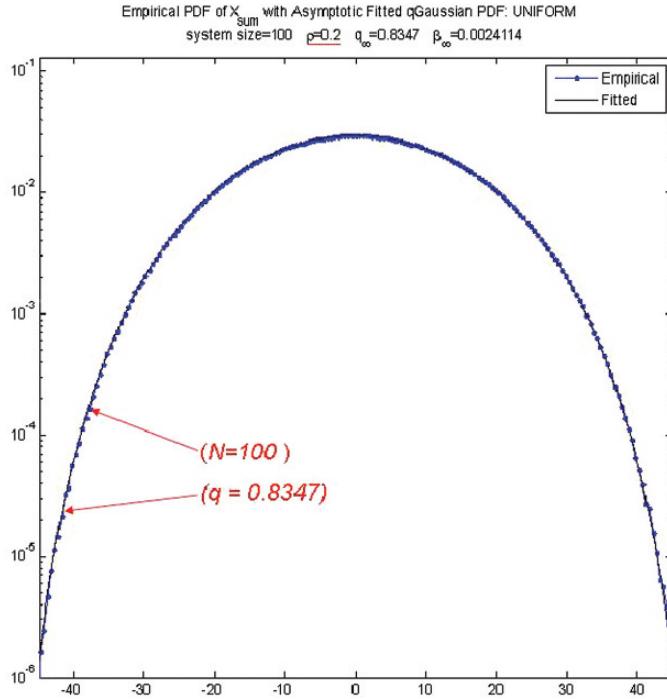
with  $-1 \leq \rho \leq 1$  ( $\rho = 0$  means *independence*;  $\rho = 1$  means *full correlation*). See Fig. 4.8 for the influence of  $\rho$  for fixed  $N$ , and Figs. 4.9 and 4.10 for the influence of  $N$  for fixed  $\rho$ . The  $N \rightarrow \infty$  limiting distribution of the sum of  $N$  random variables appears to be very well fitted by  $q$ -Gaussians with

$$q(\rho, N) = q_\infty(\rho) - \frac{A(\rho)}{N^{\delta(\rho)}}. \quad (4.56)$$

For example,  $q_\infty(0.5) \simeq 0.3545$ ,  $A(0.5) \simeq 0.5338$ , and  $\delta(0.5) \simeq 1.9535$ . We present  $q_\infty(\rho)$  in Fig. 4.11. It is well fitted by the heuristic relation



**Fig. 4.8** TMNT model for  $N = 2$  random variables with increasingly large correlation  $\rho$  ( $\rho = 0$  corresponds to independence). *Left:* Joint distribution of the two variables. *Right up:* Marginal distribution of each of the two variables. *Right bottom:* Distribution of the sum of the two variables. Notice that, whereas for  $\rho = 0$  phase-space is equally probable,  $\rho$  approaching unity concentrates the probability on only two of the four corners. Notice also that the marginal distribution does *not* depend on  $\rho$ . From [240].



**Fig. 4.9** TMNT model: Distribution of the sum of  $N = 100$  random variables with  $\rho = 0.2$ . It is remarkably well fitted by a  $q$ -Gaussian with  $q = 0.8347$  (*continuous curve*).

$$q_\infty(\rho) = \frac{1 - (5/3)\rho}{1 - \rho}. \quad (4.57)$$

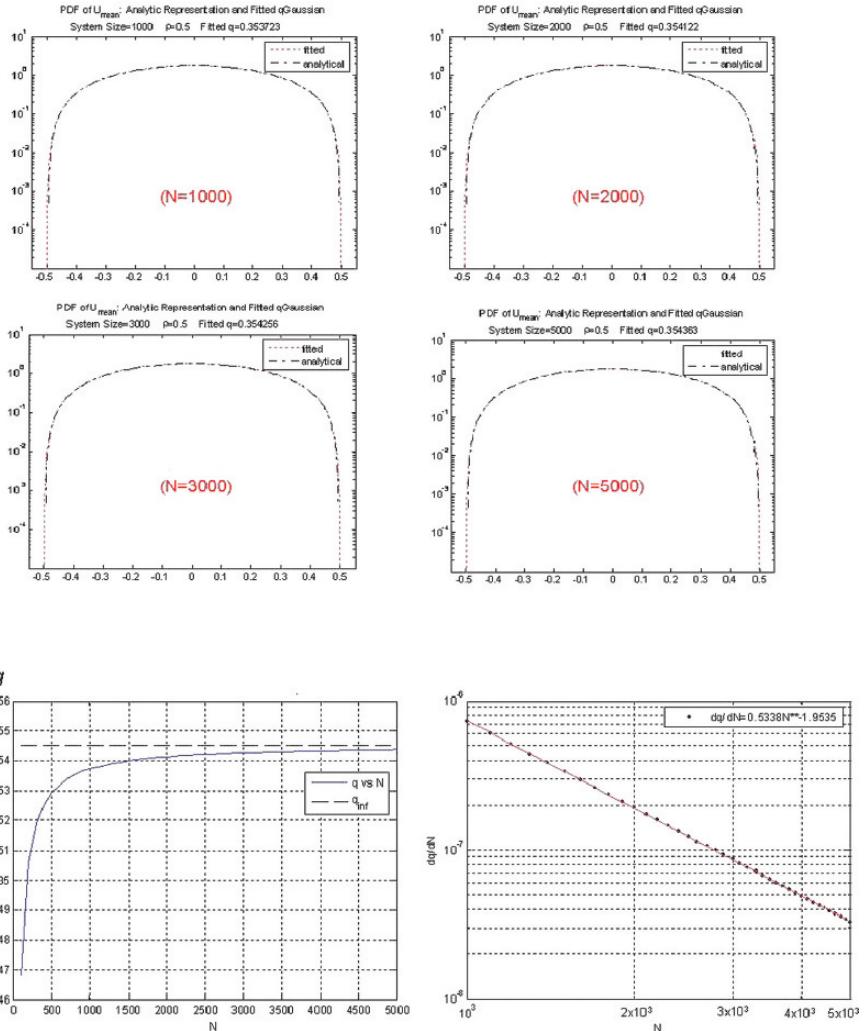
Let us now apply the present numerical approach to a model which generalizes that of matrix (4.55). We assume the following covariance matrix:

$$\begin{pmatrix} 1 & \rho(2) & \rho(3) & \dots & \rho(N) \\ \rho(2) & 1 & \rho(2) & \dots & \rho(N-1) \\ \rho(3) & \rho(2) & 1 & \dots & \rho(N-2) \\ \dots & \dots & \dots & \dots & \dots \\ \rho(N) & \rho(N-1) & \rho(N-2) & \dots & 1 \end{pmatrix} \quad (4.58)$$

with

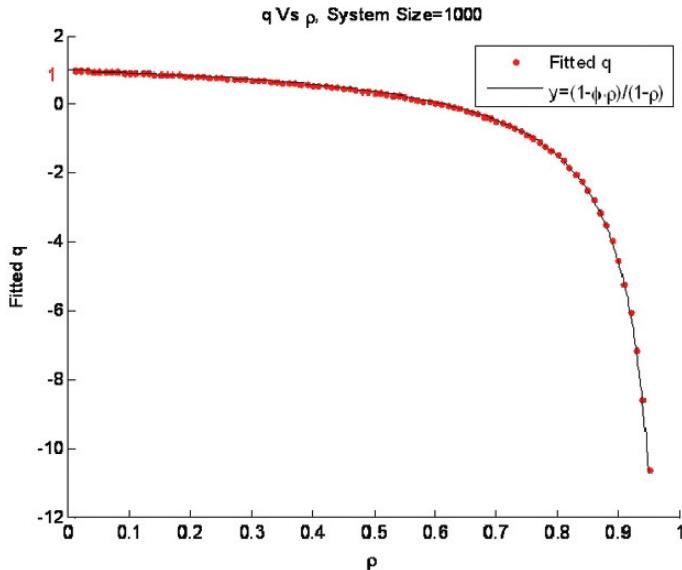
$$\rho(r) = \frac{\rho}{r^\alpha} \quad (-1 \leq \rho \leq 1; \alpha \geq 0; r = 2, 3, 4, \dots, N). \quad (4.59)$$

As in the  $\alpha = 0$  case (i.e., matrix (4.55)),  $q$ -Gaussians provide an excellent fitting. The dependence of  $q$  on  $(\rho, \alpha)$  is depicted in Fig. 4.12. This numerical result is totally consistent with what is expected in terms of the motivations of nonextensive



**Fig. 4.10** TMNT model with  $\rho = 0.5$ . *Top:* Distributions of the sum of  $N$  random variables for increasingly large values of  $N$ , and their fittings with  $q$ -Gaussians (continuous curves). *Bottom:* Influence of  $N$  on the fitting value of  $q$ . These results provide numerical support to the relation (4.56).

statistical mechanics. Indeed, for  $\rho = 0$  (independent variables) we obtain  $q = 1$ , whereas, for  $\rho \neq 0$  ( $d = 1$  system of correlated variables with periodic boundary conditions), we obtain  $q = 1$  for  $\alpha > 1$  (*short-range* correlations) and  $q \neq 1$  for  $0 < \alpha < 1$  (*long-range* correlations). This is the scenario conjectured for many-body Hamiltonian systems in the  $t \rightarrow \infty$  limit *after* the  $N \rightarrow \infty$  limit has been taken. In other words, *BG* statistical mechanics for no interactions or short-range interactions, and nonextensive statistical mechanics for long-range interactions. All



**Fig. 4.11** TMNT model: The  $\rho$ -dependence of the fitting parameter  $q_\infty$  for  $N = 1000$ . These results provide numerical support to the heuristic relation (4.57) (continuous curve, where  $\phi = 5/6$ ).

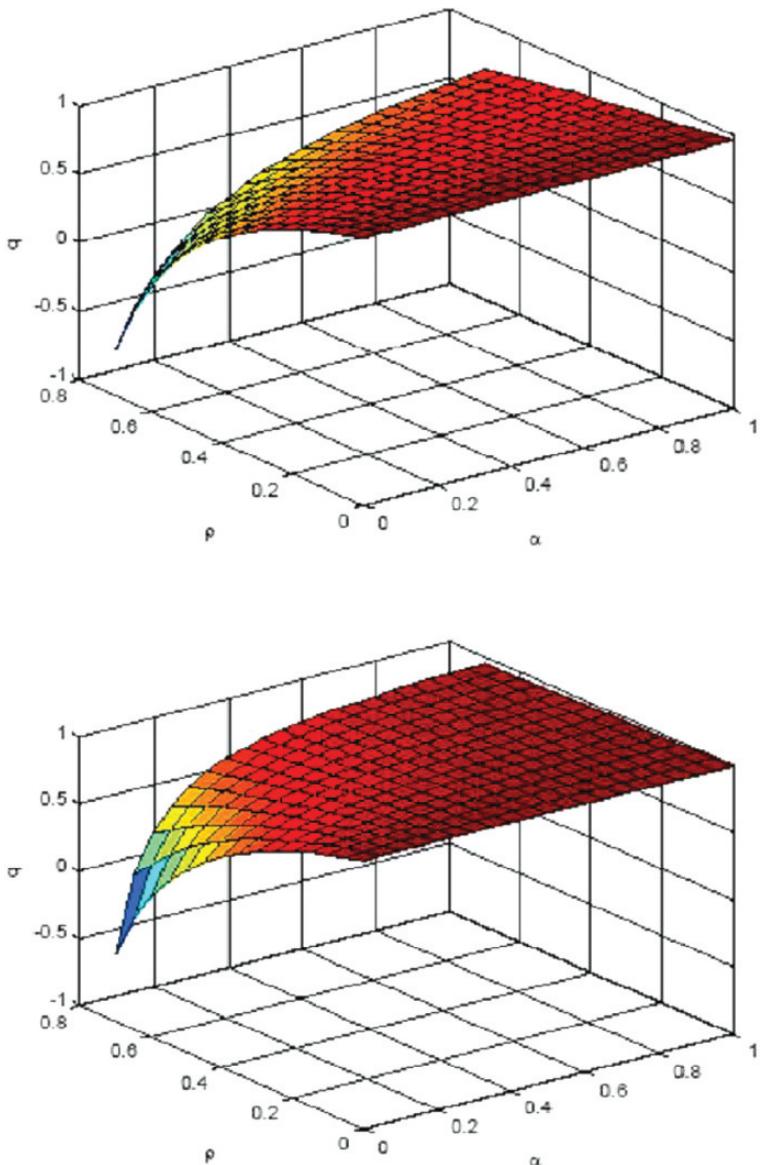
this would be just perfect, but – there is a *but!* –, as we shall show in the next subsection, the  $N \rightarrow \infty$  distributions of the *MTG* and *TMNT* probabilistic models are *not exactly*  $q$ -Gaussians, even if numerically extremely close to them.<sup>4</sup>

### 4.6.3 Analytical Approach of the MTG and TMNT Models

Here we follow [241], where the *MTG* and the  $\alpha = 0$  *TMNT* models are analytically discussed. As we shall see, the  $N \rightarrow \infty$  limiting distributions are *not*  $q$ -Gaussians, but distributions instead which numerically are *amazingly close* to  $q$ -Gaussians, although *distinctively differing from them*. It is of course trivial, – and ubiquitous in experimental, observational, and computational sciences –, the fact that a *finite* number of *finite-precision* values can *never* guarantee analytical results. History of science is full of such illustrations. Nevertheless, the present two examples are particularly instructive. Indeed, the numbers are strongly consistent with  $q$ -Gaussians. Nevertheless, the exact distributions conspire in such a way as to be numerically extremely close to  $q$ -Gaussians, and still differing from them!

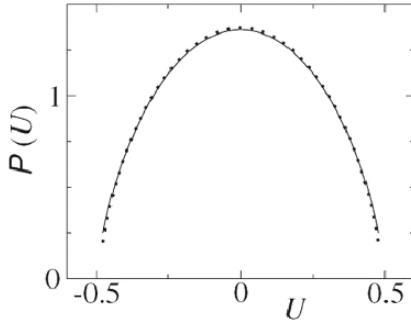
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<sup>4</sup> Anticipating the notion of *q-independence* that will soon be introduced in the context of the  $q$ -generalization of the Central Limit Theorem, this means that the  $N$  random variables introduced in the present two models are *not exactly*, but *only approximately*  $q$ -independent. If they were *exactly*  $q$ -independent, the attractors ought to *exactly* be  $q$ -Gaussians.

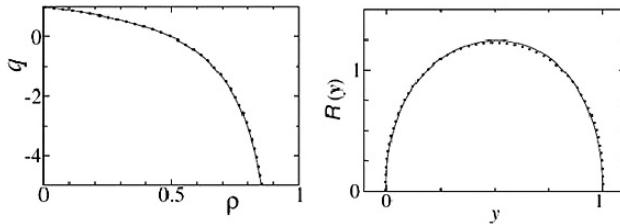


**Fig. 4.12** TMNT model: The  $(\rho, \alpha)$ -dependence of the fitting parameter  $q$  for  $N = 10$  (top) and  $N = 100$  (bottom). The  $\alpha = 0$  particular case corresponds to what is presented in Fig. 4.11. These results suggest that, in the  $N \rightarrow \infty$  limit,  $q = 1$  for  $\rho = 0$  ( $\forall \alpha$ ) as well as for  $\rho \neq 0$  and  $\alpha > 1$ ; and  $q < 1$  for  $\rho \neq 0$  and  $0 \leq \alpha < 1$ .

Let us briefly report now the analytical results in [241] (see details therein), and then discuss the possible reason for which the  $N \rightarrow \infty$  distributions do not strictly coincide, for these two models, with  $q$ -Gaussians.



**Fig. 4.13** Exact distribution (dots) for  $\rho = 7/10$  and its best  $q$ -Gaussian approximant with  $q = -5/9$  (continuous curve) (from [241]).



**Fig. 4.14** *MTG model.* *Left:* The  $\rho$ -dependence of the index  $q$  of the best  $q$ -Gaussian approximant (dots), compared to Eq. (4.63). *Right:* Exact limiting distribution for  $\rho = 7/10$  (hence  $q_{\text{correlation}} = 3/10$ ) (continuous curve), and its best  $q$ -Gaussian approximant with  $q = -4/3$  (dots) (from [241]).

Let us start with the  $\alpha = 0$  *TMNT* model. The  $N \rightarrow \infty$  distribution is given by [241]

$$P(U) = \left( \frac{2-\rho}{\rho} \right)^{1/2} \exp\left( -\frac{2(1-\rho)}{\rho} [\operatorname{erf}^{-1}(2U)]^2 \right) \quad \left( -\frac{1}{2} \leq U \leq \frac{1}{2} \right). \quad (4.60)$$

Clearly, this distribution is not a  $q$ -Gaussian, even if numerically it is amazingly close to it: see Fig. 4.13. If we approximate it by the best  $q$ -Gaussian (by imposing the matching of the second and fourth moments), we obtain for  $q$  precisely the conjectural Eq. (4.57)!

Let us address now the *MTG* model. The  $N \rightarrow \infty$  distribution is given by [241]

$$R(y) = A_\rho^{-1} (1-y)^{a_\rho} [-\ln(1-y)]^{(1-\rho)/\rho} \quad (0 \leq y \leq 1), \quad (4.61)$$

$$a_\rho \equiv \frac{2-2^\rho}{2^\rho-1}, \quad (4.62)$$

$A_\rho$  being a normalizing constant. Once again, this distribution is not a  $q$ -Gaussian, even if numerically it is very close to it: see Fig. 4.14. If we approximate it by the best  $q$ -Gaussian (by imposing the matching of the second and fourth moments), we obtain

$$q \simeq \frac{1 - 2\rho}{1 - \rho}. \quad (4.63)$$

Through the identification  $\rho \equiv 1 - q_{correlation}$ , this relation becomes

$$q \simeq 2 - \frac{1}{q_{correlation}}, \quad (4.64)$$

which, with the notation change  $(q_{correlation}, q) \rightarrow (q, q_e)$ , recovers the conjectural Eq. (4.38)!

Further understanding is obviously needed. Why these two strictly scale-invariant models (*MTG* and *TMNT*) are *so close* to  $q$ -Gaussians?, and why they do *not* precisely coincide with them? Work is presently under progress in order to solve this open problem.

#### 4.6.4 The RST1 Model and Its Analytical Approach

In Table 3.7, we have the celebrated Leibnitz triangle (merged in fact with the Pascal triangle). It satisfies the recursive relation (3.124). Consequently, it is completely determined by the marginal coefficient

$$r_{N,0}^{(1)} = \frac{1}{N+1} \quad (N = 1, 2, 3, \dots). \quad (4.65)$$

Let us now generalize this triangle by still imposing relation (3.124), and nevertheless generalizing Eq. (4.65) as follows [244]:

$$\begin{aligned} r_{N,0}^{(1)} &= \frac{1}{N+1}, \\ r_{N,0}^{(2)} &= \frac{2 \cdot 3}{(N+2)(N+3)}, \\ r_{N,0}^{(3)} &= \frac{3 \cdot 4 \cdot 5}{(N+3)(N+4)(N+5)}, \\ r_{N,0}^{(v)} &= \frac{v \cdots (2v-1)}{(N+v) \cdots (N+2v-1)} = \frac{(2v-1)!(N+v-1)!}{(v-1)!(N+2v-1)!}. \end{aligned} \quad (4.66)$$

We verify that,  $\forall v$ ,  $\lim_{N \rightarrow 0} r_{N,0}^{(v)} = 1$ , and that  $r_{N,0}^{(v)} \sim \frac{(2v-1)!}{(v-1)! N^v}$  ( $N \rightarrow \infty$ ). Also,  $\lim_{v \rightarrow \infty} r_{N,0}^{(v)} = \frac{1}{2^N}$ . As an example, the  $v = 2$  triangle (merged with the Pascal triangle) is indicated in Table 4.1.

It has been analytically shown [244] that, after appropriate centering and scaling, the  $N \rightarrow \infty$  limit of these distributions is exactly a  $q$ -Gaussian with

**Table 4.1** Merging of the Pascal triangle (the set of all *left* members) with the  $v = 2$  triangle (the set of all *right* members) associated with  $N$  equal subsystems

$(N = 0)$	$(1, 1)$						
$(N = 1)$	$(1, \frac{1}{2})$	$(1, \frac{1}{2})$					
$(N = 2)$	$(1, \frac{3}{10})$	$(2, \frac{1}{5})$	$(1, \frac{3}{10})$				
$(N = 3)$	$(1, \frac{1}{5})$	$(3, \frac{1}{10})$	$(3, \frac{1}{10})$	$(1, \frac{1}{5})$			
$(N = 4)$	$(1, \frac{1}{7})$	$(4, \frac{2}{35})$	$(6, \frac{3}{70})$	$(4, \frac{2}{35})$	$(1, \frac{1}{7})$		

$$q = \frac{v - 2}{v - 1} = 1 - \frac{1}{v - 1}. \quad (4.67)$$

Also, if we associate  $\sigma_i = \pm 1$  ( $i = 1, 2, \dots, N$ ) with the  $N$  random variables, we can easily obtain (in addition to  $\langle \sigma_i \rangle = 0, \forall i$ ) the following interesting result:

$$\langle \sigma_i \sigma_j \rangle = \frac{1}{2v + 1} \quad (\forall i \neq j; \forall N). \quad (4.68)$$

As expected, for the case of independence, i.e., when  $v \rightarrow \infty$ , the correlation vanishes.

This model, such as the MTG and TMNT ones, is strictly scale-invariant. But, in variance with those two, it asymptotically approaches a  $q$ -Gaussian.<sup>5</sup>

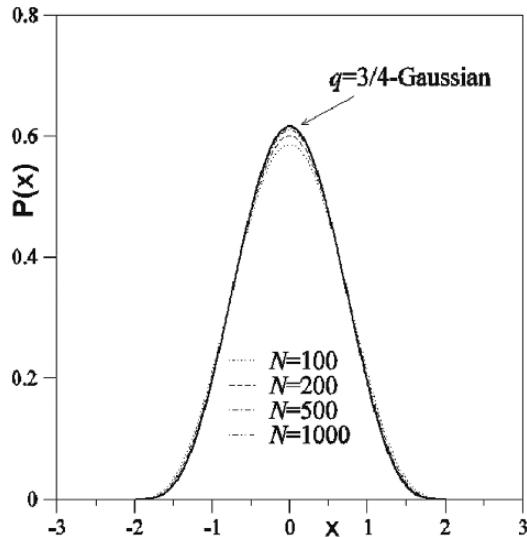
#### 4.6.5 The RST2 Model and Its Numerical Approach

We shall now define a model by discretizing (symmetrically) a  $q$ -Gaussian into  $(N + 1)$  values (identified by  $n = 0, 1, 2, \dots, N$ ) [244]. These values can be interpreted as the probabilities corresponding to  $N$  equal and distinguishable binary random variables. This model, referred to as the RST2 one, will approach *by construction* the  $q$ -Gaussian that has been discretized (in fact, two slightly different discretizations have been used). The interest of such a model is of course not its limit (since this is imposed), but *how* the limit is approached for increasingly large values of  $N$ . The relation (3.124) corresponds to strict scale-invariance. We can numerically (and in some cases analytically) follow the ratio

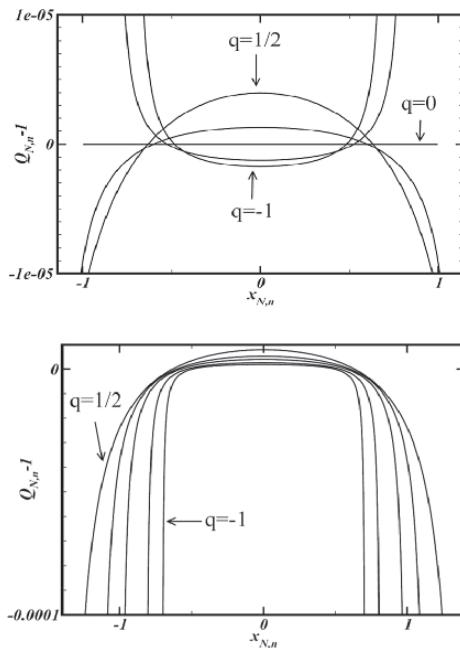
$$Q_{N,n} \equiv \frac{r_{N,n}}{r_{N+1,n} + r_{N+1,n+1}}. \quad (4.69)$$

We verify that  $Q_{N,n}$  tends to 1 (or equivalently  $(Q_{N,n} - 1) \rightarrow 0$ ) as  $N$  increases, i.e., the model is asymptotically scale-invariant. Note that  $Q_{0,0} = Q_{1,0} = Q_{1,1} = 1$  for arbitrary values of  $r_{0,0}$ ,  $r_{1,n}$ , and  $r_{2,n}$ . See Figs. 4.15, 4.16, and 4.17.

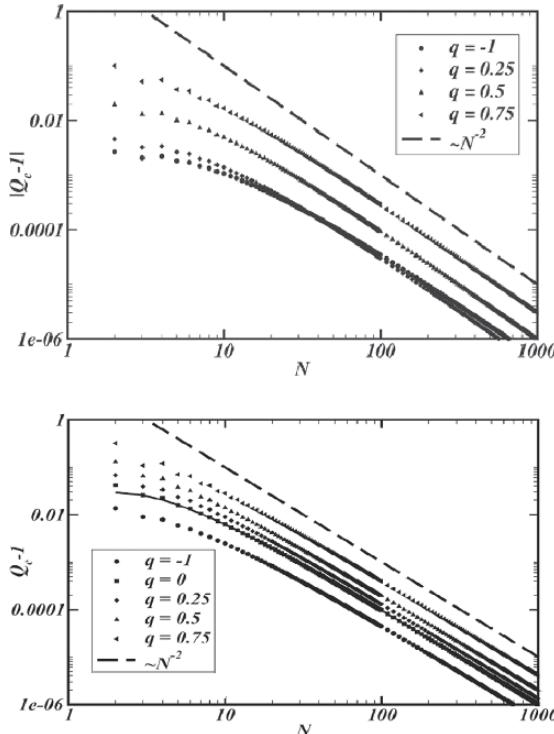
<sup>5</sup> Using the Laplace-de Finetti representation, the present RST1 model has been recently extended to *real* values of  $q$ , both above and below unity [R. Hanel, S. Thurner and C. Tsallis, *Scale-invariant correlated probabilistic model yields q-Gaussians in the thermodynamic limit* (2008), preprint].



**Fig. 4.15** Successive discretizations (with typical values of  $N$ ) of a  $q = 3/4$   $q$ -Gaussian (from [244]).



**Fig. 4.16**  $Q_{N,n} - 1$  as a function of  $n$  for  $N = 500$  and different values of  $q = -1, -1/2, 0, 1/4, 1/2$  for discretizations D1 (top) and D2 (bottom). Strict scale invariance is observed for  $q = 0$  and discretization D1 (from [244]).



**Fig. 4.17**  $Q_c - 1 = Q_{N,N/2} - 1$  as a function of  $N$  for different values of  $q$  for discretizations D1 (top) and D2 (bottom). The power law has exponent  $-2$  (from [244]).

## 4.7 Central Limit Theorems

The standard and Lèvy–Gnedenko central limit theorems (*CLT*) are  $q$ -generalized in [247–250] (see also [251–255]).

We start with a *definition*. The  $q$ -*Fourier transform* ( $q$ -FT) of a function  $f(x)$  is defined as follows:

$$F_q[f](\xi) \equiv \int dx e_q^{i\xi x} \otimes_q f(x). \quad (4.70)$$

This definition holds for any real value of  $q$ . However, its implementation is very simple for  $q \geq 1$ . We shall therefore restrict to this interval from now on.<sup>6</sup> It can be shown [247] that

<sup>6</sup> The  $q$ -Fourier transform for  $q < 1$  can be conveniently handled, as recently shown [K.P. Nelson and S. Umarov, *The relationship between Tsallis statistics, the Fourier transform, and nonlinear coupling*, 0811.3777[cs.IT]], by using the self-dual transformation  $q \leftrightarrow (5 - 3q)/(3 - q)$ , which transforms the  $q \leq 1$  interval into the  $1 \leq q < 3$  interval and reciprocally.

$$F_q[f](\xi) = \int_{-\infty}^{\infty} dx e_q^{i\xi x [f(x)]^{q-1}} f(x) \quad (q \geq 1). \quad (4.71)$$

It is transparent that this transformation is, for  $q \neq 1$ , *nonlinear*. Indeed, if we do  $f(x) \rightarrow \lambda f(x)$ ,  $\lambda$  being any constant, we verify that  $F_q[\lambda f](\xi) \neq \lambda F_q[f](\xi)$  ( $q \neq 1$ ).

This generalization of the standard Fourier transform ( $F_1[f](\xi)$ ) has a remarkable *property*: it transforms  $q$ -Gaussians into  $q$ -Gaussians. Indeed, we verify

$$F_q \left[ \frac{\sqrt{\beta}}{A_q} e_q^{-\beta x^2} \right] (\xi) = e_{q_1}^{-\beta_1 \xi^2}, \quad (4.72)$$

where

$$q_1 = \frac{1+q}{3-q}, \quad (4.73)$$

and

$$\beta_1 = \frac{3-q}{8 \beta^{2-q} A_q^{2(1-q)}}, \quad (4.74)$$

with

$$A_q = \begin{cases} \frac{2\sqrt{\pi} \Gamma(\frac{1}{1-q})}{(3-q)\sqrt{1-q} \Gamma(\frac{3-q}{2(q-1)})} & \text{if } q < 1, \\ \sqrt{\pi} & \text{if } q = 1, \\ \frac{\sqrt{\pi} \Gamma(\frac{3-q}{2(q-1)})}{\sqrt{q-1} \Gamma(\frac{1}{q-1})} & \text{if } 1 < q < 3. \end{cases} \quad (4.75)$$

It follows that the  $q$ -Fourier transform has the inverse transform in the set of  $q$ -Gaussians (see [256]) (and for the  $(q, \alpha)$ -stable distributions to be soon defined, as well).<sup>7</sup>

<sup>7</sup> Hilhorst [257] has recently produced an interesting example which is noninvertible. Consider  $f(x) = (\lambda/x)^{\frac{1}{q-1}}$  if  $a < x < b$ , and zero otherwise;  $q > 1$ ,  $0 < a < b$ , and  $\lambda > 0$ . Imposition of normalization straightforwardly yields  $\lambda = \left[ \frac{q-1}{q-2} \left( b^{\frac{q-2}{q-1}} - a^{\frac{q-2}{q-1}} \right) \right]^{-(q-1)}$ . It immediately follows that  $F_q[f](\xi) = [1 + (1-q)i\xi\lambda]^{\frac{1}{1-q}}$ . Therefore this solution is, for fixed  $q$ , *one and the same* for a one-parameter family of normalized functions  $f(x)$ . Indeed, for all  $(a, b)$  having the same  $\lambda$ , the  $q$ -Fourier transform is the same. Therefore, for this example, the inverse  $q$ -Fourier transform does not exist in the sense that it does not yield a single function, but rather a family of them. In other words, the  $q$ -Fourier transform is not invertible in the image of *all* probability density functions. To further understand the domain of impact of this example, let us consider a more general situation, namely  $F_{q'}[f](\xi) = \int_a^b dx \left[ 1 + (1-q')i\xi x [f(x)]^{q'-1} \right]^{\frac{1}{1-q'}} f(x) (q' > 1)$ , i.e.,  $F_{q'}[f](\xi) = \int_a^b dx \left[ 1 + (1-q')i\xi \lambda^{\frac{q'-1}{q-1}} x^{\frac{q-q'}{q-1}} \right]^{\frac{1}{1-q'}} f(x)$ . This integral can be expressed as a

See Fig. 4.18 for illustrations of the interesting *closure* property (4.72), which does *not* exist for *any* other of the presently known linear or nonlinear integral transforms.

Equation (4.74) can be rewritten as follows

$$\beta^{\sqrt{2-q}} \beta_1^{\frac{1}{\sqrt{2-q}}} = K(q), \quad (4.76)$$

$$K(q) \equiv \left[ \frac{3-q}{8A_q^{2(1-q)}} \right]^{\frac{1}{\sqrt{2-q}}}. \quad (4.77)$$

See Fig. 4.19.

Through direct derivation we can easily verify another interesting *property* of the  $q$ -Fourier transform, namely the following set of relations (for  $q \geq 1$ ) [258]:

$$F_q[f](0) = \int_{-\infty}^{\infty} dx f(x), \quad (4.78)$$

$$\left. \frac{dF_q[f](\xi)}{d\xi} \right|_{\xi=0} = i \int_{-\infty}^{\infty} dx x [f(x)]^q, \quad (4.79)$$

$$\left. \frac{d^2 F_q[f](\xi)}{d\xi^2} \right|_{\xi=0} = -q \int_{-\infty}^{\infty} dx x^2 [f(x)]^{2q-1}, \quad (4.80)$$

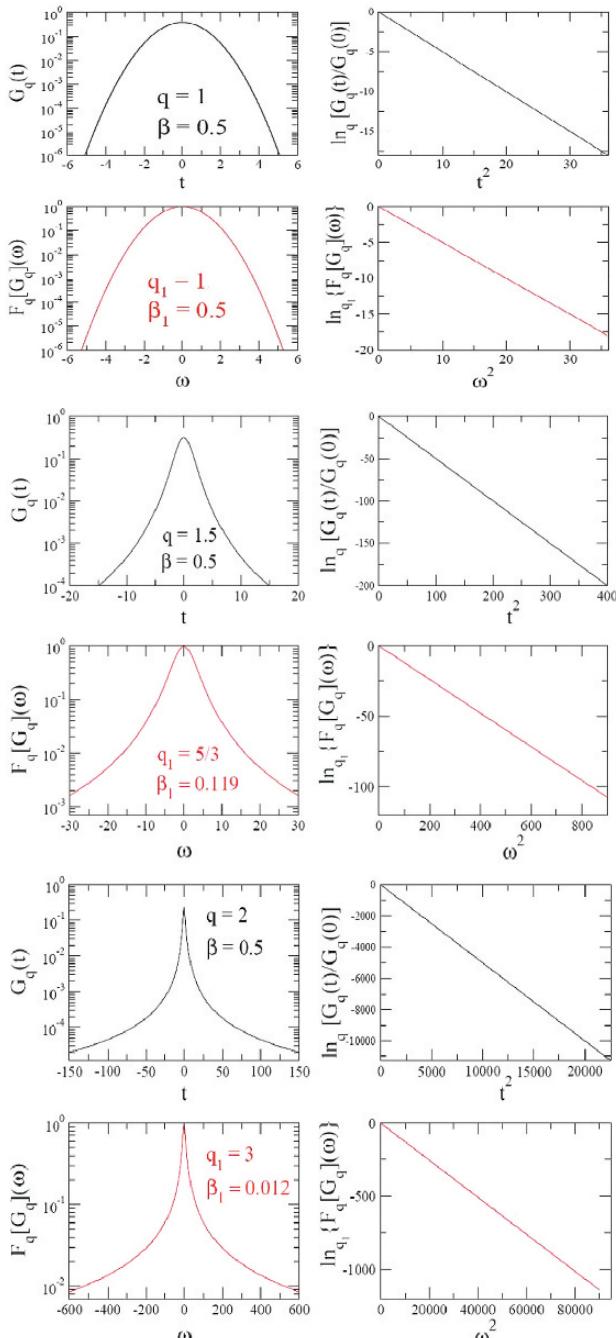
$$\begin{aligned} \left. \frac{d^n F_q[f](\xi)}{d\xi^n} \right|_{\xi=0} &= (i)^n \left\{ \prod_{m=0}^{n-1} [1 + m(q-1)] \right\} \\ &\times \int_{-\infty}^{\infty} dx x^n [f(x)]^{1+n(q-1)} \quad (n = 1, 2, 3, \dots). \end{aligned} \quad (4.81)$$

If  $f(x)$  is a real, nonnegative, integrable function, we can define a probability distribution, namely  $p(x) \equiv f(x) / \int_{-\infty}^{\infty} dx f(x)$ . We can also define a family of escort distributions, namely [258]

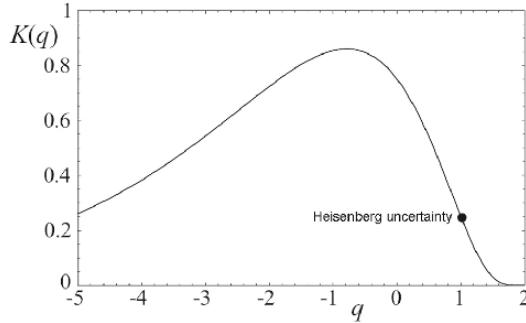
$$P^{(n)}(x) \equiv \frac{[f(x)]^{1+n(q-1)}}{\int_{-\infty}^{\infty} dx [f(x)]^{1+n(q-1)}} \quad [n = 0, 1, 2, \dots; P^{(0)}(x) = p(x); P^{(1)}(x) = P(x)]. \quad (4.82)$$

With the following definition of associated  $q$ -expectation values

combination of two hypergeometric functions, where we see through inspection that, due to the presence of  $x^{\frac{q-q'}{q-1}}$ , the one-parameter invariance has disappeared for all  $(q, q')$  such that  $q \neq q'$ . In other words, for fixed  $q$ , all  $q'$ -Fourier transforms are invertible, excepting if  $q' = q$ . Equivalently, for fixed  $q'$ , all the above functions  $f(x) = (\lambda/x)^{\frac{1}{q'-1}}$  are invertible excepting if  $q = q'$ . This discussion appears to suggest that  $F_q[f](\xi)$  is invertible for all admissible  $q$  and for all functions  $f(x)$  excepting a zero-measure class of them. It is possible that such exceptions could be handled satisfactorily by using extra information related to  $q$ -expectation values, but such discussion is out of the present scope.



**Fig. 4.18**  $q$ -Gaussians (in log-linear and  $q$ -log-quadratic scales) and their  $q$ -Fourier transforms (in log-linear and  $q$ -log-quadratic scales) for  $q = 1$  (top),  $q = 3/2$  (middle), and  $q = 2$  (bottom).



**Fig. 4.19** The function  $K(q)$ . At  $q = 1$  we recover the well-known transformation, through standard Fourier transform, of widths of Gaussians, mathematically involved in the Heisenberg uncertainty principle.

$$\langle(\dots)\rangle_n \equiv \int_{-\infty}^{\infty} dx (\dots) P^{(n)}(x) = \frac{\int_{-\infty}^{\infty} dx (\dots) [f(x)]^{1+n(q-1)}}{\int_{-\infty}^{\infty} dx [f(x)]^{1+n(q-1)}} \quad (n = 0, 1, 2, \dots), \quad (4.83)$$

we can rewrite the set of Eq. (4.81) as follows:

$$\frac{1}{v_{q_n}} \left. \frac{d^n F_q[f](\xi)}{d\xi^n} \right|_{\xi=0} = (i)^n \left\{ \prod_{m=0}^{n-1} [1 + m(q-1)] \right\} \langle x^n \rangle_n \quad (n = 1, 2, 3, \dots), \quad (4.84)$$

where

$$v_{q_n} \equiv \int_{-\infty}^{\infty} dx [f(x)]^{q_n} \quad (n = 0, 1, 2, \dots), \quad (4.85)$$

with

$$q_n = 1 + (q - 1)n \quad (n = 0, 1, 2, \dots). \quad (4.86)$$

Notice that

- (i) For  $q = 1$ , we recover the well-known relations involving the *generating function* in theory of probabilities;
- (ii) For  $n = 1$ , we obtain  $q_1 = q$ , hence the usual escort distribution (used to define the energy-related constraint under which  $S_q$  is to be extremized) emerges naturally;
- (iii) All  $q$ -expectation values in nonextensive statistical mechanics are well defined (i.e., finite) up to one and the same value of  $q$  (more precisely, for  $q < 2$  for a discrete energy spectrum);

- (iv) If we consider that  $F_q[f](\xi) = 1 + \left[ \frac{dF_q[f](\xi)}{d\xi} \right]_{\xi=0} \xi + \frac{1}{2} \left[ \frac{d^2F_q[f](\xi)}{d\xi^2} \right]_{\xi=0} \xi^2 + \frac{1}{3!} \left[ \frac{d^3F_q[f](\xi)}{d\xi^3} \right]_{\xi=0} \xi^3 + \dots$ , then  $F_q[f](\xi)$  is uniquely determined by the knowledge of the sets  $\{\langle x^n \rangle_n\}$  and  $\{v_{q_n}\}$  ( $n = 0, 1, 2, 3, \dots$ ). Finally, since the inverse  $q$ -Fourier transform exists and, under some conditions, possibly is unique [247], the same knowledge determines in principle  $f(x)$  itself [258].
- (v) If  $f(x) \sim 1/|x|^\gamma$  ( $|x| \rightarrow \infty; \gamma > 0$ ), then we define  $q = 1 + \frac{1}{\gamma}$ . This determines  $q_n = 1 + (q - 1)n$ , hence all the moments  $\langle x^n \rangle_n$ . For example, if  $f(x)$  is a  $Q$ -Gaussian, we have that  $\gamma = 2/(Q - 1)$ , hence  $1/(q - 1) = 2/(Q - 1)$ . Therefore, the upper admissible limit  $q = 2$  precisely corresponds to the well-known upper admissible value  $Q = 3$ .

Let us now introduce another *definition*. A random variable is said to have a  $(q, \alpha)$ -stable distribution  $L_{q,\alpha}(x)$ <sup>8</sup> if its  $q$ -Fourier transform has the form

$$a e^{-b|\xi|^\alpha} \quad (a > 0, b > 0, 0 < \alpha \leq 2), \quad (4.87)$$

with

$$q_{\alpha,1} \equiv \frac{\alpha q + 1 - q}{\alpha + 1 - q}, \quad (4.88)$$

i.e., if

$$F_q[L_{q,\alpha}](\xi) = a e^{-b|\xi|^\alpha} \quad (a > 0, b > 0, 0 < \alpha \leq 2). \quad (4.89)$$

Therefore,  $L_{1,2}(x)$  corresponds to Gaussians,  $L_{1,\alpha}(x)$  corresponds to  $\alpha$ -stable Lévy distributions, and  $L_{q,2}(x)$  corresponds to  $q$ -Gaussians. Notice that  $q_{2,1} = q_1 = (1 + q)/(3 - q)$ , as given by Eq. (4.73).

If we successively apply  $n$  times the  $q$ -Fourier transform onto  $L_{q,\alpha}(x)$ , we obtain the following algebra:

$$\frac{\alpha}{1 - q_{\alpha,n}} = \frac{\alpha}{1 - q} + n \quad (n = 0, \pm 1, \pm 2, \dots). \quad (4.90)$$

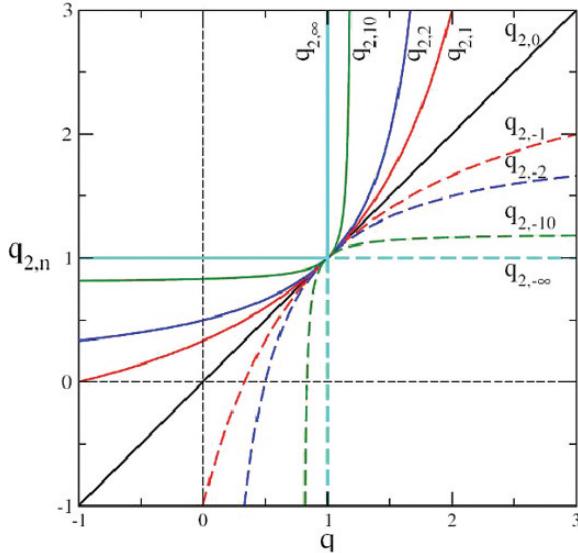
See Fig. 4.20. The  $n = 1$  case recovers relation (4.88). From Eq. (4.90) we immediately obtain

$$q_{\alpha,n} = \frac{(2 + \alpha)q_{\alpha,n+2} - 2}{2q_{\alpha,n+2} + \alpha - 2} \quad (n = 0, \pm 1, \pm 2, \dots). \quad (4.91)$$

If  $\alpha = 2$ , this recursion becomes

---

<sup>8</sup> The reason for the word *stable* will become clear soon.



**Fig. 4.20** The index  $q_{2,n}$  vs.  $q$  for typical values of  $n$ . The countable infinite family merges on a single point only for  $q = 1$ . This reflects the fact that the structure of  $BG$  statistical mechanics is considerably simpler than that of the nonextensive one.

$$q_{\alpha,n} = 2 - \frac{1}{q_{\alpha,n+2}} \quad (n = 0, \pm 1, \pm 2, \dots), \quad (4.92)$$

which, quite intriguingly, coincides with Eq. (4.38).

Let us finally introduce one more *definition*. Two random variables  $X$  (with distribution  $f_X(x)$ ) and  $Y$  (with distribution  $f_Y(y)$ ) having zero  $q$ -mean values are said *q-independent* if

$$F_q[X + Y](\xi) = F_q[X](\xi) \otimes_{\frac{1+q}{3-q}} F_q[Y](\xi), \quad (4.93)$$

i.e., if

$$\int dz e^{i\xi z} f_{X+Y}(z) = \left[ \int dx e^{i\xi x} f_X(x) \right] \otimes_{\frac{1+q}{3-q}} \left[ \int dy e^{i\xi y} f_Y(y) \right], \quad (4.94)$$

with

$$f_{X+Y}(z) = \int dx \int dy h(x, y) \delta(x+y-z) = \int dx h(x, z-x) = \int dy h(z-y, y), \quad (4.95)$$

where  $h(x, y)$  is the joint distribution. Therefore, *q-independence* means *independence* for  $q = 1$  (i.e.,  $h(x, y) = f_X(x)f_Y(y)$ ), and it means *strong correlation* (of a certain class) for  $q \neq 1$  (i.e.,  $h(x, y) \neq f_X(x)f_Y(y)$ ).

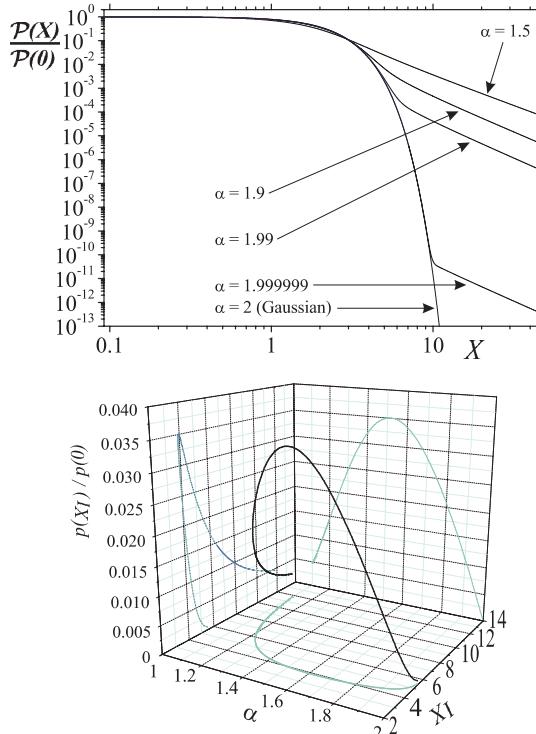
We can now present the structure of the  $q$ -generalization of the CLTs: see Fig. 4.21. To better understand the structure of the four theorems therein, we shall illustrate some crucial aspects of them.

Let us start with the  $q = 1$  cases, i.e., the standard and the Lévy–Gnedenko CLTs. The  $\alpha = 2$  attractor is a Gaussian. The asymptotic behavior of the  $\alpha < 2$  attractor is proportional to  $1/|x|^{1+\alpha}$ . Consequently, the  $\alpha \rightarrow 2$  limit yields a  $1/|x|^3$  tail, which is definitively different from a Gaussian tail. How can this occur? Through a *crossover!* (which corresponds to an inflexion point in log–log plots). The situation is depicted in Fig. 4.22.

We can also see the attractive effect in the space of distributions as  $N$  increases. If the distributions that we compose are  $q$ -Gaussians, the nature of the attractor will depend on whether the variance is finite (which occurs for  $q < 5/3$ ) or infi-

$q = 1$ [independent]	$q \neq 1$ (i.e., $Q \equiv 2q - 1 \neq 1$ ) [globally correlated]
$\sigma_Q < \infty$ ( $\alpha = 2$ )	$F(x) = \text{Gaussian } G(x)$ , with same $\sigma_1$ of $f(x)$
$\sigma_Q \rightarrow \infty$ ( $0 < \alpha < 2$ )	$F(x) = \text{Levy distribution } L_\alpha(x)$ , with same $ x  \rightarrow \infty$ behavior

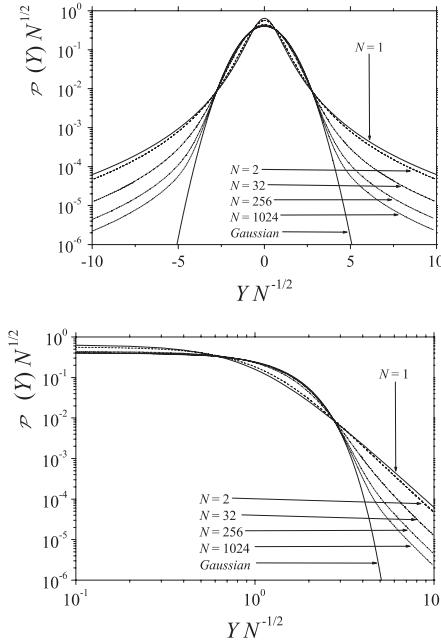
**Fig. 4.21**  $N^{1/[\alpha(2-q)]}$ -scaled attractors  $F(x)$  when summing  $N \rightarrow \infty$   $q$ -independent identical random variables with symmetric distribution  $f(x)$  with  $Q$ -variance  $\sigma_Q \equiv \int_{-\infty}^{\infty} dx x^2 [f(x)]^Q / \int_{-\infty}^{\infty} dx [f(x)]^Q$  ( $Q \equiv 2q - 1$ ;  $q_1 = (1+q)/(3-q)$ ;  $q \geq 1$ ). Top left: The attractor is the Gaussian sharing with  $f(x)$  the same variance  $\sigma_1$  (standard CLT). Bottom left: The attractor is the  $\alpha$ -stable Lévy distribution which shares with  $f(x)$  the same asymptotic behavior, i.e., the coefficient  $C_\alpha$  (Lévy–Gnedenko CLT, or  $\alpha$ -generalization of the standard CLT). Top right: The attractor is the  $q$ -Gaussian which shares with  $f(x)$  the same  $(2q - 1)$ -variance, i.e., the coefficient  $C_q$  ( $q$ -generalization of the standard CLT, or  $q$ -CLT). Bottom right: The attractor is the  $(q, \alpha)$ -stable distribution which shares with  $f(x)$  the same asymptotic behavior, i.e., the coefficient  $C_{q,\alpha}^L$  ( $q$ -generalization of the Lévy–Gnedenko CLT and  $\alpha$ -generalization of the  $q$ -CLT). The case  $\alpha < 2$ , for both  $q = 1$  and  $q \neq 1$  (more precisely  $q > 1$ ), further demands specific asymptotics for the attractors to be those indicated; essentially the divergent  $q$ -variance must be due to fat tails of the power-law class, excepting for possible logarithmic corrections (for the  $q = 1$  case see, for instance, [340] and references therein).



**Fig. 4.22** *Top:* Gaussian and  $\alpha$ -stable Lévy distributions for  $\alpha$  approaching 2 in the inverse Fourier transform of  $e^{-|\xi|^\alpha}$ . For values of  $\alpha$  closer to 2, the Lévy distribution becomes almost equal to a Gaussian up to some characteristic value above which the power law behavior emerges. *Bottom:* Locus of the inflection point of the same  $\alpha$ -stable Lévy distributions. Contrarily to what happens with  $q$ -Gaussians, when Lévy distributions are represented in a log-log scale, they exhibit an inflection point which goes to infinity as  $\alpha \rightarrow 1$  (Cauchy–Lorentz distribution, i.e.,  $q = 2$ ) and  $\alpha \rightarrow 2$  (Gaussian distribution) too. We also show the projections onto the planes  $\frac{p(X_I)}{p(0)} - X_I$ ,  $\frac{p(X_I)}{p(0)} - \alpha$ , and  $\alpha - X_I$  (from [252]).

nite (which occurs for  $q \geq 5/3$ ). Both cases are illustrated in Figs. 4.23 and 4.24, respectively.

Let us see now the  $q > 1$  cases. The attractors are now  $q$ -Gaussians when the  $(2q - 1)$ -variance is finite (i.e.,  $\alpha = 2$ ), and  $(q, \alpha)$ -stable distributions when it diverges (i.e.,  $0 < \alpha < 2$ ). These distributions must somehow match with  $q$ -Gaussians when  $\alpha$  approaches 2, and must match with  $\alpha$ -stable Lévy distributions when  $q$  approaches 1. This happens through a *double crossover!* See Fig. 4.25. We see that, while  $|x|$  increases, the distribution goes essentially through *two* different power-law regimes, a *distant one*, which will match with  $\alpha$ -distributions when  $q$  approaches unity, and an *intermediate one*, which will match with  $q$ -Gaussians when  $\alpha$  approaches 2. See Figs. 4.26 and 4.27.



**Fig. 4.23** Both panels represent probability density function  $\mathcal{P}(Y)$  vs.  $Y$  (properly scaled) in log–linear (*top*) and log–log (*bottom*) scales, where  $Y$  represents the sum of  $N$  independent variables  $X$  each of them having a  $q$ -Gaussian distribution with  $q = 3/2 (< 5/3)$ . Since the variables are independent and the variance is finite,  $\mathcal{P}(Y)$  converges to a Gaussian as it is visible. It is also visible in the log–linear representation that, although the central part of the distribution approaches a Gaussian, the power-law decay subsists even for large  $N$  as depicted in log–log representation (from [252]).

## 4.8 Generalizing the Langevin Equation

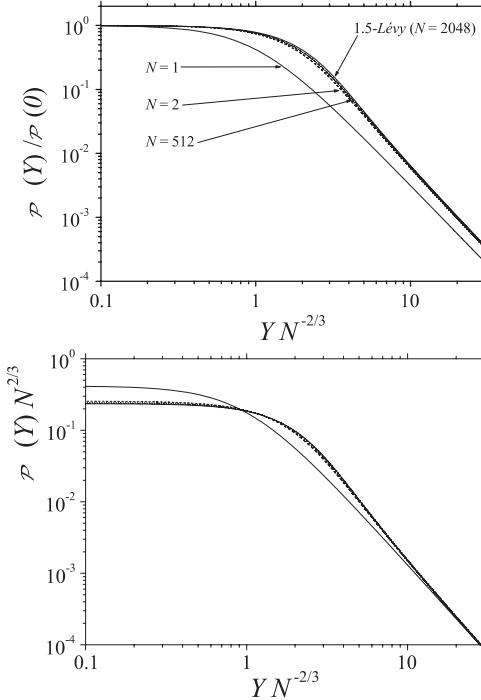
The standard Langevin equation is given by [302, 303]

$$\dot{x} = f(x) + \eta(t), \quad (4.96)$$

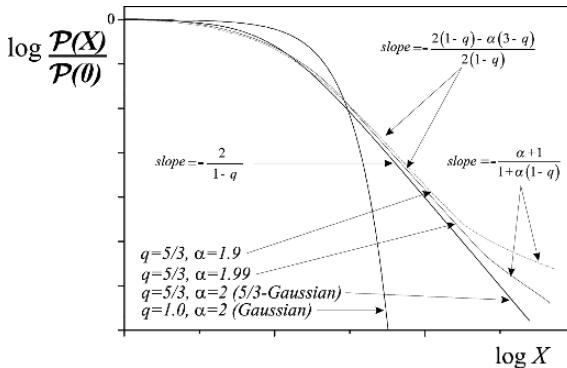
where  $x(t)$  is a stochastic variable,  $f(x)$  is an arbitrary function which represents some deterministic drift, and  $\eta(t)$  is a Gaussian-distributed zero-mean white noise satisfying

$$\langle \eta(t) \eta(t') \rangle = 2 A \delta(t - t'). \quad (4.97)$$

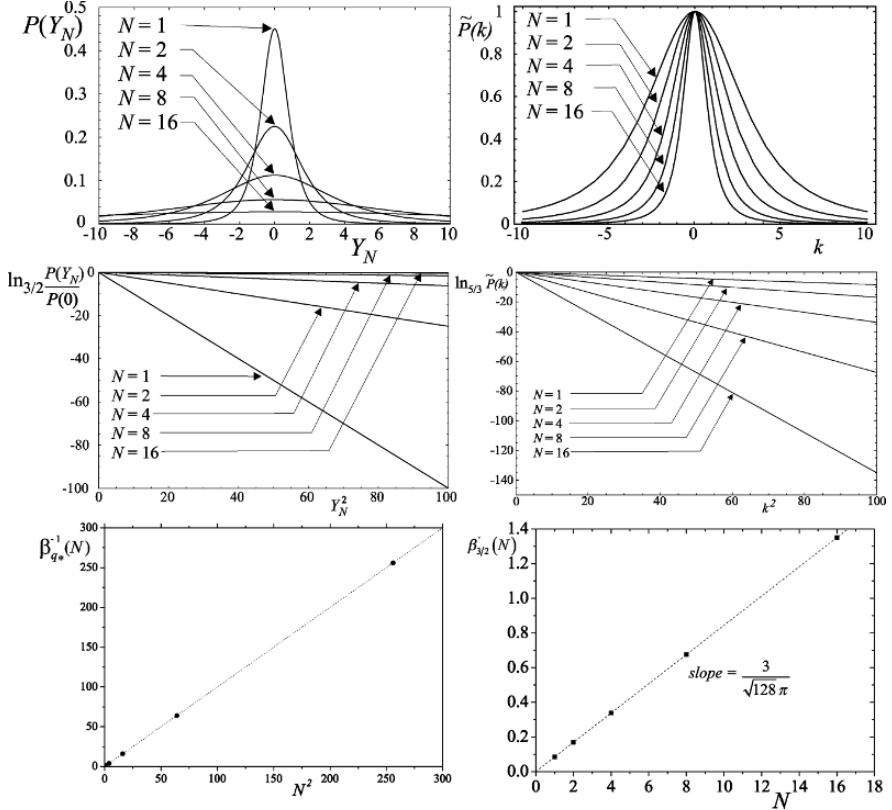
The noise amplitude  $A \geq 0$  stands for *additive*. The deterministic drift  $f(x)$  can be interpreted either as a damping force (whenever  $x$  is a velocity-like quantity) or as an external force (when motion is overdamped and  $x$  represents a position coordinate). Other interpretations are possible as well, depending on the particular system we are focusing on. This equation is known to lead to the standard Fokker–Planck equation (Fourier’s *heat equation*), whose basic solutions are Gaussians in the variable  $x/\sqrt{t}$ .



**Fig. 4.24** Both panels represent probability density function  $\mathcal{P}(Y)$  vs.  $Y$  (properly scaled) in two different log–log scales, where  $Y$  represents the sum of  $N$  independent variables  $X$  each of them having a  $q$ -Gaussian distribution with  $q = 9/5 (> 5/3)$ . Since the variables are independent and the variance diverges,  $\mathcal{P}(Y)$  converges to a Lévy distribution as it is visible (from [252]).



**Fig. 4.25** Outline of  $(q, \alpha)$ -stable distributions (inverse  $q$ -Fourier transforms of  $a e_q^{-b |\xi|^\alpha}$ ) for the case in which the correlation is given by  $q_1 = 2$ . As  $\alpha$  approaches 2, the  $(q, \alpha)$ -stable distributions become closer and closer to a  $q$ -Gaussian with  $= 5/3$ , with an exponent  $[2(q - 1) + \alpha(3 - q)] / [2(q - 1)]$ . However, since  $\alpha \neq 2$ , for some value  $X^*$ , a crossover occurs through which the distribution changes from the intermediate regime towards the distant regime with a tail exponent  $(\alpha + 1) / (1 + \alpha q - \alpha)$ . The inequalities  $2/(q - 1) \geq [2(q - 1) + \alpha(3 - q)] / [2(q - 1)] > (1 + \alpha) / [1 + \alpha(q - 1)]$  are satisfied (from [253]).

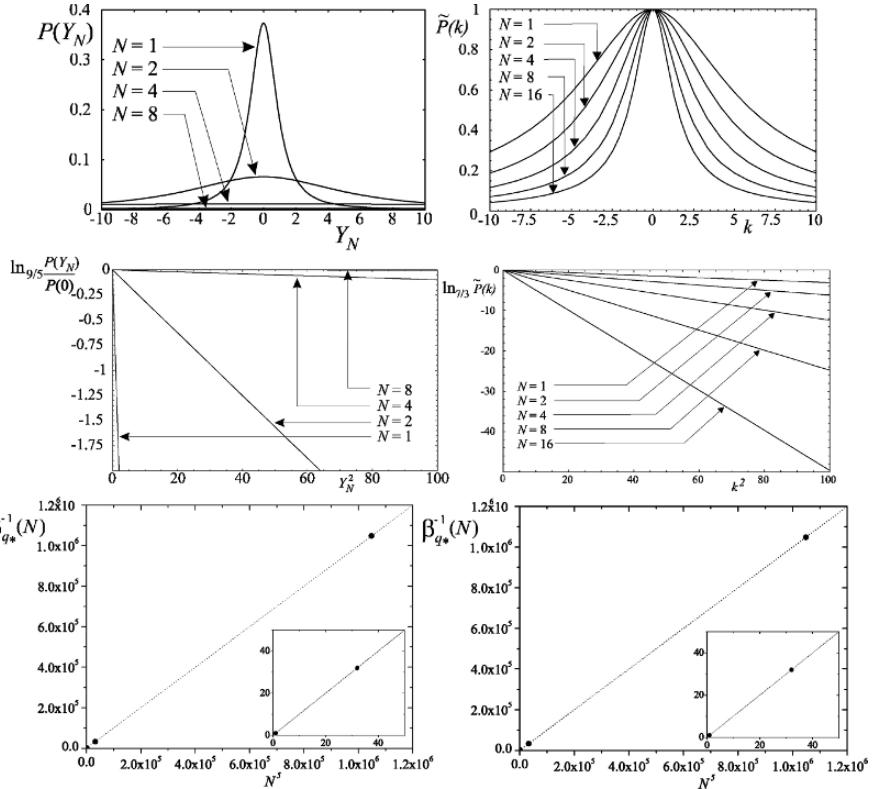


**Fig. 4.26** Top: Probability distribution  $P(Y_N)$  vs.  $Y_N$ , with  $Y_N \equiv \sum_{i=1}^N X_i$ ,  $X_i$  being  $(q = \frac{5}{3})$ -independent random variables associated with a  $\mathcal{G}_{\frac{5}{3}}(X)$  distribution with  $\beta = 1$  (left), and the respective  $(q = \frac{3}{2})$ -Fourier Transform,  $\tilde{P}(k)$ , vs.  $k$  (right). Middle: Same as above, in  $\ln_{\frac{3}{2}}$ -squared scale (left), and  $\ln_{\frac{5}{3}}$ -squared scale (right). The straight lines indicate that  $P(Y_N)$  and  $\tilde{P}(k)$  are  $q$ -Gaussians with  $q = \frac{3}{2}$  and  $q = \frac{5}{3}$ , respectively. Their slopes are  $\beta_{q_*=3/2}^{-1}(N)$  for left panel curves and  $\beta'_{q_*}(N)$  for right panel curves. Bottom:  $\beta_{q_*=3/2}^{-1}(N)$  vs.  $N^2$ , which is a straight line with slope 1 (left);  $\beta'_{q_*=3/2}(N)$  vs.  $N$  which is also a straight line but with slope  $\frac{3-q_*}{8 C_{q_*}^{2(q_*-1)}} \Big|_{q_*=3/2} = 0.088844\dots$  (right) (from [253]).

This historical equation has been generalized in very many ways. Some of them yield exact solutions which are  $q$ -Gaussians. Two such examples are described in [304] (simultaneous presence of uncorrelated additive and multiplicative noises) and in [306] (dichotomous colored noise). Because of its particularly simple nature, we shall present here the first example in detail. Let us consider the following generalization of Eq. (4.96):

$$\dot{x} = f(x) + g(x)\xi(t) + \eta(t), \quad (4.98)$$

where  $g(x)$  is an arbitrary function satisfying  $g(0) = 0$ , and  $\xi(t)$  is a Gaussian-distributed zero-mean white noise satisfying



which is the value of  $x$  to be used in  $g(x)$ . This is the well-known Itô–Stratonovich controversy [303, 307]. In the Itô definition, the value before the pulse must be used, whereas in the Stratonovich definition, the values before and after the pulse contribute in a symmetric way. In the particular instance when noise is purely additive, both definitions agree. In what follows, we shall adopt the Stratonovich definition (the Itô definition leads in fact to very similar results). By using standard procedures [303, 304], Eq. (4.98) leads to

$$\frac{\partial P(u, t)}{\partial t} = -\frac{\partial j(u, t)}{\partial u}, \quad (4.100)$$

where the *current* is defined as follows:

$$j(u, t) \equiv J(u)P(u, t) - \frac{\partial[D(u)P(u, t)]}{\partial u}, \quad (4.101)$$

with

$$J(u) \equiv f(u) + Mg(u)g'(u), \quad (4.102)$$

$$D(u) \equiv A + M[g(u)]^2. \quad (4.103)$$

Equation (4.100) can be rewritten as a Fokker–Planck equation, namely

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial[f(x)P(x, t)]}{\partial x} + M\frac{\partial}{\partial x}\left(g(x)\frac{\partial[g(x)P(x, t)]}{\partial x}\right) + A\frac{\partial^2 P(x, t)}{\partial x^2}. \quad (4.104)$$

In some processes, the deterministic drift derives from a potential-like function  $V(x) = (\tau/2)[g(x)]^2$ , where  $\tau$  is some nonnegative proportionality constant. Therefore, using  $f(x) = -dV/dx$ , we obtain the condition

$$f(x) = -\tau g(x)g'(x). \quad (4.105)$$

Let us note that the particular case  $g(x) \propto f(x) \propto x$ , which is a natural first choice for a physical system, verifies this condition. However, since no extra calculational difficulties emerge, we will discuss here the more general case of Eq. (4.105). Notice that, in the absence of deterministic forcing, condition (4.105) is satisfied for any  $g(x)$  by setting  $\tau = 0$ .

We shall restrict here to the stationary solutions corresponding to no flux boundary conditions (i.e.,  $j(-\infty) = j(\infty) = j(u) = 0$ ), although more general conditions could in principle also be considered. If Eq. (4.105) is satisfied, the stationary solution  $P(u, \infty)$  is of the  $q$ -exponential form, namely

$$P(u, \infty) \propto e_q^{-\beta[g(u)]^2}, \quad (4.106)$$

with<sup>10</sup>

$$q = \frac{\tau + 3M}{\tau + M}, \quad (4.107)$$

and

$$\beta \equiv \frac{1}{kT} = \frac{\tau + M}{2A}. \quad (4.108)$$

( $T$  can be generically seen as the amplitude of an effective noise). For the typical case  $\tau > 0$ , we have that  $q \geq 1$  if  $M \geq 0$ , the value  $q = 1$  corresponding to vanishing multiplicative noise. If  $|g(u)|$  grows, for  $|u| \rightarrow \infty$ , faster than  $|u|^{1+\tau/M}$ ,  $P(u, \infty)$  decreases faster than  $1/|u|$ , and is therefore normalizable. The condition (4.105) is in fact not necessary for having solutions of the  $q$ -exponential form. The interested reader can see the details in [304].

Let us mention that we have discussed here a case in which  $q$ -Gaussian distributions emerge from a *linear* Fokker–Planck equation (Eq. (4.104)). It is clear that this mechanism differs from the one focused on in Eq. (4.9), which is a *nonlinear* Fokker–Planck equation. For the Langevin discussion, i.e., from mesoscopic first principles, of this nonlinear Fokker–Planck equation, see [305] (with the notation change  $q \rightarrow 2 - q$ ). It turns out that if we consider a mechanism involving strongly non-Markovian processes, i.e., long memory effects, the nonlinear Fokker–Planck equation (Eq. (4.9)) naturally comes out.

Finally, as mentioned above, another Langevin process has been studied [306] which includes a colored symmetric dichotomous noise. Although not identified in this manner by the author, the stationary state has a  $q$ -Gaussian distribution with

$$q = \frac{1 - 2\gamma/\lambda}{1 - \gamma/\lambda}, \quad (4.109)$$

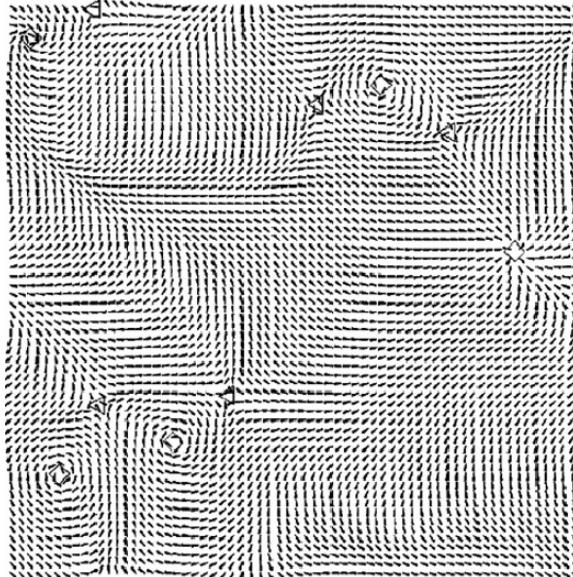
where  $\gamma$  and  $\lambda$  are mesoscopic parameters of the model.

## 4.9 Time-Dependent Ginzburg–Landau $d$ -Dimensional $O(n)$ Ferromagnet with $n = d$

The standard Langevin and Fokker–Planck equations are by no means equivalent to *BG* statistical mechanics, but they surely are consistent with it. One expects something similar to occur in the case of nonextensive statistical mechanics. It is our purpose here to exhibit one such example, even if the authors did not make the connection in their original papers [350, 351].

An interesting short-range-interacting  $d$ -dimensional ferromagnetic system is that whose symmetry is dictated by rotations in  $n$  dimensions, i.e., the so-called

<sup>10</sup> Incidentally, if we had used the Itô convention, we would have obtained  $q = \frac{\tau+4M}{\tau+2M}$ .



**Fig. 4.28** A typical vortex configuration in a  $256 \times 256$   $n = d = 2$  system. The arrow on each site represents the order parameter at that point. Not all the lattice sites are shown. The squares and triangles are in the core regions of  $+1$  and  $-1$  vortices, where the magnitude of the order parameter is near zero (from [351]).

$O(n)$  symmetry ( $n = 2$  corresponds to the  $XY$  model,  $n = 3$  corresponds to the Heisenberg model, and so on; the analytic limit  $n \rightarrow 1$  would yield the Ising model). We specifically address the kinetics of point defects (see the vortices in Fig. 4.28) during a quenching from high temperature to zero temperature for the  $d = n$  model. The theoretical description is done in terms of a time-dependent Ginzburg–Landau equation (similar to a Langevin equation). As a main outcome, one obtains that the distribution of the vortex velocity  $\mathbf{v}$  is, although not written in this manner by the authors [350, 351], given by

$$P(\mathbf{v}) \propto e_q^{-|\mathbf{v}|^2/v_0^2}, \quad (4.110)$$

with

$$q = \frac{d+4}{d+2}, \quad (4.111)$$

$v_0$  being a reference velocity which approaches zero for time increasing after the moment at which the quenching was done. It is certainly very interesting, although yet unexplained, to notice that the value of  $q$  precisely is the one which separates the finite from the infinite variance regions of  $q$  at  $d$  dimensions (see Eq. (4.30)).

# Chapter 5

## Deterministic Dynamical Foundations of Nonextensive Statistical Mechanics

*Il dépend de celui qui passe, Que je sois tombe ou trésor, Que je parle ou me taise, Ceci ne tient qu'à toi, Ami n'entre pas sans désir.*

Paul Valéry, *Palais de Chaillot*

In this chapter, we focus on *microscopic*-like nonlinear dynamical systems, in the sense that the time evolution is expressed exclusively with *deterministic* ingredients. We will first discuss, analytically and numerically, low-dimensional dissipative maps, and then low-dimensional conservative maps. We address next, numerically, many-body problems, first symplectic systems constituted by coupled simple low-dimensional conservative maps, and finally classical Hamiltonian systems. Our intention is to focus, in an unified manner, on those common aspects which relate to nonextensive statistical mechanical concepts. We shall see that, every time we have nonlinear dynamics which is only weakly chaotic (typically at the frontier between regular motion and strong chaos), the need systematically emerges to  $q$ -generalize various concepts and functions, and very especially the entropy.

### 5.1 Low-Dimensional Dissipative Maps

#### 5.1.1 One-Dimensional Dissipative Maps

Let us start by defining the maps we are going to deal with. We focus on unimodal one-dimensional maps. Some of them are since long well known in the literature; others have been recently introduced with the purpose of illustrating specific features that we are interested in.

The  $z$ -*logistic map* is defined as follows (see, for instance, [128]):

$$x_{t+1} = 1 - a|x_t|^z \quad (z > 1; 0 \leq a \leq 2; |x_t| \leq 1). \quad (5.1)$$

The standard case is recovered for  $z = 2$ , and its primary edge of chaos occurs at  $a_c(2) = 1.40115518909\dots$ . For this simple  $z = 2$  case, and with  $y \equiv x + 1/2$ , we obtain the traditional form

$$y_{t+1} = \mu y_t(1 - y_t) \quad (0 \leq \mu \leq 4; 0 \leq y_t \leq 1). \quad (5.2)$$

The  $z$ -periodic map is defined as follows [129]:

$$x_{t+1} = d \cos(\pi |x_t - 1/2|^{z/2}) \quad (z > 1; d > 0; |x_t| \leq d). \quad (5.3)$$

It belongs to the same universality class of the  $z$ -logistic map since they both share an extremum with inflection of order  $z$ . The standard case is recovered for  $z = 2$ , and its primary edge to chaos occurs at  $d_c(2) = 0.8655\dots$

The  $z$ -circular map is defined as follows [132]:

$$\theta_{t+1} = \Omega + [\theta_t - \frac{1}{2\pi} \sin(2\pi\theta_t)]^{z/3} \quad (z > 0). \quad (5.4)$$

The case  $z = 3$  recovers the standard case, and its primary edge to chaos occurs at  $\Omega_c(3) = 0.6066\dots$ . Various interesting properties and analytical results can be seen in [145].

The  $z$ -exponential map is defined as follows [146]:

$$x_{t+1} = 1 - a e^{-1/|x_t|^z} \quad (z > 0; a \in [0, a^*(z)]; |x_t| \leq 1), \quad (5.5)$$

where  $a^*(z)$  depends slowly from  $z$  (e.g.,  $a^*(0.5) \simeq 5.43$ ). This map was introduced [146] in order to have an extremum *flatter than any power*, which is the case of the  $z$ -logistic and the  $z$ -periodic ones. It shares with the  $z$ -logistic and  $z$ -periodic maps the same topological properties, although they differ in the metric ones. The case  $z = 1/2$  is a typical one, and its primary edge to chaos occurs at  $a_c(1/2) = 3.32169594\dots$

### 5.1.1.1 Sensitivity to the Initial Conditions

The sensitivity to the initial conditions  $\xi$  for a one-dimensional dynamical system is, as previously addressed, defined as follows:

$$\xi \equiv \lim_{\Delta x(0) \rightarrow 0} \frac{\Delta x(t)}{\Delta x(0)}, \quad (5.6)$$

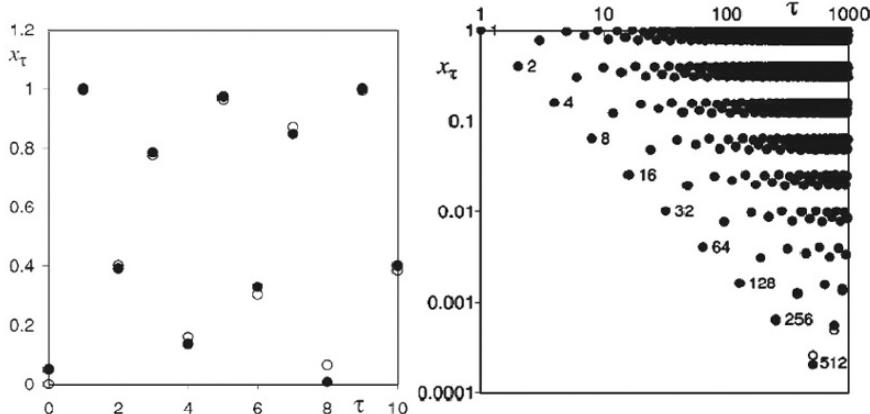
where  $x$  denotes the phase-space variable. The sensitivity  $\xi$  is quite generically expected to satisfy

$$\frac{d\xi}{dt} = \lambda_{q_{sen}} \xi^{q_{sen}}, \quad (5.7)$$

hence [127, 141, 142, 150]

$$\xi = e^{\lambda_{q_{sen}} t}, \quad (5.8)$$

where  $q_{sen} = 1$  if the Lyapunov exponent  $\lambda_1 \neq 0$  (*strongly sensitive* if  $\lambda_1 > 0$ , and *strongly insensitive* if  $\lambda_1 < 0$ ), and  $q_{sen} \neq 1$  otherwise; *sen* stands for *sensitivity*. At the edge of chaos,  $q_{sen} < 1$  (*weakly sensitive*), and at both the period-doubling and



**Fig. 5.1** *Left:* Absolute values of positions of the first 10 iterations  $\tau$  for two trajectories of the logistic map at the edge of chaos, with initial conditions  $x_0 = 0$  (empty circles) and  $x_0 = \delta \simeq 5 \times 10^{-2}$  (full circles). *Right:* The same (in log–log plot) for the first 1000 iterations, with  $\delta = 10^{-4}$  (from [142]).

tangent bifurcations,  $q_{sen} > 1$  (*weakly insensitive*). The case  $q_{sen} < 1$  (with  $\lambda_{q_{sen}} > 0$ ) yields, in Eq. (5.8), a power-law behavior  $\xi \propto t^{1/(1-q_{sen})}$  in the limit  $t \rightarrow \infty$ . This power-law asymptotics were since long known in the literature [122–126]. The case  $q_{sen} < 1$  is in fact more complex than indicated in Eq. (5.8). This equation only reflects the maximal values of an entire family, fully (and not only asymptotically) described in [150, 155]. See Figs. 5.1 and 5.2 from [142].

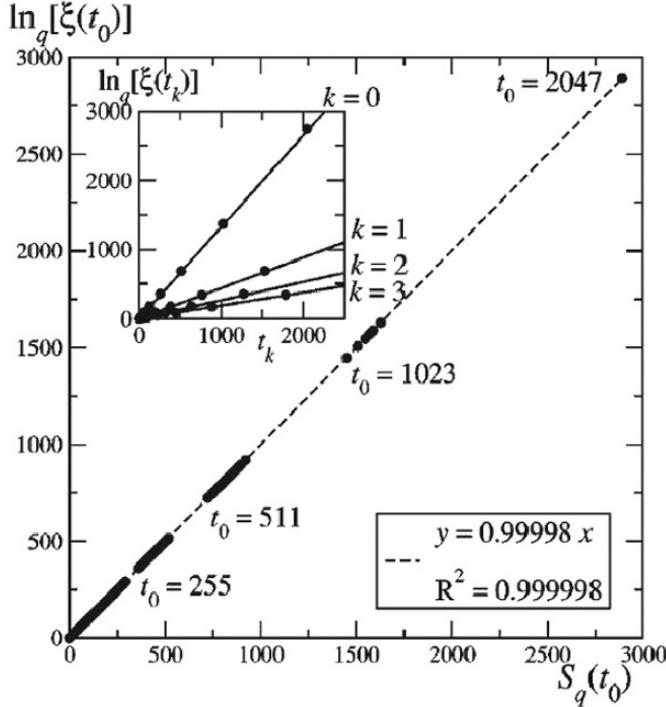
### 5.1.1.2 Multifractality

Multifractals are conveniently characterized by the multifractal function  $f(\alpha)$  [212]. Typically, this function is concave, defined in the interval  $[\alpha_{min}, \alpha_{max}]$  with  $f(\alpha_{min}) = f(\alpha_{max}) = 0$ ; within this interval it attains its maximum  $d_H$ ,  $d_H$  being the *Hausdorff or fractal dimension*.

It has been proved [129, 142], that, at the edge of chaos, we have<sup>1</sup>

$$\frac{1}{1 - q_{sen}} = \frac{1}{\alpha_{min}} - \frac{1}{\alpha_{max}} \quad (q_{sen} < 1). \quad (5.9)$$

<sup>1</sup> Virtually all the  $q$ -formulae of the present book admit the limit  $q \rightarrow 1$ . This is not the case of Eq. (5.9), since the left member diverges whereas the right member vanishes. Indeed,  $q = 1$  typically corresponds to the case of dynamics with positive Lyapunov exponent, hence mixing, hence ergodic, hence leading to an Euclidean, nonfractal, geometry. For such a standard one-dimensional geometry, it should be  $\alpha_{min} = \alpha_{max} = f(\alpha_{min}) = f(\alpha_{max}) = 1$ , which clearly makes the right member of Eq. (5.9) to vanish. A relation more general than Eq. (5.9) is therefore needed before taking the  $q \rightarrow 1$  limit. A relation such as  $\frac{1}{1-q_{sen}} = \frac{1}{\alpha_{min}-f(\alpha_{min})} - \frac{1}{\alpha_{max}-f(\alpha_{max})}$  for instance. Indeed, it recovers Eq. (5.9) for  $f(\alpha_{min}) = f(\alpha_{max}) = 0$ , and also admits  $q \rightarrow 1$ , being now possible for both members to diverge. It should be however noticed that this more general relation is totally heuristic: we do not yet dispose of numerical indications, and even less of a proof.



**Fig. 5.2** Numerical corroboration (full circles) of the  $q$ -generalized Pesin-like identity  $K_q^{(k)} = \lambda_q^{(k)}$  at the edge of chaos the logistic map. On the ordinate we plot the  $q$ -logarithm of  $\xi_{t_k}$  (equal to  $\lambda_q^{(k)} t$ ), and in the abscissa  $S_q$  (equal to  $K_q^{(q)} t$ ), both for  $q = 0.2445 \dots$ . The dashed line is a linear fit. Inset: The full lines are from the analytic result (from [147]).

For unimodal maps with inflection  $z$ , negative Schwarzian derivative in the bounded interval, and partition scale  $b$  we have

$$\begin{aligned} \alpha_{\max}(z) &= \frac{\ln b}{\ln \alpha_F(z)}, \\ \alpha_{\min}(z) &= \frac{\ln b}{z \ln \alpha_F(z)}, \end{aligned} \quad (5.10)$$

where  $\alpha_F$  is the so-called Feigenbaum constant. Hence

$$\frac{1}{1 - q_{sen}(z)} = (z - 1) \frac{\ln \alpha_F(z)}{\ln b}. \quad (5.11)$$

For the universality class of the  $z$ -logistic map, we have  $b = 2$  hence

$$\frac{1}{1 - q_{sen}(z)} = (z - 1) \frac{\ln \alpha_F(z)}{\ln 2}. \quad (5.12)$$

Broadhurst calculated the  $z = 2$  Feigenbaum constant  $\alpha_F$  with 1018 digits [352]. Through Eq. (5.12), it straightforwardly follows that

$$q_{sen}(2) = 0.244487701341282066198 \dots \quad (5.13)$$

See [128] for  $q_{sen}(z)$ .

The same type of information is available for the edge of chaos of other unimodal maps. For example, for the universality class of the  $z$ -circular map, we must use [132]  $b = (\sqrt{5} + 1)/2 = 1.6180 \dots$  into Eq. (5.11). We then obtain [132]  $q_{sen}(3) = 0.05 \pm 0.01$ . Similar results are available for the universality class of the  $z$ -exponential map [146].

### 5.1.1.3 Entropy Production and the Pesin Theorem

There are quite generic circumstances under which the entropy increases with time, typically while dynamically exploring the phase-space of the system. If this increase is (asymptotically) linear with time we may define an *entropy production per unit time*, which is the rate of increase of the entropy. One such concept, based on single trajectories as already mentioned, is the so-called *Kolmogorov–Sinai entropy rate* or just *KS entropy* [84]. It satisfies, under quite general conditions, an identity, namely that it is equal to the sum of all positive Lyapunov exponents (which reduces to the single Lyapunov exponent if the system is one-dimensional). This equality is frequently referred in the literature as the *Pesin identity*, or the *Pesin theorem* [86]. Here, instead of the KS entropy (computationally very inconvenient), we shall use  $K_q$ , the ensemble-based entropy production rate that we defined in Section 3.2. We refer to Eq. (3.59). A special value of  $q$ , noted  $q_{ent}$ , generically exists such that  $K_{q_{ent}}$  is finite, whereas  $K_q$  vanishes (diverges) for any  $q > q_{ent}$  ( $q < q_{ent}$ ). For systems strongly chaotic (i.e., whose single Lyapunov exponent is positive), we have  $q_{ent} = 1$ , thus recovering the usual case of ergodic systems and others. For systems weakly chaotic (i.e., whose single Lyapunov exponent vanishes, such as in the case of an edge of chaos), we have  $q_{ent} < 1$ . Many nonergodic (but certainly not all) systems belong to this class.

For quite generic systems we expect [127] (see Section 5.2)

$$q_{ent} = q_{sen}, \quad (5.14)$$

and

$$K_{q_{ent}} = \lambda_{q_{sen}}. \quad (5.15)$$

For  $q_{ent} = 1$ , this entropy production is expected to coincide, quite generically, with the KS entropy rate. Although a rigorous proof is, to the best of our knowledge, still lacking, examples can be seen in [133, 139, 147]. For many  $K_1 = \lambda_1 = 0$

systems, we expect the straightforwardly  $q$ -generalized Kolmogorov–Sinai entropy rate to coincide with  $K_{q_{ent}}$ .

The properties that have been exhibited here for the sensitivity to the initial conditions and the entropy production have also been checked [143, 144] for other entropies directly related to  $S_q$ . The scheme remains the same, excepting for the slope  $K_{q_{ent}}$ , which does depend on the particular entropy. The slope for  $S_q$  turns out to be the maximal one among those that have been analyzed. For all these  $q \neq 1$  examples, the Renyi entropy  $S_q^R$  fails in providing a *linear* time dependence: it provides instead a *logarithmic* time dependence.

### 5.1.1.4 Relaxation

In the previous paragraphs, we were dealing with the value of  $q$ ,  $q_{sen}$ , associated with the sensitivity to the initial conditions, and also with multifractality and the entropy production. We address now a different property, namely relaxation. As we shall see, a new value of  $q$ , denoted  $q_{rel}$  (where *rel* stands for *relaxation*), emerges. Typically  $q_{rel} \geq 1$ , the equality holding for strongly chaotic systems (i.e., when  $q_{sen} = 1$ ). Relaxation was systematically studied for the  $z$ -logistic map in [148]. The procedure consists in starting, at the edge of chaos, with a distribution of  $M \gg 1$  initial conditions which is uniform in phase-space ( $x_0 \in [-1, 1]$  for the  $z$ -logistic map), and let evolve the ensemble towards the multifractal attractor. A partition of the phase-space is established with  $W(0) \gg 1$  little equal cells, and then the covering is followed along time by only counting those cells which have at least one point at time  $t$ . This determines  $W(t)$ , which gradually decreases since the measure of the multifractal attractor is zero. In the  $M \rightarrow \infty$  and  $W(0) \rightarrow \infty$  limits, and disregarding small oscillations, it is verified

$$\frac{W(t)}{W(0)} \simeq e^{-t/\tau_{q_{rel}}}, \quad (5.16)$$

with  $q_{rel}(z) \geq 1$  and  $\tau_{q_{rel}}(z) > 0$ . If it is taken into account the fact that, for the  $z$ -logistic map, also the Hausdorff dimension depends on  $z$ , it can be numerically verified the following quite intriguing, and yet unexplained, relation:

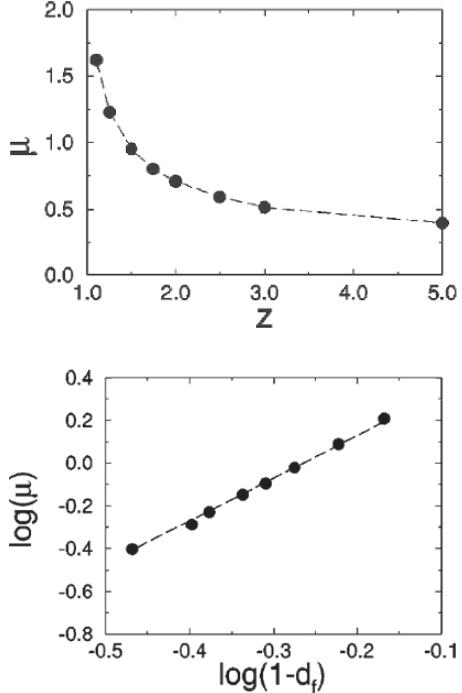
$$\frac{1}{q_{rel}(z) - 1} \simeq a [1 - d_H(z)]^2 \quad (z \in [1.1, 5.0]), \quad (5.17)$$

with  $a = 3.3 \pm 0.3$ . See Fig. 5.3. Higher precision calculations are available for  $z = 2$ , namely  $1/[q_{rel}(2) - 1] = 0.800138194\dots$ , hence  $q_{rel}(2) = 2.249784109\dots$  [149, 152].<sup>2</sup>

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<sup>2</sup> These two references concern the *approach* to the multifractal attractor as a function of time. However, [149] contains a general criticism concerning also the time evolution *within* the attractor. This is rebutted in [150] (see also [151]).

**Fig. 5.3** The exponent  $\mu \equiv 1/(q_{rel} - 1)$  for the  $z$ -logistic map, as a function of  $z$  (*top*), and of the fractal dimension  $d_H \equiv d_f$  (*bottom*). From [148].



For the  $z$ -circular map, it is numerically found [148]  $q_{rel}(z) \rightarrow \infty$  and  $d_H(z) = 1$ ,  $\forall z$ , which also is consistent with a relation such as Eq. (5.17) ( $q_{rel} \rightarrow \infty$  suggests a logarithmic behavior instead of the asymptotic power-law in Eq. (5.16)).<sup>3</sup>

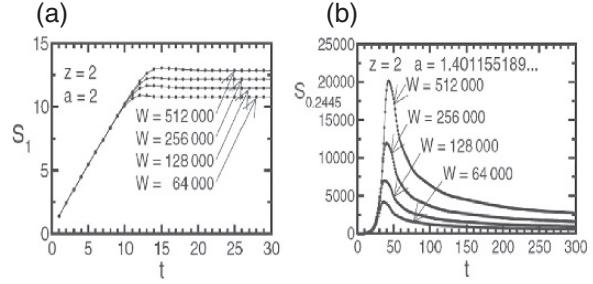
An alternative way for studying  $q_{rel}$  has been proposed in [140]. If we consider  $S_1(t)$  for a map which is strongly chaotic (or  $S_{q_{ent}}(t)$  for a map which is weakly chaotic) for a given number  $W(0)$  of little cells within which the phase-space has been partitioned, we typically observe the following behavior. For small values of  $t$  there is a transient; for intermediate values of  $t$  there is a *linear* regime (which enables the calculation of the entropy production per unit time, and becomes longer and longer with increasing  $W(0)$ ); finally, for larger values of  $t$  the entropy approaches (typically from above!) its saturation value  $S_q(\infty)$ . Therefore,  $S_q(t) - S_q(\infty)$  vanishes with diverging  $t$ , and it does so as follows:

$$S_{q_{ent}}(t) - S_{q_{ent}}(\infty) \propto e^{-t/\tau_{q_{rel}}}, \quad (5.18)$$

which enables the determination of  $q_{rel}$ , as well as that of  $\tau_{q_{rel}}$ . See Fig. 5.4.

<sup>3</sup> The  $d$ -dimensional generalization of Eq. (5.17) might well be  $1/(q_{rel}-1) \propto (d-d_H)^2$ . Therefore, all the so-called *fat-fractal* dynamical attractors (i.e.,  $d_H = d$ ) would yield  $q_{rel} \rightarrow \infty$ .

**Fig. 5.4** Time evolution of  $S_{q_{ent}}$  for the  $z = 2$  logistic map, for strongly chaotic (a) and weakly chaotic (b) cases. In all cases,  $S_{q_{ent}}(t) < \ln_{q_{ent}} W$  (however, for a given  $W$ , the maximal value attained by  $S_{q_{ent}}(t)$  is very close to  $\ln_{q_{ent}} W$  (from [140]).



### 5.1.1.5 Influence of Averaging

We briefly present here how results are modified [146, 153] when averaging is done over the initial conditions. Depending on the “experimental” setup of computational or real experiments, we might be interested in the dynamics related to essentially one or many initial conditions. To illustrate these effects, we focus on averages done over initial conditions that are uniformly distributed within the phase-space of the system. We numerically verify the following behaviors:

$$\langle \ln_{q_{sen}^{av}} \xi \rangle(t) = \lambda_{q_{sen}^{av}} t , \quad (5.19)$$

and

$$\langle S_{q_{ent}^{av}} \xi \rangle(t) = K_{q_{ent}^{av}} t , \quad (5.20)$$

with

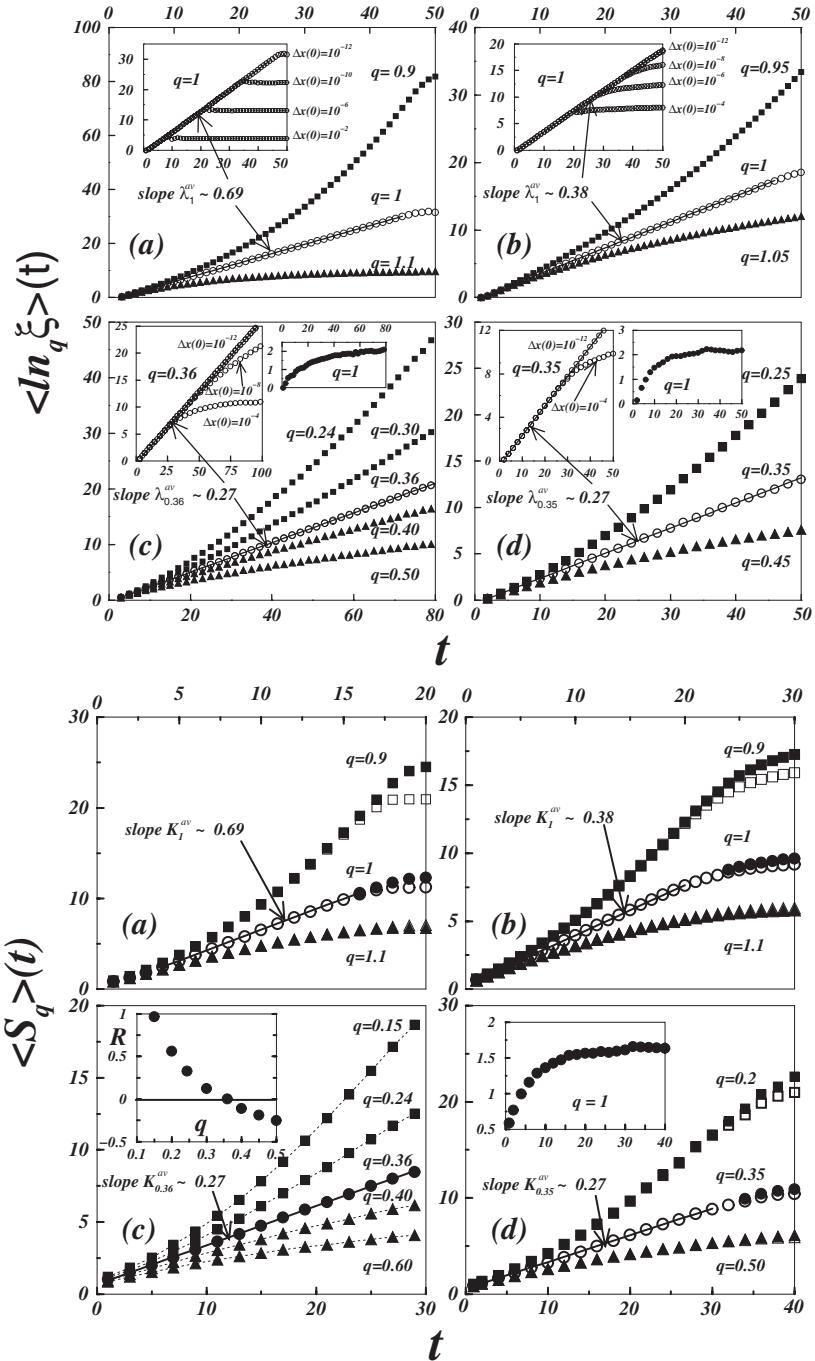
$$q_{ent}^{av} = q_{sen}^{av} , \quad (5.21)$$

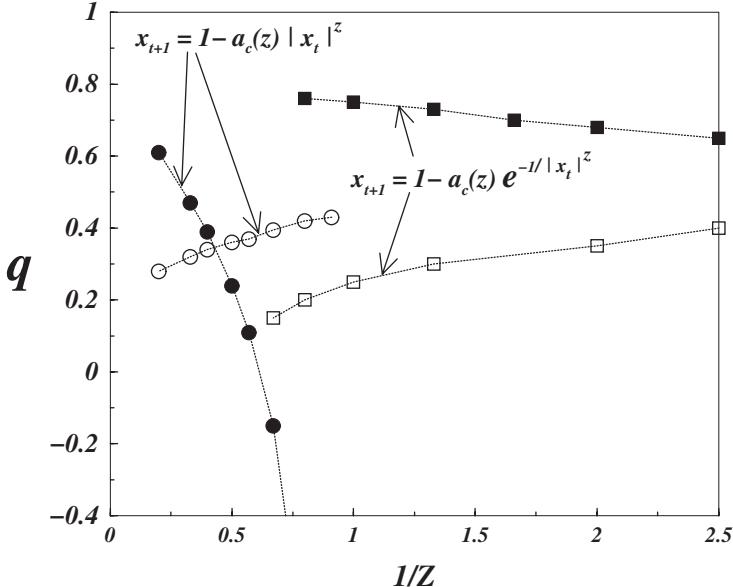
and

$$K_{q_{ent}^{av}} = \lambda_{q_{ent}^{av}} , \quad (5.22)$$

where *av* stands for *average*. See Fig. 5.5. Notice however that, although the structure and properties remain the same, the values of  $(q_{sen}^{av}, \lambda_{q_{sen}^{av}})$  differ from  $(q_{sen}, \lambda_{q_{sen}})$ , being  $q_{sen} < q_{sen}^{av} < 1$  (see Fig. 5.6). The analytical discussion of these facts is by no means trivial and has not yet been undertaken. Indeed, it involves the simultaneous consequences of the gradual approach to the multifractal attractor and the time evolution on the attractor itself.

Averaging introduces a further complication. Let us illustrate it with the  $z$ -logistic map. The edge of chaos that we have been primarily focusing on is that which emerges as an accumulation point of successive bifurcations (noted *cycle 2*). But there are edges of chaos corresponding to the accumulation points of trifurcations (noted *cycle 3*), or the various penta-furcations (noted *cycle 5*) and so on. They all

**Fig. 5.5** (continued).



**Fig. 5.6**  $z$ -dependence of  $q_{sen}^{av}$  (empty circles and squares: present work) and  $q_{sen}$  (filled circles: from [128, 129]; filled squares: from [146]). Dotted lines are guides to the eye.

belong to the same universality class in the sense that  $q_{sen}(z)$  is one and the same for all of them. But it is not so for  $q_{sen}^{av}(z)$ . The situation is depicted in Figs. 5.7, 5.8, and 5.9. Also, we numerically verify an intriguing relation between  $q_{sen}^{av}(\text{cycle } n; z)$  and  $q_{rel}(\text{cycle } n; z)$ , namely (see Fig. 5.10).

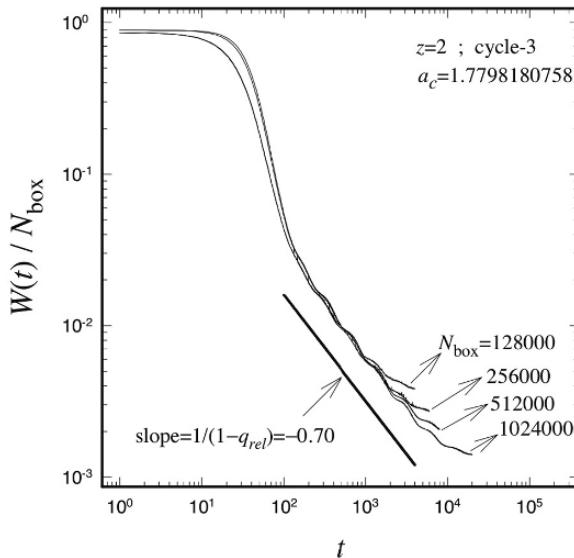
$$q_{rel}(\text{cycle } n; z) - 1 \simeq A_n [1 - q_{sen}^{av}(\text{cycle } n; z)]^{\alpha_n} \quad (A_n > 0; \alpha_n > 0; n = 2, 3, 5, \dots). \quad (5.23)$$

The limit  $q_{rel}(\text{cycle } n; z) = q_{sen}^{av}(\text{cycle } n; z) = 1$  corresponds to the BG case. Finally, we verify (see Fig. 5.11) that

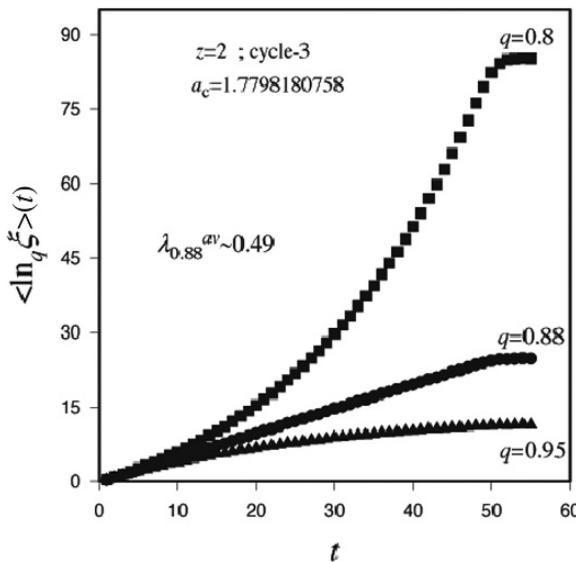
$$q_{sen}^{av}(\text{cycle } 3; z) \simeq 2.5 q_{sen}^{av}(\text{cycle } 2; z) - 0.03, \quad (5.24)$$

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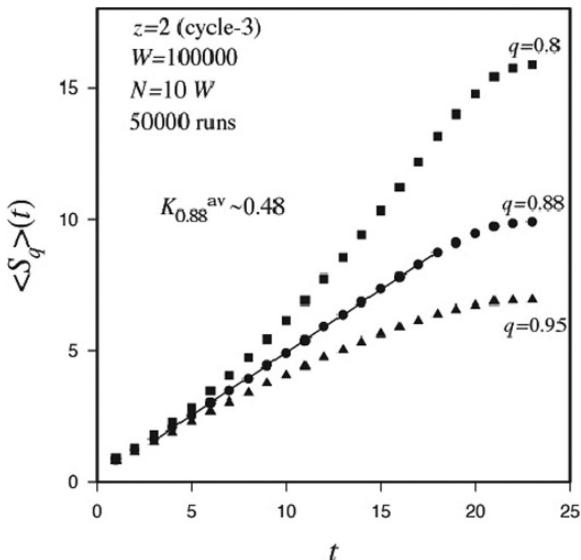
**Fig. 5.5** (continued) Time dependence of  $\langle \ln_q \xi \rangle$  and  $\langle S_q \rangle$ :  $z = 2$  logistic map for strong [(a)  $a = 2$ ] and weak [(c)  $a = 1.401155189$ ] chaos, and  $z = 0.5$  exponential map for strong [(b)  $a = 4$ ] and weak [(d)  $a = 3.32169594$ ] chaos. **Sensitivity function**  $\langle \ln_q \xi \rangle(t)$ : averages over  $10^5$  ( $10^7$ ) runs for (a) and (b) ((c) and (d)); we use  $\Delta x(0) = 10^{-12}$  as the initial discrepancy unless otherwise indicated; in the insets, we show the linear tendency of the sensitivity function for  $q_{sen}^{av}$  with various values of  $\Delta x(0)$ ; at the edge of chaos ((c) and (d)) we exhibit the  $q = 1$  curve nonlinearity. **Entropy**  $\langle S_q \rangle(t)$ : (a,b) 3000 runs with  $N = 10W$  with  $W = 10^5$  and  $W = 3.10^5$  (empty and filled symbols, respectively); 50,000 runs with  $N = 10W$  with  $W = 10^5$  (for (c)) and  $W = 5.10^4$  and  $W = 10^5$  (for (d)). (c) inset: determination of  $q_{sen}^{av}$  (see text). (d) inset: we exhibit the  $q = 1$  curve nonlinearity.



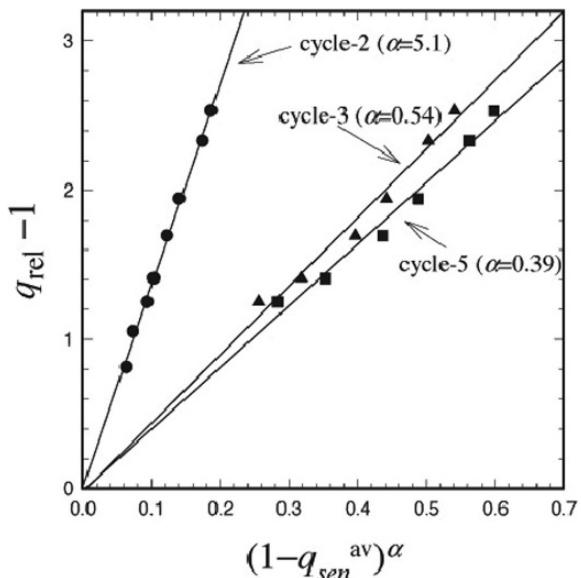
**Fig. 5.7** The volume occupied by the ensemble as a function of discrete time. After a transient period, which is the same for all  $N_{\text{box}}$  values, the power-law behavior is evident. For each case, a set of  $10N_{\text{box}}$  identical copies of the system is followed.



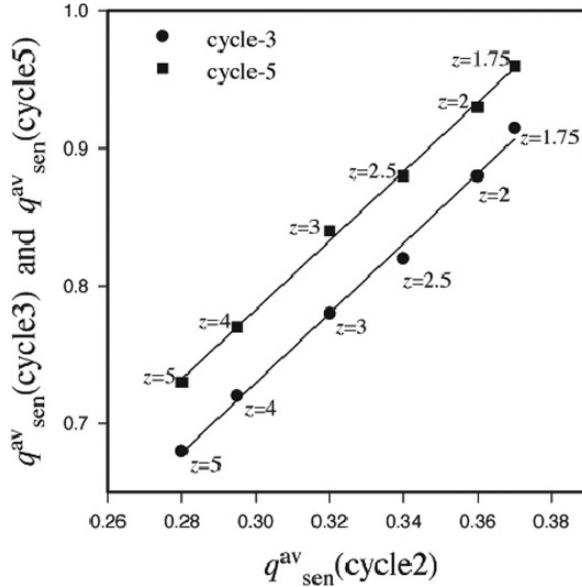
**Fig. 5.8** The behavior of  $\langle \ln_q \xi \rangle$  as a function of time (from [153]).



**Fig. 5.9** The behavior of  $\langle S_q \rangle$  as a function of time (from [153]).



**Fig. 5.10** Straight lines:  $q_{rel}(\text{cycle 2}) - 1 = 13.5 [1 - q_{sen}^{av}(\text{cycle 2})]^{5.1}$ ,  $q_{rel}(\text{cycle 3}) - 1 = 4.6 [1 - q_{sen}^{av}(\text{cycle 3})]^{0.54}$ , and  $q_{rel}(\text{cycle 5}) - 1 = 4.1 [1 - q_{sen}^{av}(\text{cycle 5})]^{0.39}$ . The  $q_{rel} = q_{sen}^{av} = 1$  corner corresponds to the Boltzmann-Gibbs limit (from [153]).



**Fig. 5.11** Straight lines:  $q_{sen}^{av}(\text{cycle 3}) = 2.5 q_{sen}^{av}(\text{cycle 2}) - 0.03$  and  $q_{sen}^{av}(\text{cycle 5}) = 2.5 q_{sen}^{av}(\text{cycle 2}) + 0.03$ , which suggests  $q_{sen}^{av}(\text{cycle 5}) - q_{sen}^{av}(\text{cycle 3}) \simeq 0.06$  (from [153]).

$$q_{sen}^{av}(\text{cycle 5}; z) \simeq 2.5 q_{sen}^{av}(\text{cycle 2}; z) + 0.03, \quad (5.25)$$

hence

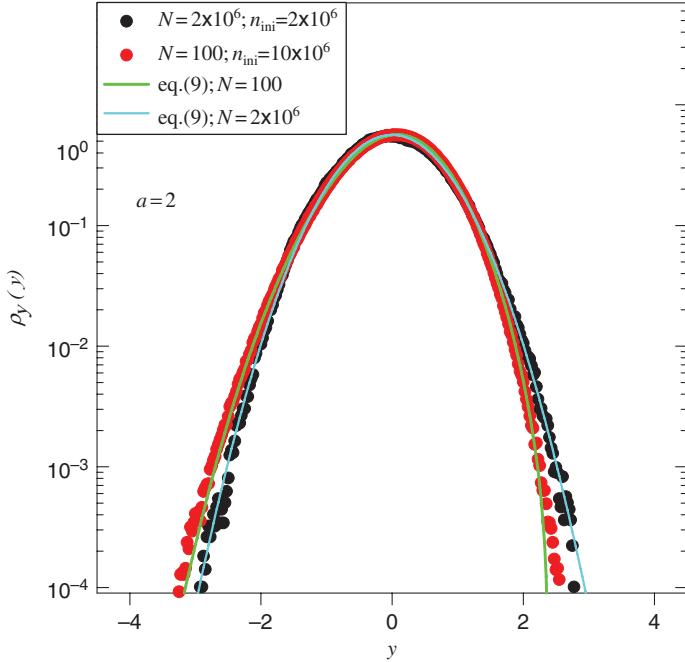
$$q_{sen}^{av}(\text{cycle 5}; z) - q_{sen}^{av}(\text{cycle 3}; z) \simeq 0.06. \quad (5.26)$$

The full understanding of all these relations remains an open problem.

### 5.1.1.6 Attractor

Let us now focus on an important limiting property, directly related to the Central Limit Theorem (CLT). It is in fact a dynamical version of the CLT. As an example of unimodal one-dimensional map, let us consider the  $z$ -logistic one for values of the control parameter  $a$  such that the Lyapunov exponent  $\lambda_1$  is *positive* (i.e., a strongly chaotic map), and start from a given initial condition  $x_0$ . The successive  $N$  iterates  $x_1, x_2, x_3 \dots$ , constitute a time series which associates, with each value of  $x_0$ , the uniquely defined sum of the first  $N$  terms. For fixed  $N$ , we may consider a large set of initial conditions uniformly distributed within the allowed phase-space. The distribution of the sums, appropriately centered and scaled, approaches, for  $N \rightarrow \infty$ , a Gaussian [154]. See Figs. 5.12, 5.13, and 5.14 (from [370]).

The situation changes dramatically if we are at the edge of chaos, where  $\lambda_1 = 0$  (i.e., a weakly chaotic map). The limiting distribution appears to be a  $q$ -Gaussian with  $q = q_{stat} \simeq 1.7$  (*stat* stands for *stationary state*; this qualification will become



**Fig. 5.12** Probability density of rescaled sums of iterates of the logistic map with  $a = 2$ ;  $N = 2 \cdot 10^6$  and  $N = 100$ . The number of initial values contributing to the histogram is  $n_{ini} = 2 \cdot 10^6$ , respectively  $n_{ini} = 10^7$ . The solid lines correspond to the analytical expressions for finite  $N$  (from [370]).

more transparent later on) [370]. See Figs. 5.15 and 5.16. In these figures we can appreciate relatively well the tails of the distributions. The central part can be seen in Fig. 5.17.<sup>4</sup>

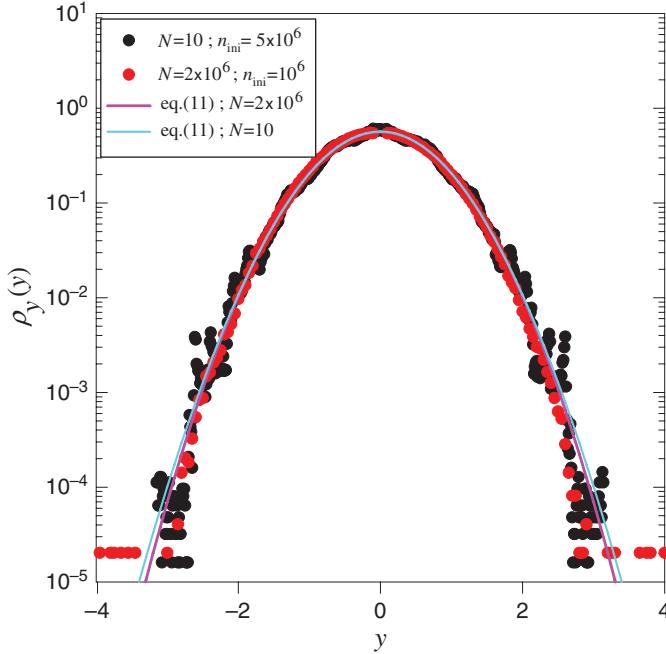
Let us summarize the case of simple one-dimensional dissipative maps at the edge of chaos by reminding that we have established the existence of a basic  $q$ -triplet. In particular, for the  $z = 2$  logistic map we have  $(q_{sen}, q_{rel}, q_{stat}) \simeq (0.24, 2.2, 1.7)$ . Later on, we turn back onto  $q$ -triplets (as well as other values of  $q$ ; see, for instance, [150, 155]).

### 5.1.2 Two-Dimensional Dissipative Maps

Although not with the same detail as for the one-dimensional ones, some two-dimensional dissipative maps have been studied as well [156–158]. More specifically, the Henon and the Lozi maps. Let us illustrate with the Henon map. It is defined as follows:

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<sup>4</sup> An illustration on a different map can be seen in G. Ruiz and C. Tsallis, *Nonextensivity at the edge fo chaos of a new universality class of one-dimensional maps*, Eur. Phys. J. B. (2009), in press, 0901.4292 [cond-mat.stat-mech].



**Fig. 5.13** Probability density of rescaled sums of iterates of the cubic map (which belongs to the same universality class of the logistic map) for  $N = 10^7$  and  $N = 10$ . The number of initial values is  $n_{ini} = 10^6$ ,  $n_{ini} = 5 \cdot 10^6$ , respectively. The solid lines correspond to the analytical expressions for finite  $N$  (from [370]).

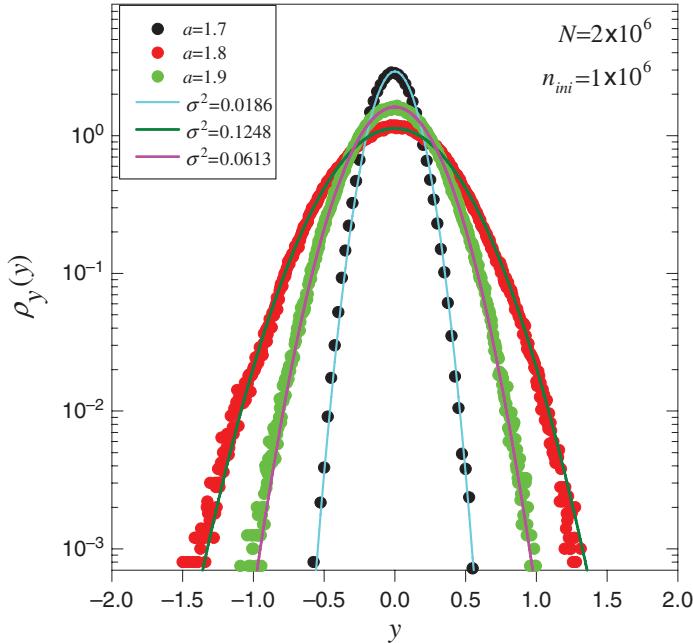
$$x_{t+1} = 1 - ax_t^2 + y_t \quad (5.27)$$

$$y_{t+1} = bx_t. \quad (5.28)$$

The  $b = 0$  particular case corresponds precisely to the  $z = 2$  logistic map. For  $b \geq 0$ , a line (an infinite number of them, in fact) exists in the  $(a, b)$  space on which the system is at the edge of chaos, with vanishing Lyapunov exponents. It is since long well known (see [159] and references therein) that two universality classes exist along this line, namely the dissipative (logistic map) universality map  $\forall b \neq 1$ , and the conservative universality class for  $b = 1$ . One consistently expects that the values of  $q$  should follow the same classes. In particular, the value of  $q_{sen}$  for  $0 < b < 1$  should be the same as that for  $b = 0$ , i.e.,  $q_{sen} = 0.2445 \dots$ . Indeed, precisely this, within some numerical precision, has been verified in [156–158].

## 5.2 Low-Dimensional Conservative Maps

We remind that a  $d$ -dimensional map has  $d$  Lyapunov exponents  $\lambda_1^{(1)}, \lambda_1^{(2)}, \dots, \lambda_1^{(d)}$  ([286] and references therein). If it is *conservative*, it satisfies



**Fig. 5.14** Probability density of rescaled sums of iterates of the logistic map for  $a = 1.7, 1.8, 1.9$  and  $N = 2 \cdot 10^6$ ,  $n_{ini} = 10^6$ . The solid lines show Gaussians  $e^{-y^2/(2\sigma^2)}/\sqrt{2\pi\sigma^2}$  with variance parameter  $\sigma^2$  (from [370]).

$$\sum_{i=1}^d \lambda_1^{(i)} = 0. \quad (5.29)$$

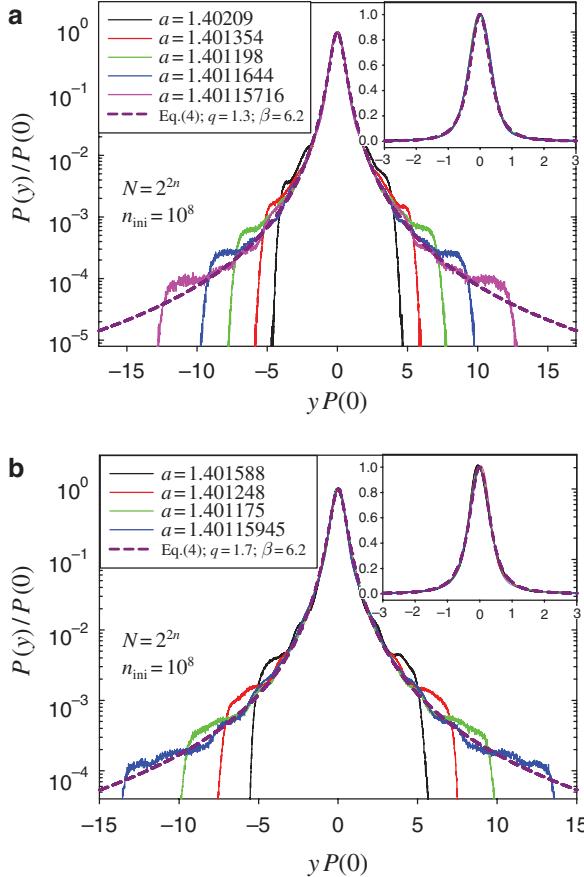
If, in addition to that, it is symplectic,  $d$  is an even integer, and we can therefore conveniently define  $d = 2N$  ( $N = 1, 2, \dots$ ). Furthermore, the Lyapunov exponents are in pairs which differ only in the sign. Obviously, two-dimensional conservative maps are necessarily symplectic.

Entropic properties in low-dimensional maps have already been addressed for  $d = 2$  ([85, 138, 356–358], among others) and  $d = 4$  ([356, 357], among others). The review of some of their peculiarities will pave the understanding of many-body Hamiltonian systems, the primary object of study in statistical mechanics.

### 5.2.1 Strongly Chaotic Two-Dimensional Conservative Maps

In order to illustrate relevant properties, we shall focus here on three paradigmatic (strongly chaotic, area-preserving, and transforming the unit square into itself), two-dimensional conservative maps, first the so-called *baker map*, second the *generalized cat map* [85], and third the *standard map* [85, 356].

The *baker map* is defined as follows [138]:



**Fig. 5.15** Probability density of the quantity  $y/\sigma$  at the critical point  $a_c$  for  $z = 2$ ,  $N = 2^{14}$ , and  $N = 2^{15}$  (from [371]).

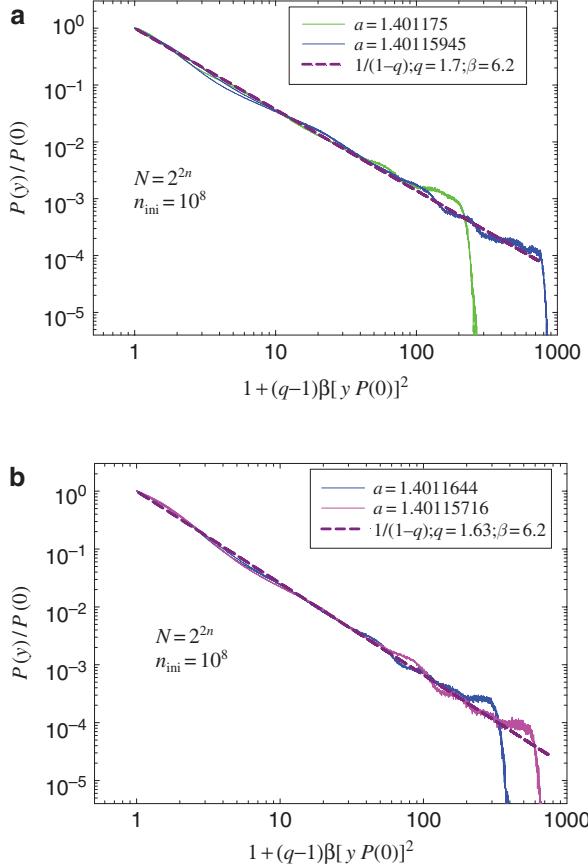
$$(x_{t+1}, y_{t+1}) = \begin{cases} (2x_t, y_t/2) & (0 \leq x_t < 1/2) \\ (2x_t - 1, (y_t + 1)/2) & (1/2 \leq x_t \leq 1). \end{cases} \quad (5.30)$$

We verify that  $|\partial(x_{t+1}, y_{t+1})/\partial(x_t, y_t)| = 1$ , and  $\lambda_1^{(1)} = -\lambda_1^{(2)} = \ln 2$ . See Fig. 5.18. The time dependence of the entropy  $S_q(t)$  is depicted in Figs. 5.19 and 5.20.

The *generalized cat map* is defined as follows [85]

$$\begin{aligned} p_{t+1} &= p_t + k x_t \quad (\text{mod } 1) \\ x_{t+1} &= p_t + (1+k)x_t \quad (\text{mod } 1) \quad (k \geq 0). \end{aligned} \quad (5.31)$$

We verify that  $|\partial(p_{t+1}, x_{t+1})/\partial(p_t, x_t)| = 1$ , and  $\lambda_1^{(1)} = -\lambda_1^{(2)} = \ln \frac{2+k+\sqrt{k^2+4k}}{2}$ . For typical values of  $k$ , it has been numerically verified in [85] that



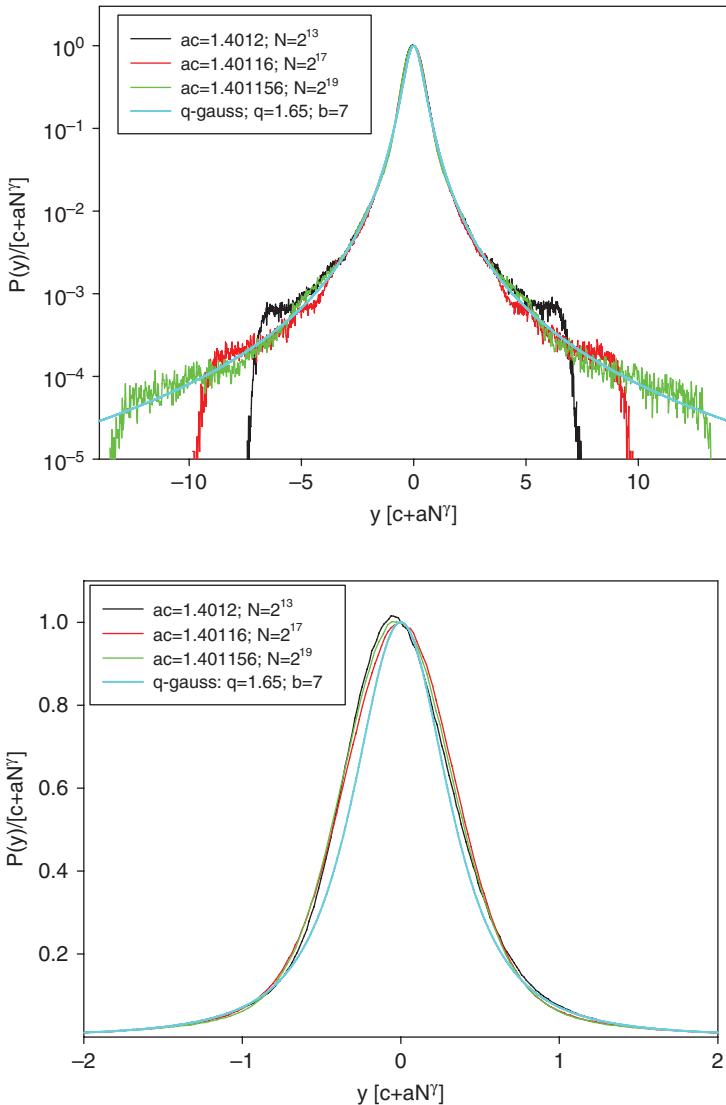
**Fig. 5.16** Probability density of the quantity  $y/\sigma$  at the critical point  $a_c$  for  $z = 1.75, 2, 3$  (from [371]).

$\lim_{t \rightarrow \infty} \lim_{W \rightarrow \infty} \lim_{M \rightarrow \infty} S_{BG}(t)/t = \lambda_1^{(1)}$ . An analytic proof would naturally be most welcome.

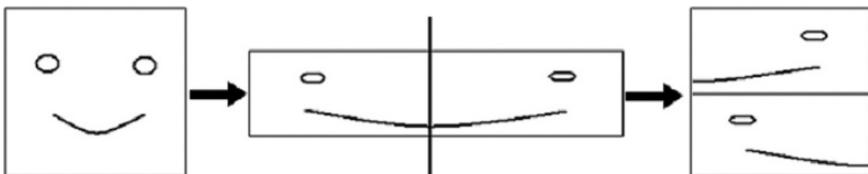
The *standard map* (or *kicked rotor map*) is defined as follows [85, 356]:

$$\begin{aligned} p_{t+1} &= p_t + \frac{a}{2\pi} \sin(2\pi\theta_t) \quad (\text{mod } 1) \\ \theta_{t+1} &= \theta_t + p_{t+1} \quad (\text{mod } 1) \quad (a \geq 0). \end{aligned} \quad (5.32)$$

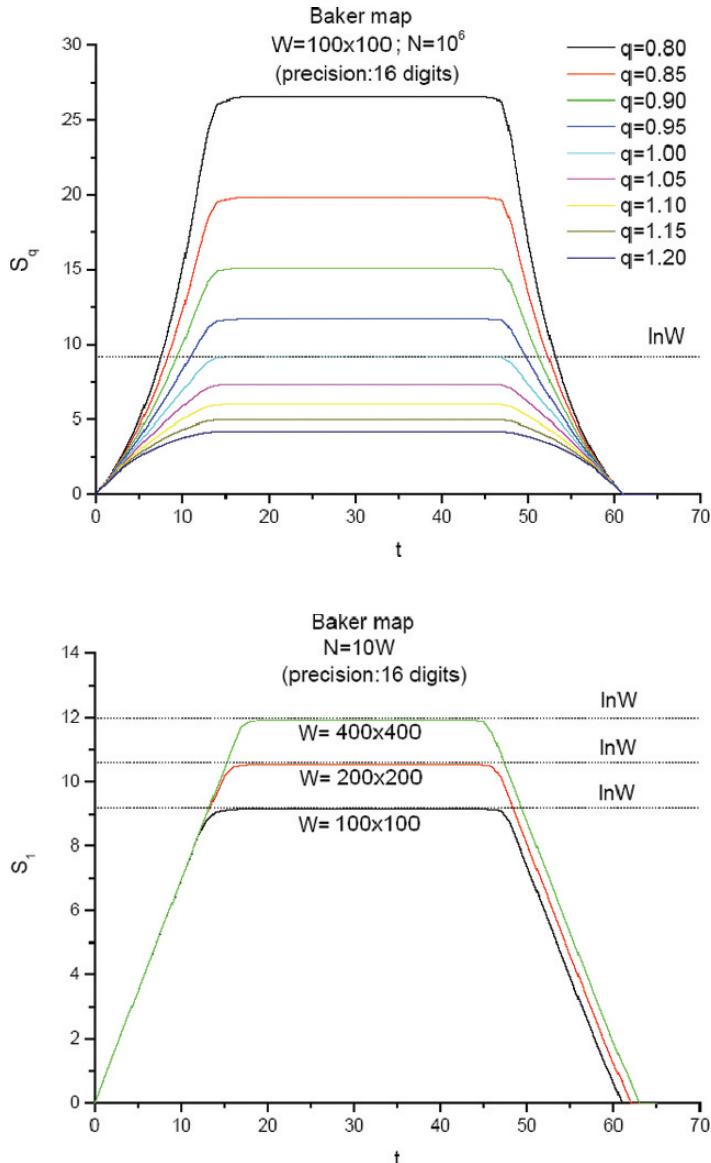
This map is only partially chaotic (i.e., the size of the “chaotic sea” is smaller than the unit square), and the percentage of chaos increases for increasing  $a$ . Inside the chaotic sea, it has been numerically verified [85] that  $\lim_{t \rightarrow \infty} \lim_{W \rightarrow \infty} \lim_{M \rightarrow \infty} S_{BG}(t)/t = \lambda_1^{(1)}$  equals 0.98, 1.62, and 2.30 for  $a = 5, 10$ , and 20, respectively. It is instructive to define [356] a *dynamical “temperature”*  $T$  as the variance of the angular momentum, i.e.,  $T \equiv \langle (p - \langle p \rangle)^2 \rangle = \langle p^2 \rangle - \langle p \rangle^2$ , where  $\langle \rangle$  denotes ensemble



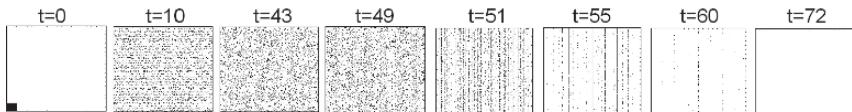
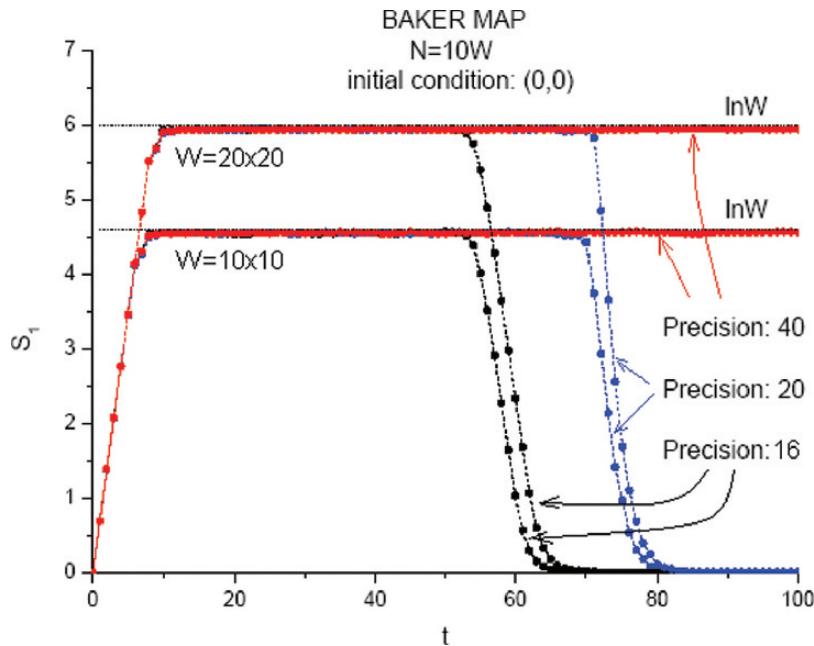
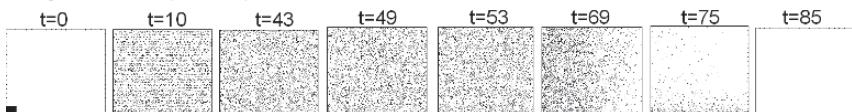
**Fig. 5.17** Distribution for the  $z = 2$  logistic map at the edge of chaos ( $a = a_c$ ). The value of  $N$  must increase together with the degree of precision used to approximate  $a_c$  (from [371]).



**Fig. 5.18** The nondissipative baker map. From [138].

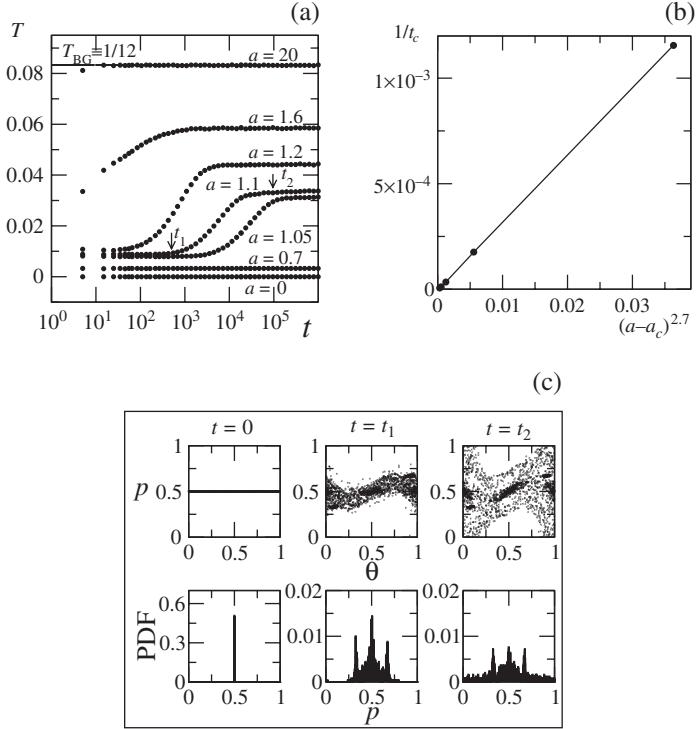


**Fig. 5.19** Time evolution of the  $q$ -entropy for the non-dissipative baker map, using 16 digit calculations. *Top:*  $S_q(t)$  for entropic indices  $q = 0.80, 0.85, 0.90, 0.95, 1.00, 1.05, 1.10, 1.15, 1.20$  (from top to bottom) when  $W = 10^4$  and  $N = 10^6$ . *Bottom:*  $S_1(t)$  for typical values of  $W$  ( $W = 10^4, 4 \times 10^4, 16 \times 10^4$ ;  $N = 10W$ ). Notice that the bounding value for the  $q = 1$  entropy corresponds, in all cases, to equiprobability, i.e.,  $\ln W$ . The slope  $dS_1(t)/dt$  (on the left side) recovers the well-known values for the Lyapunov exponents  $\lambda_1^{(1)} = -\lambda_1^{(2)} = \ln 2$  (from [138]).

16-digit calculations ( $W=10 \times 10$ ):20-digit calculations ( $W=10 \times 10$ ):

**Fig. 5.20** Numerical study of the baker map, with controlled fixed precision. The sequences of the top figure exhibit the evolution in phase-space with a fixed precision. The corresponding curves for  $S_1(t)$  are shown in the bottom figure. The evolution of  $S_1(t)$  corresponding to a higher fixed precision experiment (40 digits) is shown as well; the time reversal of the entropy is not observed before  $t = 100$  (from [138]).

average. The temperature associated with the uniform ensemble (that we will call *BG temperature*  $T_{BG}$  because of its similarity with the equal-a-priori-probability postulate) is given by  $T_{BG} = \int_0^1 dp p^2 - (\int_0^1 dp p^2)^2 = 1/12$ . Notice that, in the present conservative model, the “temperature”  $T$  is necessarily bounded since  $p$  itself is bounded, in contrast with a true thermodynamical temperature, which is of course unbounded. The time evolution of the system and of  $T$ , for typical values of  $a$  are depicted in Fig. 5.21.

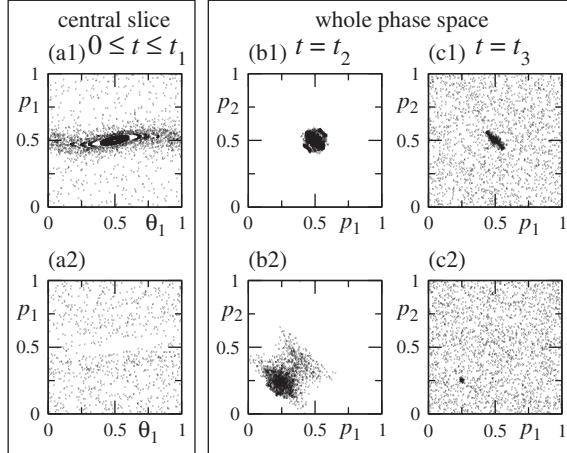


**Fig. 5.21** (a) Time evolution of the dynamical temperature  $T$  of a standard map, for typical values of  $a$ . We start with “water bag” initial conditions ( $M = 2500$  points in  $0 \leq \theta \leq 1$ ,  $p = 0.5 \pm 10^{-4}$ ). In order to eliminate cyclical fluctuations, the dots represent average of 10 iteration steps; moreover, each curve is the average of 50 realizations. (b) Inverse crossover time  $t_c$  (inflection point between the QSS and the BG regimes) vs.  $1/(a - a_c)^{2.7}$ . No inflection points subsist if  $t$  is linearly represented. (c) Time evolution of the ensemble in (a) for  $a = 1.1$  (first row) and PDF of its angular momentum (second row).  $t = 0$ : “water bag” initial conditions;  $t = t_1 = 500$ : the ensemble is mostly restricted by cantori;  $t = t_2 = 10^5$ : the ensemble is confined inside KAM-tori (from [356]).

### 5.2.2 Strongly Chaotic Four-Dimensional Conservative Maps

In the previous subsection we considered  $N = 1$  particle. Let us consider here  $N = 2$ , on the road to the thermodynamic limit  $N \rightarrow \infty$  [85, 356, 357]. We shall focus on a simple symplectic system of two coupled standard maps, defined as follows:

$$\begin{aligned}\theta_1(t+1) &= p_1(t+1) + \theta_1(t) + b p_2(t+1), \\ p_1(t+1) &= p_1(t) + \frac{a_1}{2\pi} \sin[2\pi\theta_1(t)], \\ \theta_2(t+1) &= p_2(t+1) + \theta_2(t) + b p_1(t+1), \\ p_2(t+1) &= p_2(t) + \frac{a_2}{2\pi} \sin[2\pi\theta_2(t)],\end{aligned}\tag{5.33}$$



**Fig. 5.22** Phase-space analysis of the evolution of “water bag” ensembles for two coupled standard maps for  $(\tilde{a}, b) = (0.4, 2)$ . First row: “Water bag” initial conditions  $0 \leq \theta_1, \theta_2 \leq 1, p_1, p_2 = 0.5 \pm 5 \cdot 10^{-3}$ . Second row: “Water bag” initial conditions  $0 \leq \theta_1, \theta_2 \leq 1, p_1, p_2 = 0.25 \pm 5 \cdot 10^{-3}$ . (a) Projection on the  $(\theta_1, p_1)$ -plane of the central slice of the phase-space ( $\theta_2, p_2 = 0.5 \pm 10^{-2}$ ), for the orbit  $0 \leq t \leq t_1 = 10^4$ . (c),(c) Projection on the  $(p_1, p_2)$ -plane of whole phase-space for the iterate at time  $t_2 = 15$  and  $t_3 = 2 \cdot 10^4$  (from [356]).

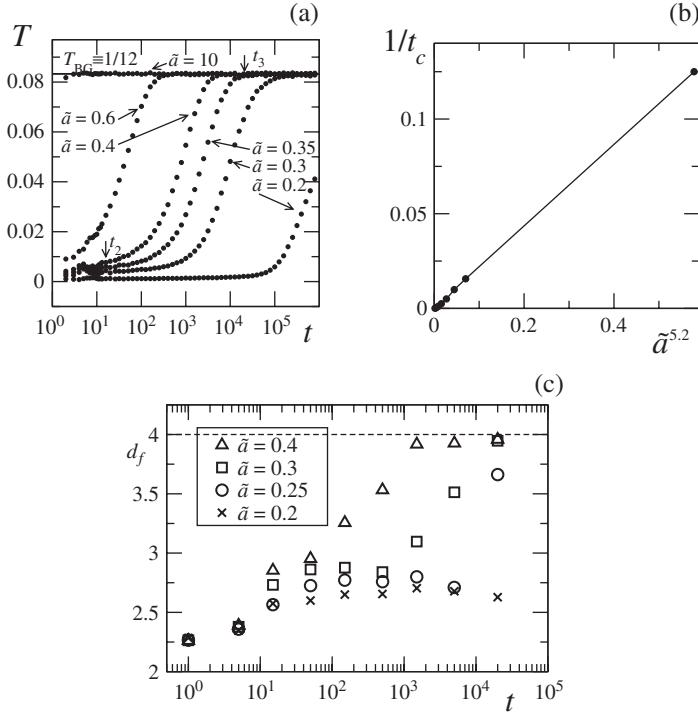
where  $a_1, a_2, b \in \mathbb{R}$ ,  $t = 0, 1, \dots$ , and all variables are defined mod 1. If the coupling constant  $b$  vanishes the two standard maps decouple; if  $b = 2$  the points  $(0, 1/2, 0, 1/2)$  and  $(1/2, 1/2, 1/2, 1/2)$  are a 2-cycle for all  $(a_1, a_2)$ , hence we preserve in phase-space the same referential that we had for a single standard map. For a generic value of  $b$ , all relevant present results remain qualitatively the same. Also, we set  $a_1 = a_2 \equiv \tilde{a}$  so that the system is invariant under permutation  $1 \leftrightarrow 2$ . Since we have two rotors now, the *dynamical temperature* is naturally given by  $T \equiv \frac{1}{2} (\langle p_1^2 \rangle + \langle p_2^2 \rangle - \langle p_1 \rangle^2 - \langle p_2 \rangle^2)$ , hence the BG temperature remains  $T_{BG} = 1/12$ . The time evolution of the system is depicted in Figs. 5.22, 5.23, and 5.24.

### 5.2.3 Weakly Chaotic Two-Dimensional Conservative Maps

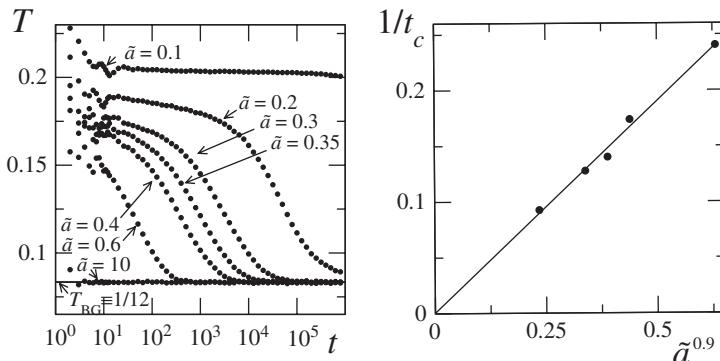
In the previous subsections we have analyzed low-dimensional systems that are strongly chaotic. We shall dedicate the present subsection to weakly chaotic two-dimensional systems, namely the *Casati–Prosen map* (or *triangle map*) [8–10] and the *Moore map* [134–136], the former as focused on in [358], the latter as focused on in [138].

The *Casati–Prosen map*  $z_{n+1} = T(z_n)$  is defined on a torus  $z = (x, y) \in [-1, 1] \times [-1, 1]$

$$\begin{aligned} y_{n+1} &= y_n + \alpha \operatorname{sgn} x_n + \beta \quad (\text{mod } 2), \\ x_{n+1} &= x_n + y_{n+1} \quad (\text{mod } 2), \end{aligned} \tag{5.34}$$



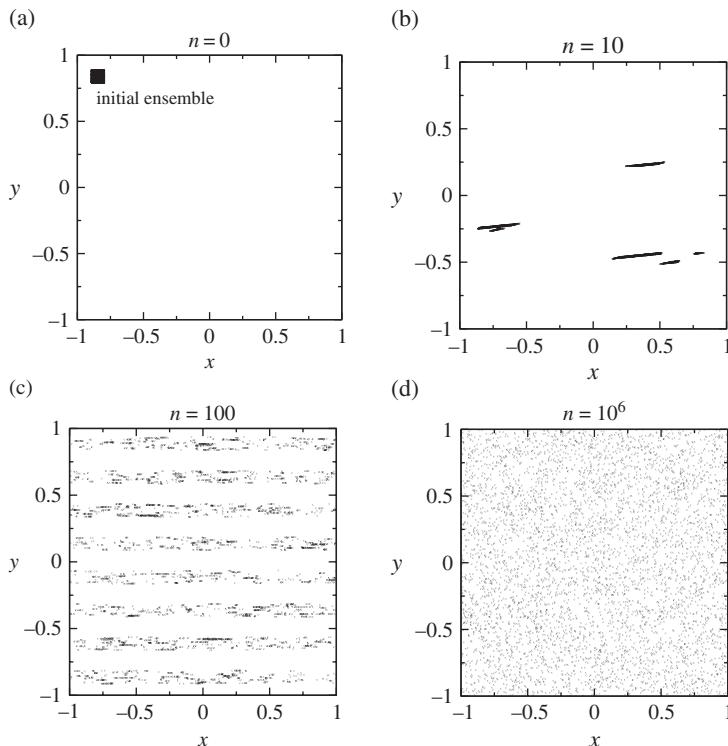
**Fig. 5.23** (a) Time evolution of the dynamical temperature  $T$  of two coupled standard maps, for  $b = 2$  and typical values of  $\tilde{a}$ . We start with water bag initial conditions ( $M = 1296$  points with  $0 \leq \theta_1, \theta_2 \leq 1$ , and  $p_1, p_2 = 0.25 \pm 5 \cdot 10^{-3}$ ); moreover, an average was taken over 35 realizations. See Fig. 5.22 for  $t_2$  and  $t_3$ . (b) Inverse crossover time  $t_c$  vs.  $1/\tilde{a}^{5.2}$ . (c) Time evolution of the fractal dimension of a single initial ensemble in the same setup of (a) (from [356]).



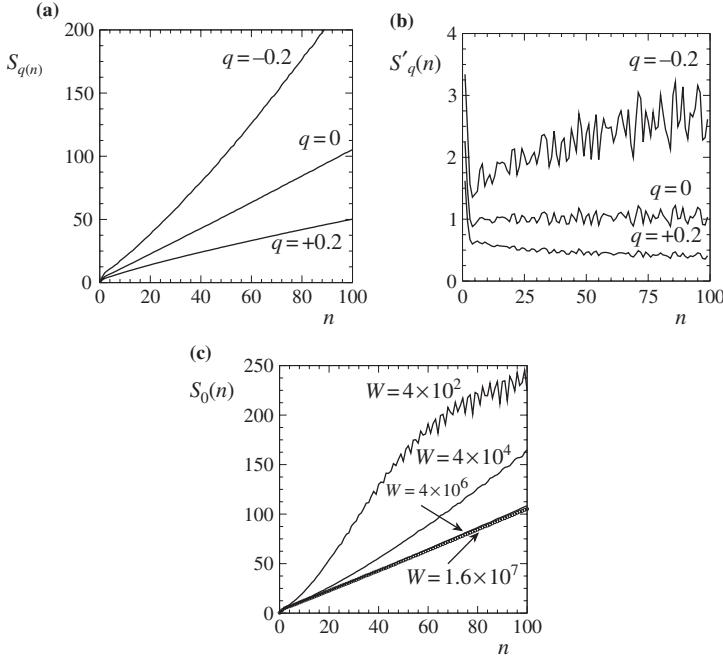
**Fig. 5.24** Same as Fig. 5.23(a),(b) but with “double water bag” initial conditions:  $0 \leq \theta_1, \theta_2 \leq 1$ ;  $p_1, p_2$  randomly distributed inside one of the two regions  $p_1, p_2 = 0 + 10^{-2}, p_1, p_2 = 1 - 10^{-2}$  (from [356]).

where  $\text{sgn}x = \pm 1$  is the sign of  $x$ , and  $\alpha, \beta$  are two parameters ( $n = 0, 1, \dots$ ). This map is linearly unstable. For rational values of  $\alpha, \beta$  the system is in principle integrable, as the dynamics is confined on invariant curves. If  $\beta = 0$  and  $\alpha$  is irrational, the dynamics is ergodic but the phase-space is filled very slowly, while for incommensurate irrational values of  $\alpha, \beta$  the dynamics is ergodic and mixing with dynamical correlation function decaying as  $t^{-3/2}$  (i.e.,  $q_{\text{rel}} = 5/3$ , according to a notation that will be discussed later on). This map does not have any secondary time scales, and the exploration of the phase-space by a given orbit is arbitrarily close to that of a random model.

For the sake of definiteness, in the following we will fix (see [358]) the parameter values  $\alpha = [\frac{1}{2}(\sqrt{5} - 1) - e^{-1}]/2$ ,  $\beta = [\frac{1}{2}(\sqrt{5} - 1) + e^{-1}]/2$  although it should be noticed that qualitatively identical results are obtained for other irrational parameter values. Figure 5.25 shows the mixing process of an ensemble of points initially localized inside a small square. The action of the map (5.34) initially divides the area covered by the ensemble into different unconnected portions, each essentially stretched along a straight line. After a certain amount of time, these portions overlap until a slow relaxation process to a complete mixing is observed. We can verify in



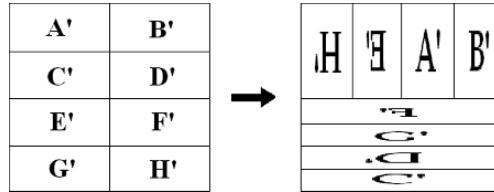
**Fig. 5.25** Time evolution of an ensemble of points in phase-space. (a) The ensemble is initially located inside a single cell. (b, c, and d) Phase-space distribution after  $n = 10, 10^2, 10^6$  map iterations (from [358]).



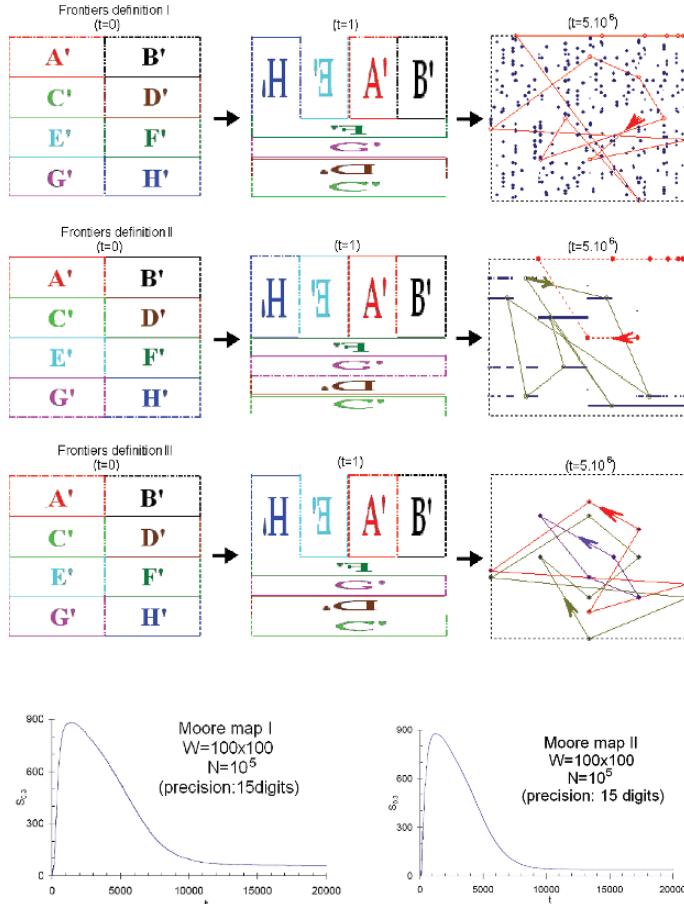
**Fig. 5.26** Time-evolution of the statistical entropy  $S_q$  for different values of  $q$ . The phase-space has been divided into  $W = 4000 \times 4000$  equal cells of size  $l = 5 \times 10^{-4}$  and the initial ensemble is characterized by  $N = 10^3$  points randomly distributed inside a partition-square. Curves are the result of an average over 100 different initial squares randomly chosen in phase-space. The analysis of the derivative of  $S_q$  in (b) shows that only for  $q = 0$  a linear behavior is obtained. In fact, a linear regression provides  $S_0(n) = 1.029 n + 1.997$  with a correlation coefficient  $R = 0.99993$ . (c) shows that the linear growth for  $S_0$  is reached from above, in the limit  $W \rightarrow \infty$ . (from [358]).

Fig. 5.26 that  $q_{ent} = 0$ . The linear time-dependence [8,9] of the sensitivity  $\xi$  implies  $q_{sen} = 0$ , which, as usual, coincides with  $q_{ent}$ . Furthermore, we can verify that the  $q$ -generalized Pesin-like identity is once again satisfied.

In conclusion, while positivity of Lyapunov exponents is *sufficient* for a meaningful statistical description (the *BG* statistical mechanics), it might be *not necessary*. Indeed, we have illustrated, for a conservative, mixing and ergodic nonlinear dynamical system, that the use of the more general entropy  $S_q$  (with the value  $q = 0$  for this case) provides a satisfactory frame for handling nonlinear dynamical systems whose maximal Lyapunov exponent vanishes. In particular, we have shown that (the upper bound of) the coefficient  $\lambda_q$  of the sensitivity to the initial conditions *coincides* with the entropy production per unit time, in total analogy with the Pesin theorem for standard chaotic systems. These results suggest that a thermostatistical approach of such systems is possible. Indeed, the structure that we have exhibited here for the time dependence of  $S_q$  is totally analogous to the one that has been recently exhibited [199] for the  $N$ -dependence of  $S_q$ , where  $N$  is the number of elements of a many-body system. When the number of nonzero-probability states of the system increases as a power of  $N$  (instead of exponentially with  $N$  as usually),



**Fig. 5.27** The Moore map. Alphabetic symbols are written on the cells to show how local dynamics evolves (from [138]).

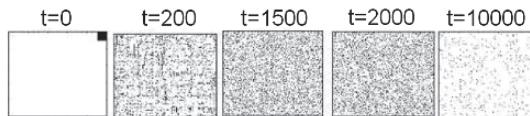


**Fig. 5.28** Time evolution of three Moore maps (denoted by I, II, and III) which differ just in the definition of the mapping of the frontiers. Alphabetic symbols are written inside the cells, and different types of colored lines are also traced, to help the description of the evolution of their frontiers. *Top figures:* Snapshots of the evolution in phase-space ( $t = 0$ ,  $t = 1$ , and  $t = 5 \times 10^6$ ), when starting with points exclusively *on* the frontiers. In the  $t = 5 \times 10^6$  squares, we have also indicated typical trajectories. *Bottom figures:* Time evolution of  $S_{0,3}$  for maps I and II, starting with a set of initial conditions within a small cell ( $W = 10^4$ ;  $N = 10^5$ ) (from [138]).

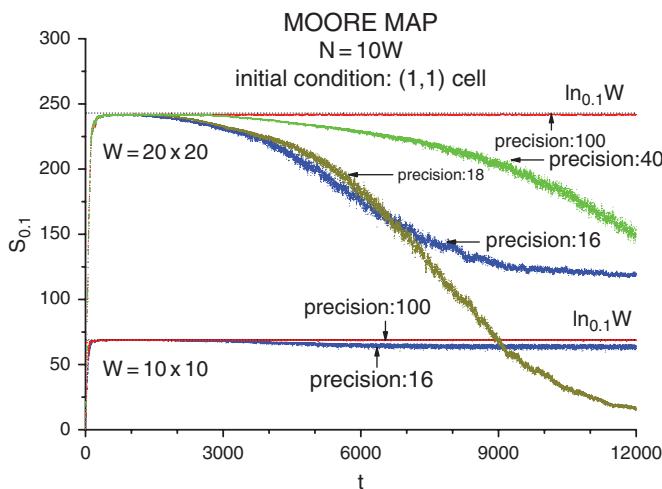
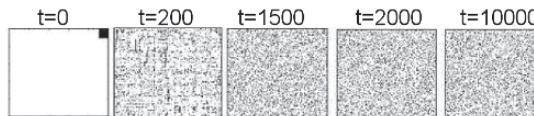
a special value of  $q$  below unity exists such that  $S_q$  is *extensive*. In other words,  $S_q$  asymptotically increases *linearly* with  $N$ , whereas  $S_{BG}$  does not.

The *Moore map* we shall study is a paradigmatic one belonging to the generalized shift family of maps proposed by Moore [134]. This class of dynamical systems poses some sort of undecidability, as compared with other low-dimensional chaotic systems [134, 135]. It is equivalent to the piecewise linear map shown in Fig. 5.27. When this map is recurrently applied, the area in phase-space is conserved, while the corresponding shape keeps changing in time, becoming increasingly complicated. This map appears to be ergodic, possibly exhibits a Lyapunov exponent  $\lambda_1 = 0$ , and, presumably, the divergence of close initial conditions follows a power-law behavior [137]. When we consider a partition of  $W$  equal cells and select  $N$  random initial conditions inside one random cell, the points spread much slower than they do on the baker map. More precisely, they spread, through a slow relaxation process, all over the phase-space, each orbit appearing to gradually fill up the entire square. See Figs. 5.28, 5.29, and 5.30.

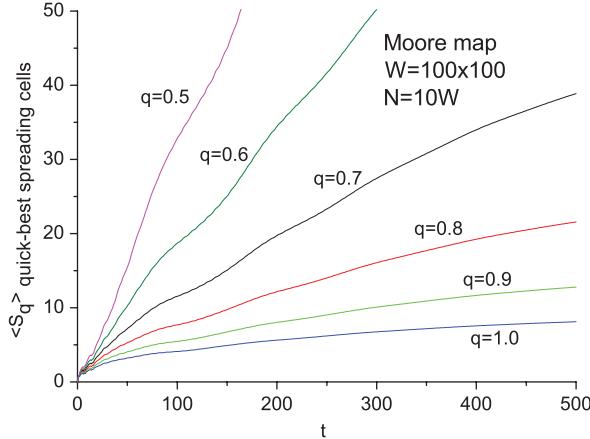
16-digit calculations ( $W=10 \times 10$ ):



100-digit calculations ( $W=10 \times 10$ ):



**Fig. 5.29** Numerical study of the Moore map I. *Top figures:* Evolution of occupancy in phase-space. *Bottom figure:* Evolution of  $S_{0.1}$ .



**Fig. 5.30** Time dependence of  $S_q$  averaged over the 10% quick-best spreading cells, on the far-from-equilibrium regime, for typical values of  $q$ .

In order to have a *finite* entropy production for  $S_q$  we need a value of  $q$  which is definitively smaller than unity, i.e., the Boltzmann–Gibbs entropy does not appear as the most adequate tool. Deeper studies are needed in order to establish whether another value of  $q$  can solve this problem.

### 5.3 High-Dimensional Conservative Maps

The model we focus on here [359] is a set of  $N$  symplectically coupled (hence conservative) standard maps, where the coupling is made through the *coordinates* as follows:

$$\begin{aligned} \theta_i(t+1) &= \theta_i(t) + p_i(t+1) \quad (\text{mod } 1), \\ p_i(t+1) &= p_i(t) + \frac{a}{2\pi} \sin[2\pi\theta_i(t)] + \\ &\quad \frac{b}{2\pi N} \sum_{\substack{j=1 \\ j \neq i}}^N \frac{\sin[2\pi(\theta_i(t)-\theta_j(t))]}{r_{ij}^\alpha} \quad (\text{mod } 1), \end{aligned} \tag{5.35}$$

where  $t$  is the discrete time  $t = 1, 2, \dots$ , and  $\alpha \geq 0$ . The  $a$  parameter is the usual nonlinear constant of the individual standard map, whereas the  $b$  parameter modulates the overall strength of the long-range coupling. Both parameters contribute to the nonlinearity of the system; it becomes integrable when  $a = b = 0$ . For simplicity, we have studied only the cases  $a > 0$ ,  $b > 0$ , but we expect similar results when one or both of these parameters are negative. The systematic study of the whole parameter space is certainly welcome. Notice that, in order to describe a system whose phase-space is bounded, we are considering, as usual, only the

torus (mod 1). Additionally, the maps are placed in a one dimensional ( $d = 1$ ) regular lattice with periodic boundary conditions. The distance  $r_{ij}$  is the minimum distance between maps  $i$  and  $j$ , hence it can take values from unity to  $\frac{N}{2}$  ( $\frac{N-1}{2}$ ) for even (odd) number  $N$  of maps. Note that  $r_{ij}$  is a fixed quantity that, modulated with the power  $\alpha$ , enters Eq. (5.35) as an effective time-independent coupling constant. As a consequence,  $\alpha$  regulates the range of the interaction between maps. The sum is global (i.e., it includes every pair of maps), so the limiting cases  $\alpha = 0$  and  $\alpha = \infty$  correspond, respectively, to infinitely long range and nearest neighbors. In our case  $d=1$ , thus  $0 \leq \alpha \leq 1$  ( $\alpha > 1$ ) means *long-range* (*short-range*) coupling. Moreover, the coupling term is normalized by the sum [177, 360]  $\tilde{N} \equiv d \int_1^{N^{1/d}} dr r^{d-1} r^{-\alpha} = \frac{N^{1-\alpha/d} - \alpha/d}{1-\alpha/d}$ , to yield a non-diverging quantity as the system size grows (for simplicity, we have replaced here the exact discrete sum over integer  $r$  by its continuous approximation).

If  $G(\bar{x})$  denotes a map system, then  $G$  is symplectic when its Jacobian  $\partial G / \partial \bar{x}$  satisfies the relation [83]:

$$\left( \frac{\partial G}{\partial \bar{x}} \right)^T J \left( \frac{\partial G}{\partial \bar{x}} \right) = J, \quad (5.36)$$

where the superindex  $T$  indicates the transposed matrix, and  $J$  is the Poisson matrix, defined by

$$J \equiv \begin{pmatrix} 0 & I \\ -I & 0 \end{pmatrix}, \quad (5.37)$$

$I$  being the  $N \times N$  identity matrix. A consequence of Eq. (5.36) is that the Jacobian determinant  $|\partial G / \partial \bar{x}| = 1$ , indicating that the map  $G$  is (*hyper*)volume-preserving. In particular, for our model

$$\frac{\partial G}{\partial \bar{x}} = \begin{pmatrix} I & I \\ B & (I + B) \end{pmatrix}, \quad (5.38)$$

where  $\bar{x}$  is the  $2N$ -dimensional vector  $\bar{x} \equiv (\bar{p}, \bar{\theta})$ , and

$$B = \begin{pmatrix} K_{\theta_1} & c_{21} & \dots & c_{N1} \\ c_{12} & K_{\theta_2} & \dots & c_{N2} \\ \vdots & \vdots & \vdots & \vdots \\ c_{1N} & c_{2N} & \dots & K_{\theta_N} \end{pmatrix}, \quad (5.39)$$

with

$$K_{\theta_i} \equiv a \cos[2\pi\theta_i(t)] + \frac{b}{\tilde{N}} \sum_{j \neq i} \frac{\cos[2\pi(\theta_i(t) - \theta_j(t))]}{r_{ij}^\alpha}, \quad (5.40)$$

and

$$c_{ij} = c_{ji} \equiv -\frac{b}{\tilde{N}} \frac{\cos[2\pi(\theta_i(t) - \theta_j(t))]}{r_{ij}^\alpha}, \quad (5.41)$$

where  $i, j = 1, \dots, N$ . It can be seen that,

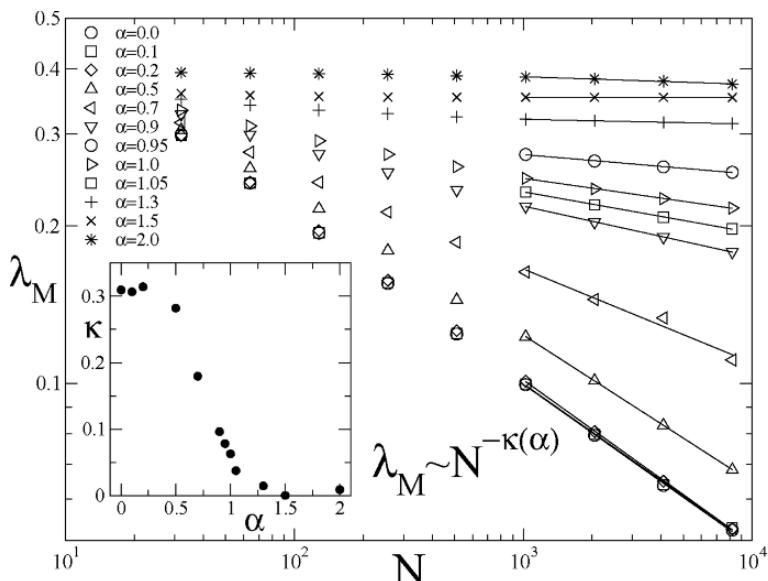
$$\left( \frac{\partial G}{\partial \bar{x}} \right)^T = \begin{pmatrix} I & B \\ I & (I + B) \end{pmatrix}, \quad (5.42)$$

hence

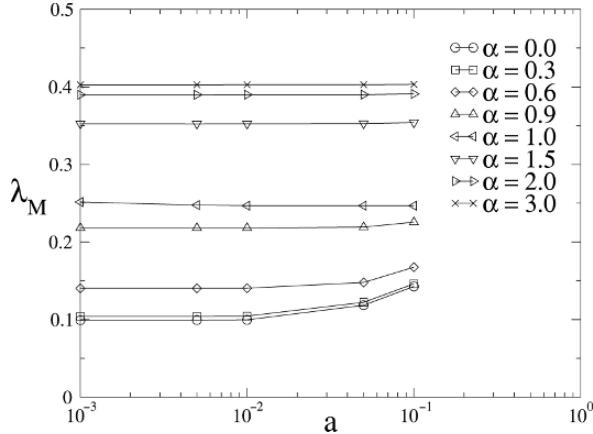
$$\left( \frac{\partial G}{\partial \bar{x}} \right)^T J = \begin{pmatrix} -B & I \\ -(I + B) & I \end{pmatrix}. \quad (5.43)$$

This quantity, multiplied (from the right side) by the matrix (5.38) yields  $J$ . Therefore our system is symplectic. Consequently, the  $2N$  Lyapunov exponents  $\lambda_1 \equiv \lambda_M, \lambda_2, \lambda_3, \dots, \lambda_{2N}$  are coupled two by two as follows:  $\lambda_1 = -\lambda_{2N} \geq \lambda_2 = -\lambda_{2N-1} \geq \dots \geq \lambda_N = -\lambda_{N+1} \geq 0$ . In other words, as a function of time, an infinitely small *length* typically diverges as  $e^{\lambda_1 t}$ , an infinitely small *area* diverges as  $e^{(\lambda_1 + \lambda_2)t}$ , an infinitely small *volume* diverges as  $e^{(\lambda_1 + \lambda_2 + \lambda_3)t}$ , an infinitely small  $N$ -dimensional *hypervolume* diverges as  $e^{(\sum_{i=1}^N \lambda_i)t}$  ( $\sum_{i=1}^N \lambda_i$  being in fact equal to the Kolmogorov–Sinai entropy rate, in agreement with the Pesin identity), an infinitely small  $(N + 1)$ -hypervolume diverges as  $e^{(\sum_{i=1}^{N+1} \lambda_i)t}$ , and so on. For example, a  $(2N - 1)$ -hypervolume diverges as  $e^{\lambda_1 t}$ , and finally a  $2N$ -hypervolume remains constant, thus recovering the conservative nature of the system (of course, this corresponds to the Liouville theorem in classical Hamiltonian dynamics).

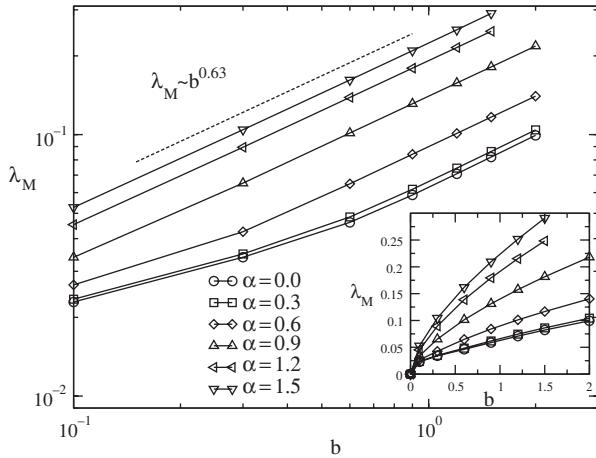
Typical results are depicted in Figs. 5.31, 5.32, 5.33, 5.34, and 5.35.



**Fig. 5.31** Lyapunov exponent dependence on system size  $N$  in log–log plot, showing that  $\lambda_M \sim N^{-\kappa(\alpha)}$ . Initial conditions correspond to  $\theta_0 = 0.5$ ,  $8\theta = 0.5$ ,  $p_0 = 0.5$ , and  $\delta p = 0.5$ . Fixed parameters are  $a = 0.005$  and  $b = 2$ . We averaged over 100 realizations. *Inset:*  $\kappa$  vs.  $\alpha$ , exhibiting weak chaos in the limit  $N \rightarrow \infty$  when  $0 \leq \alpha \lesssim 1$  (from [359]).



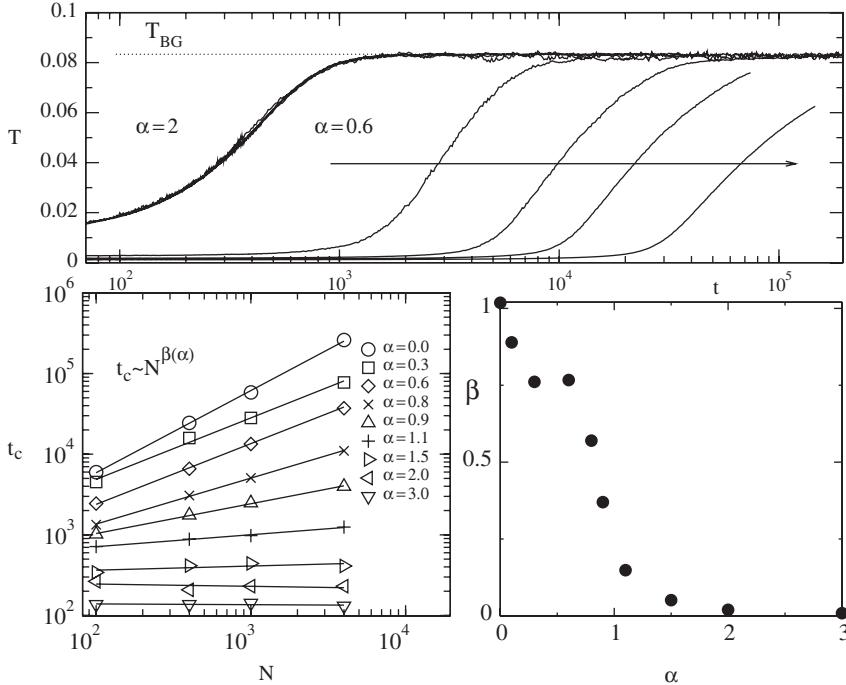
**Fig. 5.32** Lyapunov exponent dependence on  $a$  for different values of  $\alpha$ . Fixed constants are  $N = 1024$  and  $b = 2$ . Initial conditions correspond to  $\theta_0 = 0.5$ ,  $\delta\theta = 0.5$ ,  $p_0 = 0.5$ , and  $\delta p = 0.5$ . We averaged over 100 realizations (from [359]).



**Fig. 5.33** Lyapunov exponent dependence on  $b$  in log-log plot. Fixed constants are  $N = 1024$  and  $a = 0.005$ . Initial conditions correspond to  $\theta_0 = 0.5$ ,  $\delta\theta = 0.5$ ,  $p_0 = 0.5$  and  $\delta p = 0.5$ . We averaged over 100 realisations. *Inset:* Same data in linear-linear plot (from [359]).

## 5.4 Many-Body Long-Range-Interacting Hamiltonian Systems

In this section, we focus on a central question, namely many-body Hamiltonian systems with interactions that can have a long-range character (i.e.,  $0 \leq \alpha/d \leq 1$  for classical systems). To isolate the role of the range of the interaction from any other influence, we shall consider interactions which present no particular difficulty at the origin (consequently, Newtonian gravitation is excluded since it has a divergent

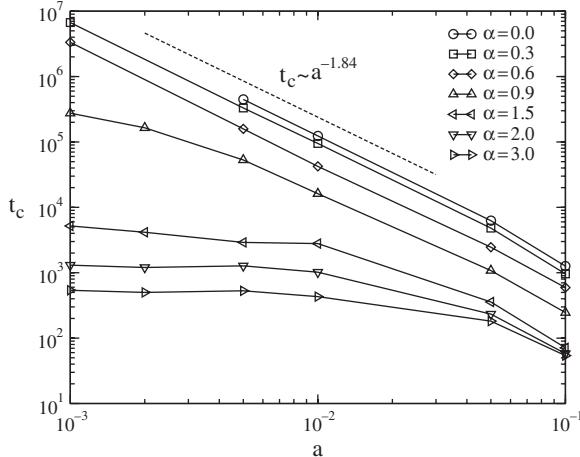


**Fig. 5.34** *Upper panel:* Temperature evolution for  $\alpha = 2$  and  $\alpha = 0.6$  and four system sizes  $N = 100, 400, 1000, 4000$ . Initial conditions correspond to  $\theta_0 = 0.5$ ,  $\delta\theta = 0.5$ ,  $p_0 = 0.3$ , and  $\delta p = 0.05$ . Fixed constants are  $a = 0.05$  and  $b = 2$ . For  $\alpha = 2$  the four curves coincide almost completely, all having a very fast relaxation to  $T_{BG}$ . For  $\alpha = 0.6$  the same sizes are shown, growing in the direction of the arrow. *Left bottom panel:* crossover time  $t_c$  vs.  $N$ , showing a power-law dependence  $t_c \sim N^{\beta(\alpha)}$  with  $\beta(\alpha) \geq 0$ . *Right bottom panel:*  $\beta$  vs.  $\alpha$  shows that for long-range interactions the QS state life-time diverges in the thermodynamic limit. Note that when  $\alpha = 0$ ,  $\beta = 1$ , and hence  $t_c \propto N$ . Given the nonneglectable error bars due to finite size effects, the relation  $\beta = 1 - \alpha$  is not excluded as possibly being the exact one; more precisely, it is nonunplausible that  $t_c \propto \frac{N^{1-\alpha}-1}{1-\alpha}$  (from [359]).

attraction at the origin). More precisely, either we shall assume that the elements of the system (e.g., classical rotors) are localized on a lattice, and the long-range manifests itself through a slowly decaying coupling constant, or the elements of the system (e.g., point atoms of a gas) are free to move translationally but then a short-distance strong repulsion (such as the  $1/r^{12}$  potential term in the Lennard-Jones model for a real gas) inhibits them from being too close to each other.

As a paradigmatic system along the above lines, we shall focus on the following model of classical planar rotors [177]. The Hamiltonian is assumed to be

$$\mathcal{H} = \frac{1}{2} \sum_{i=1}^N p_i^2 + \frac{1}{2} \sum_{i \neq j} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^\alpha} \equiv K + V \quad (\alpha \geq 0), \quad (5.44)$$



**Fig. 5.35** Temperature dependence on  $a$ . Fixed constants are  $N = 100$  and  $b = 2$ . Initial conditions correspond to  $\theta_0 = 0.5$ ,  $\delta\theta = 0.5$ ,  $p_0 = 0.3$ , and  $\delta p = 0.05$ . We averaged over 100 realizations (from [359]).

where the rotors are localized on a lattice (e.g., a translationally invariant Bravais lattice, a quasi-crystal, a hierarchical network). If the lattice is a  $d$ -dimensional hypercubic one (with periodic boundary conditions) we have  $r_{ij} = 1, 2, 3, \dots$  if  $d = 1$ ,  $r_{ij} = 1, \sqrt{2}, 2, \dots$  if  $d = 2$ , and  $r_{ij} = 1, \sqrt{2}, \sqrt{3}, 2, \dots$  if  $d = 3$ . The potential energy has been written in this particular manner so that its value for the ground state (i.e.,  $\theta_i = \theta_j \forall (i, j)$ ) vanishes in all cases. We have considered unit momenta of inertia and unit first-neighbor coupling constant without loss of generality, and  $(p_i, \theta_i)$  are conjugate canonical pairs. Due to the periodic boundary conditions, the model is defined on a torus in  $d$  dimensions (i.e., a ring for  $d = 1$ ). Consequently, between any  $(i, j)$  pair of spins, there are more than one distances; in every case we consider as  $r_{ij}$  in the Hamiltonian the minimal of those distances. The model basically is a classical inertial  $XY$  ferromagnet (coupled rotators), and the limiting cases  $\alpha \rightarrow \infty$  and  $\alpha = 0$  correspond to the first-neighbor and mean-field-like models, respectively. Clearly, the  $\alpha = 0$  case does not depend on the particular lattice on which the spins are localized. This Hamiltonian is extensive (in the thermodynamical sense) if  $\alpha/d > 1$ , and nonextensive if  $0 \leq \alpha/d \leq 1$ . Indeed, in contrast with its kinetic energy, which scales like  $N$ , the potential energy scales like  $NN^*$ , where

$$N^* \equiv \sum_{j=1}^N \frac{1}{r_{ij}^\alpha}. \quad (5.45)$$

See also Eq. (3.69). For instance, for  $\alpha = 0$ ,  $N^* = N$ , and for  $\alpha/d \geq 1$  and  $N \rightarrow \infty$ ,  $N^* \rightarrow \text{constant}$ . Since the variables  $\{p_i\}$  involve a first derivative with respect to time, if we define  $t' = \sqrt{N^*} t$ , Hamiltonian  $\mathcal{H}$  in Eq. (5.44) is transformed

(see details in [177]) into  $\mathcal{H}' = \mathcal{H}/N^*$ , where

$$\mathcal{H}' = \frac{1}{2} \sum_{i=1}^N (p'_i)^2 + \frac{1}{2N^*} \sum_{i \neq j} \frac{1 - \cos(\theta_i - \theta_j)}{r_{ij}^\alpha} \quad (\alpha \geq 0). \quad (5.46)$$

It is in this form, *and omitting the “primes,”* that this system is usually presented in the literature. Although physically meaningless (since it involves microscopic coupling constants which, through  $N^*$ , depend on  $N$ ), it has the advantage of being (artificially) extensive, such as the familiar short-range-interacting ones. Unless explicitly declared otherwise, we shall from now on conform to this frequent use. For the  $\alpha = 0$  instance, it will present the widespread mean-field-like form, frequently referred to in the literature as the *HMF* model [833] (see also [834–836]),

$$\mathcal{H} = \frac{1}{2} \sum_{i=1}^N p_i^2 + \frac{1}{2N} \sum_{i \neq j} [1 - \cos(\theta_i - \theta_j)]. \quad (5.47)$$

This model, as well as its generalizations and extensions, are being intensively studied (see [372, 373, 376, 377] and references therein) in the literature through various procedures. A particularly interesting one is the molecular dynamical approach of an isolated  $N$ -sized system. Its interest comes from the fact that this is a *first-principles* calculation, since it is exclusively based on Newton’s law of motion, and therefore constitutes a privileged viewpoint to try to understand in depth the microscopic dynamical foundations of statistical mechanics<sup>5</sup> (both the *BG* and the nonextensive theories). The time evolution of the system depends on the class of initial conditions that are being used. Two distinct such classes are frequently used, namely *thermal-equilibrium*-like ones (characterized by a initial Gaussian distribution of velocities) and the *water-bag*-ones (characterized by a initially uniform distribution of velocities within an interval compatible with the assumed total energy  $U(N)$  of the system). The initial angle distribution ranges usually from all spins being aligned (say to the  $\theta_i = 0$  axis), which corresponds to maximal average *magnetization* (i.e.,  $m = 1$ ), to angularly completely disordered spins, which corresponds to minimal average *magnetization* (i.e.,  $m = 0$ ). The simplest model (*HMF*) presents, in its microcanonical version, a second order phase transition at the scaled total energy  $u_c = 0.75$ , where  $u \equiv U(N)/NN^*$  or  $u \equiv U(N)/N$ , depending on whether we are adopting Hamiltonian (5.44) or (5.46), respectively. For  $0 \leq u \leq u_c$ , the system tends to be ordered in a *ferromagnetic* phase, whereas for  $u > u_c$  it is in a disordered *paramagnetic* phase.

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<sup>5</sup> This is sometimes referred to as the *Boltzmann program*. Boltzmann himself died without having accomplished it, and rigorously speaking it so remains until today!

### 5.4.1 Metastability, Nonergodicity, and Distribution of Velocities

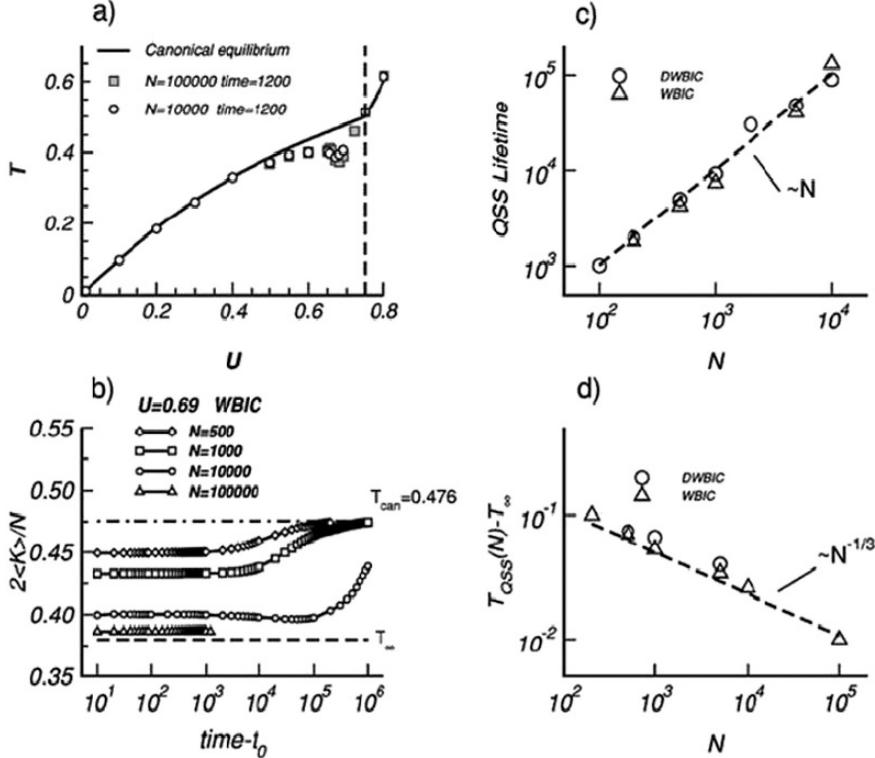
The model is analytically solvable in the *BG* canonical ensemble (equilibrium with a thermostat at temperature  $T$ ). The molecular dynamics approach coincides with it if the initial conditions for the velocities are described by a Gaussian. But, if we use a water-bag, a longstanding *metastable* or *quasi-stationary state* (QSS), appears at values of  $u$  below 0.75 and not too small (typically between 0.5 and 0.75). A value at which the effect is numerically very noticeable is  $u = 0.69$ , hence many studies are done precisely at this value. See Figs. 5.36 and 5.37. In Fig. 5.38 we can see the influence on  $T_{QSS}$  of the initial value of  $m$ .

On the thermal equilibrium plateau one expects, for all  $\alpha/d$ , the velocity distribution to be, for  $N \rightarrow \infty$ , one and the same Maxwellian distribution for both ensemble-average and time-average. This is of course consistent with the *BG* result for the canonical ensemble, based on the hypothesis of ergodicity. The situation is completely different on the QSS plateau<sup>6</sup> emerging for long-range interactions (i.e.,  $0 \leq \alpha/d \leq 1$ ). Indeed, the ensemble- and time-averages do *not* coincide [45, 46], thus exhibiting *nonergodicity* (which, as we shall see, is consistent with the fact that, along this longstanding metastable state, the entire Lyapunov spectrum collapses onto zero when  $N \rightarrow \infty$ ). The situation is illustrated in Figs. 5.39, 5.40, 5.41, 5.42, 5.43, 5.44, 5.45, and 5.46.

### 5.4.2 Lyapunov Spectrum

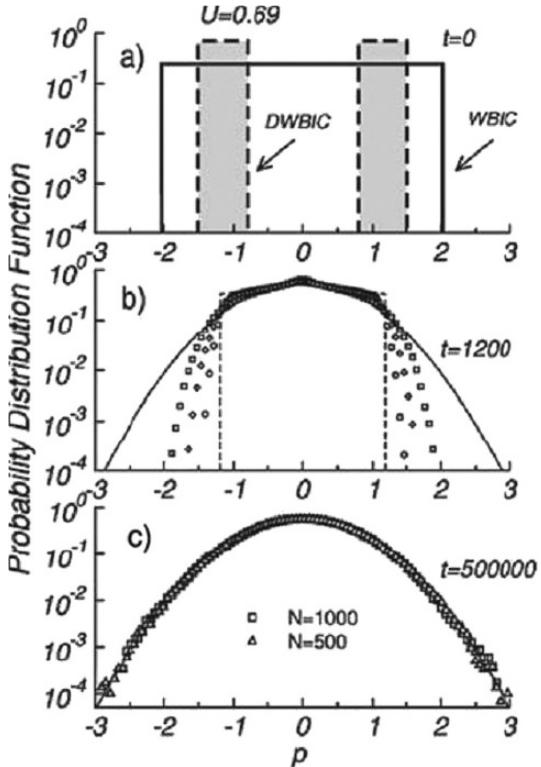
A set of  $2dN$  Lyapunov exponents is associated with the  $d$ -dimensional Hamiltonian (5.44), half of them positive and half of them negative (coupled two by two in absolute value) since the system is symplectic. We focus on the maximal value  $\tilde{\lambda}_N^{max}$ ; if this value vanishes, the entire spectrum vanishes. This property is extremely relevant for the foundations of statistical mechanics. Indeed, if  $\tilde{\lambda}_N^{max} > 0$ , the system will be *mixing* and *ergodic*, which is the basis of BG statistical mechanics. If  $\tilde{\lambda}_N^{max}$  vanishes, there is no such guarantee. This is the realm of nonextensive statistical mechanics, as we have already verified for paradigmatic dissipative and conservative low-dimensional maps. The scenario for the  $d = 1$   $\alpha$ -XY model is described in Figs. 5.47 and 5.48. The corresponding scenarios for  $d = 2, 3$  have been discussed

<sup>6</sup> The lifetime  $\tau_{QSS}$  of this QSS plateau has been conjectured (see Fig. 4 in [63], where  $\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty}$  is expected to yield the standard BG canonical thermal equilibrium and  $\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty}$  is expected to yield the nonextensive statistical mechanics results) to diverge, for fixed  $\alpha \leq d$  if  $N \rightarrow \infty$ . Also, for the  $d = 1$  model, it has been suggested [374] that, for fixed  $N$ ,  $\tau_{QSS}$  decreases exponentially with  $\alpha$  increasing above zero. All these results are consistent with  $\tau_{QSS} \propto (N^*)^a$  with  $N^*$  given in Eq. (3.69) and  $a > 0$ . Indeed, such scaling yields, for  $0 \leq \alpha/d < 1$ ,  $\tau_{QSS}(\alpha/d, N) \propto N^{a[1-(\alpha/d)]}$  ( $N \rightarrow \infty$ ), which implies  $\tau_{QSS}(0, N) \propto N^a$ , and exponentially decreasing with  $\alpha/d$  for fixed  $N$ . All authors do not always use the same definition for  $\tau_{QSS}$ . The definition used in [373] implies  $a = 1$ ; the definitions used by other authors imply  $a > 1$ .



**Fig. 5.36** (a) Caloric curve: microcanonical ensemble results for  $N = 10,000, 100,000$  are compared with equilibrium theory in the BG canonical ensemble. The dashed vertical line indicates the critical energy: Water bag initial conditions (WBIC) and initial  $m = 1$  are used in the numerical simulations. Temperature is computed from  $2\langle K(N) \rangle / N$ , where  $\langle \dots \rangle$  denotes time averages after a short transient time  $t_0 = 100$  (not reported here). The time step used was 0.2 [839–842]. Microcanonical time evolution of  $T$ , for the energy density  $u = 0.69$  and different sizes. Each curve is an average over typically 100–1000 events (*ensemble average*). The dot-dashed line represents the BG canonical temperature  $T_{BG} = 0.476$ . The quantity  $T$ , which starts from 1.38 ( $V = 0$  and  $K = UN$  for WBIC), does not relax immediately to the temperature  $T_{BG}$ . The system lives in a QSS with a plateau temperature  $T_{QSS}(N)$  smaller than the canonically expected value 0.476. The lifetime of the QSS increases with  $N$ , and the value of their temperature converges, as  $N$  increases, to the temperature 0.38, reported as a dashed line. Log-log plots for the QSS lifetime (c) and the difference  $T_{QSS}(N) - T_\infty$  (with  $T_\infty \equiv T_{QSS}(\infty)$ ) (d) are reported as functions of  $N$ . The QSS lifetime diverges roughly as  $N$ , and  $T_{QSS} - 0.38$  vanishes roughly as  $1/N^{1/3}$  (see fit shown as a dashed line). Note that from the caloric curve one gets  $m^2 = T + 1 - 2u = T - 0.38$ . Therefore, from the behavior reported in panel (d), being  $T_\infty = 0.38$ , one gets  $M_{QSS} \sim 1/N^{1/6}$ . Results are similar when we consider double water bag initial conditions (DWBIC), more precisely initial  $m = 1$  and velocities uniformly distributed within  $(-p_2, -p_1)$  and  $(p_2, p_1)$ . In the figure, we report the case  $p_1 = 0.8$  and  $p_2 = 1.51$  (from [373]).

**Fig. 5.37** Time evolution of the velocity probability distribution function (PDF) for  $u (= U) = 0.69$  and different sizes. (a) At time  $t = 0$  we start with simple WBIC, or DWBIC, velocity PDF. (b) In the transient regime, where  $T$  shows a plateau corresponding to  $T_{QSS}$  and the system lives in a QSS, the velocity PDFs do not change in time and are very different from the Gaussian BG canonical equilibrium distribution (*full curve*). The PDFs at  $t = 1200$  and  $N = 1000, 10, 000$ , and  $100, 000$  show a convergence towards a non-Gaussian PDF. (c) We show the numerical PDFs at  $t = 500, 000$  for  $N = 500$  and  $1000$ . We get an excellent agreement with the Maxwellian BG canonical equilibrium distribution at  $T = 0.476$  (from [373]).

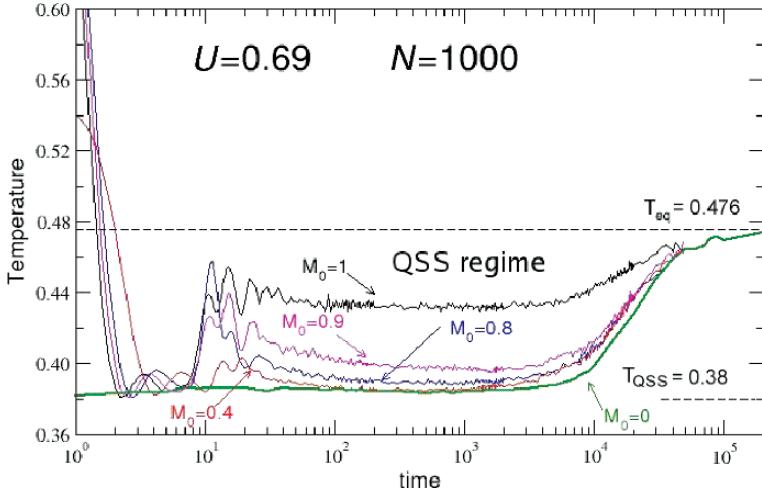


in [178], and are illustrated in Figs. 5.49, 5.50, and 5.51. They are completely analogous to that of the  $d = 1$  case, and strongly suggest that the relevant exponent  $\kappa$  does not depend separately on  $\alpha$  and  $d$ , but, like  $N^*$  (see Eq. (3.69)), only on the ratio  $\alpha/d$ .

The above molecular dynamical results concerned the disordered (paramagnetic) phase. Also are available results [375, 376] for the ordered (ferromagnetic) phase of the  $d = 1$  model, more precisely for its QSS. For reasons that are not totally transparent, the value for  $\kappa$  obtained on the QSS (below  $u_c$ ), turns out to numerically be  $1/3$  of its value above  $u_c$ : See Fig. 5.52.

### 5.4.3 Aging and Anomalous Diffusion

The very fact that, for  $u < u_c$  and fixed  $N$ , a QSS exists which, after a time of the order of  $\tau_{QSS}$ , eventually goes to thermal equilibrium implies that the system has some sort of *internal clock*. This immediately suggests that *aging* should be expected. More precisely, if we consider a two-time autocorrelation function  $C(t + t_w, t_w)$  of some dynamical variables of the system, we expect this quantity to depend not only on time  $t$ , but also on the waiting time  $t_w$ . This is precisely what is verified



**Fig. 5.38** Time evolution of the HMF temperature for the energy density  $u(= U) = 0.69$ ,  $N = 1000$  and several initial conditions with different magnetizations. After a very quick cooling, the system remains trapped into metastable long-living Quasi-Stationary States (*QSS*) at a temperature smaller than the equilibrium one. Then, after a lifetime that diverges with the size, the noise induced by the finite number of spins drives the system towards a complete relaxation to the equilibrium value. Although from a macroscopic point of view the various metastable states seem similar, they actually have different microscopic features and correlations which depend in a sensitive way on the initial magnetization (from [41]).

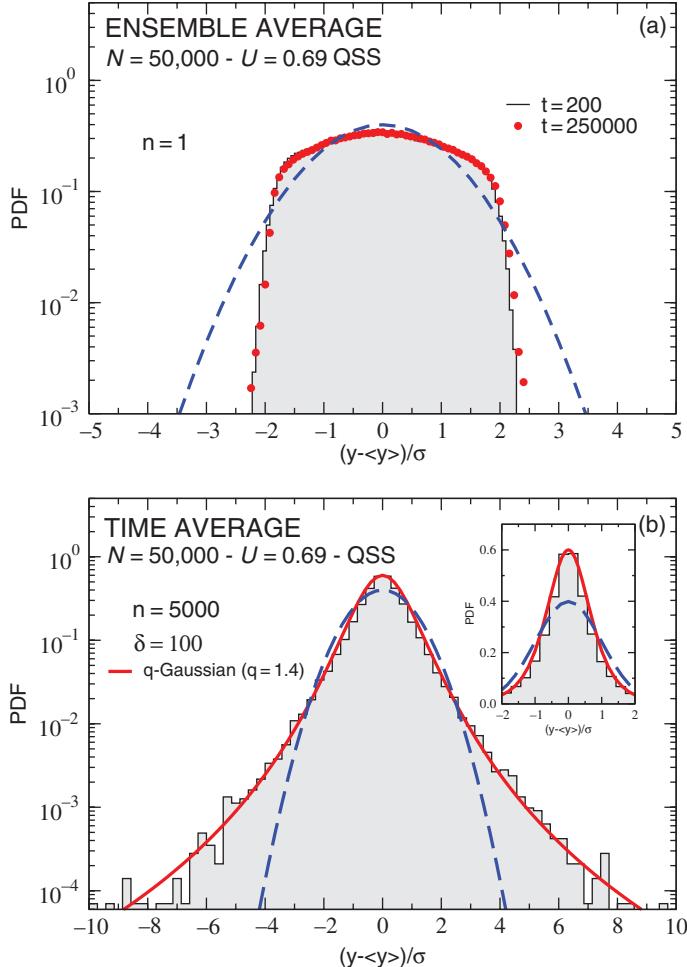
in [41, 44, 379, 380]: See Figs. 5.53, 5.54 and 5.60. It is quite remarkable that  $q$ -exponential decays are observed in these (and other) cases, and that data collapse, in the form

$$C(t + t_W, t_W) = e_q^{-Bt/t_W^\beta} \quad (B > 0; \beta \geq 0) \quad (5.48)$$

is possible (such as in usual spin-glasses). The value  $q \simeq 2.35$  (corresponding to the  $(p, \theta)$ -space [44]) is essentially what elsewhere (namely, in the context of the  $q$ -triplet to be soon discussed) is noted  $q_{\text{rel}}$ . Another remarkable fact (see Fig. 5.55) is that, for  $u > u_c$ , Eq. (5.48) is still satisfied *with the same value of*  $q \simeq 2.35$ , but with  $\beta = 0$ , i.e., without aging. Let us stress that, for a standard BG system (e.g., if  $\alpha/d > 1$ ), one normally observes, both above and below the critical point,  $q = 1$  and  $\beta = 0$ .

Let us now focus on the diffusion of the angles  $\{\theta_i\}$  by allowing them to freely move within  $-\infty$  to  $+\infty$ . The probability distributions, and corresponding anomalous diffusion exponent  $\gamma$ , can be seen in Figs. 5.56, 5.57, 5.58, 5.59, and 5.60. From the data in Fig. 5.60 we can verify (see Fig. 5.61) the agreement, within a 10% error, with the scaling predicted in Eq. (4.16).

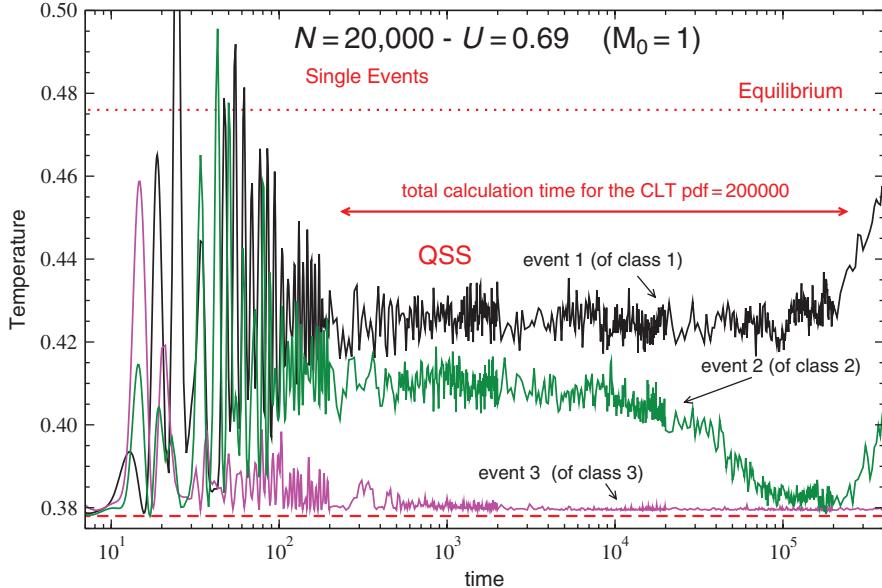
For phenomena occurring at the edge of chaos of simple maps and related to those described above, see [42, 43].



**Fig. 5.39** Numerical simulations for the HMF model for  $N = 50,000$ ,  $U = 0.69$  and  $M_1$  initial conditions in the QSS regime. **(a)** We plot the PDFs of single rotor velocities at the times  $t = 200$  and  $t = 250,000$  (ensemble average over 100 realizations). **(b)** We plot the time average PDF for the variable  $y$  calculated over *only one single realization* in the QSS regime and after a transient time of 200 units. In this case, we used  $\delta = 100$  and  $n = 5000$ , in order to cover a very large portion of the QSS. Again, a  $q$ -Gaussian reproduces very well the calculated PDF both in the tails and in the central part (see inset). See text for further details (from [45]).

#### 5.4.4 Connection with Glassy Systems

We have seen in the previous subsection that there is aging at the QSS below the critical point, whereas no such phenomenon survives above  $u_c$ . We expect then to have some sort of glassy behavior during the QSS, and no such behavior above  $u_c$ . This is precisely what we see in Fig. 5.62 (see also [42, 43]).



**Fig. 5.40** Time evolution of the temperature (calculated as twice the average kinetic energy per particle) for three single events representative of the three different classes observed at  $U = 0.69$  for initial magnetization  $M_0 = 1$ . The size of the system is  $N = 20,000$  (from [46]).

## 5.5 The $q$ -Triplet

Let us further consider the ordinary differential equations that we addressed in Section 3.1.

The solution of the differential equation

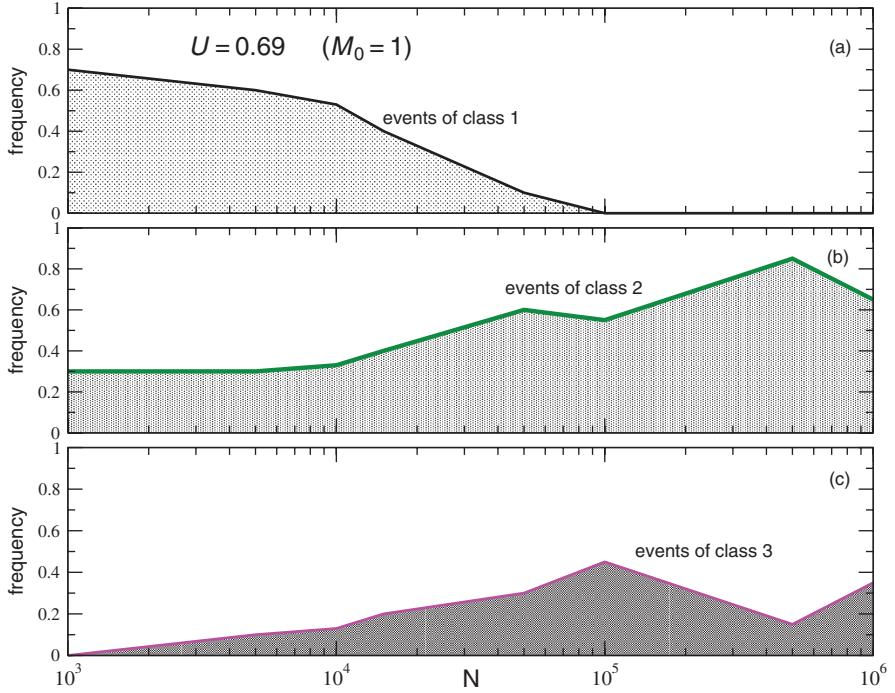
$$\frac{dy}{dx} = a y \quad (y(0) = 1) \quad (5.49)$$

is given by

$$y = e^{ax}. \quad (5.50)$$

We may heuristically think of it in three different physical manners, related respectively to the sensitivity to the initial conditions, to the relaxation in phase-space, and, if the system is Hamiltonian, to the distribution of energies at thermal equilibrium. In the first interpretation we reproduce Eq. (2.31). In the second interpretation, we focus some relaxing relevant quantity

$$\Omega(t) \equiv \frac{O(t) - O(\infty)}{O(0) - O(\infty)}, \quad (5.51)$$



**Fig. 5.41** Relative frequency of occurrence for the three classes of events shown in Fig. 1 as a function of  $N$ . A total of 20 realizations for each  $N$  was considered. The three curves add up to unity (from [46]).

where  $O$  is some dynamical observable essentially related to the evolution of the system in phase-space (e.g., the time evolution of entropy while the system approaches equilibrium). We typically expect

$$\Omega(t) = e^{-t/\tau_1}, \quad (5.52)$$

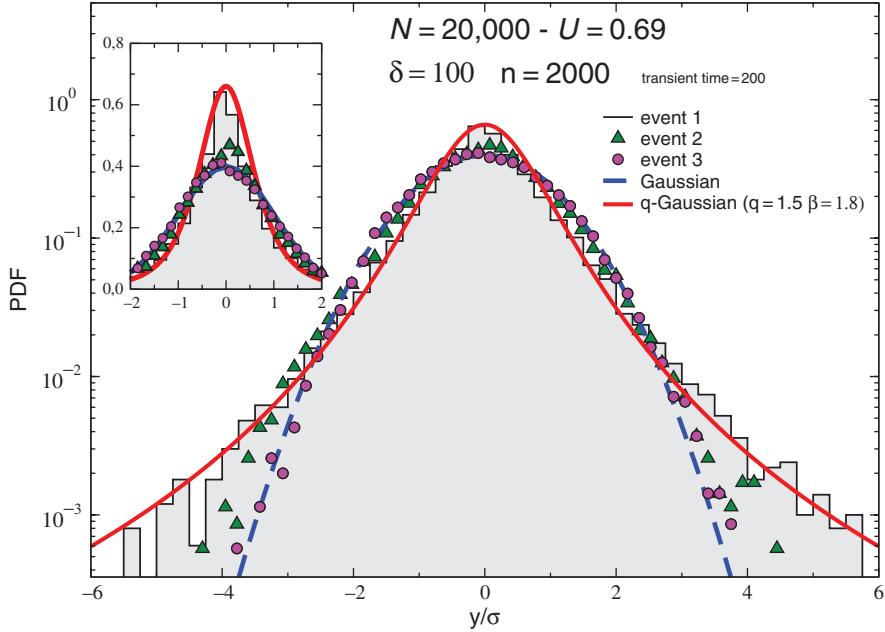
where  $\tau_1$  is the relaxation time. Finally, in the third interpretation, we have Eq. (2.64) with Eq. (2.65), i.e.,

$$Z_1 p_i = e^{-\beta E_i}, \quad (5.53)$$

where  $Z_1 \equiv \sum_{j=1}^W e^{-\beta E_j}$  is the partition function. The various interpretations are summarized in Table 5.1.

Let us now generalize these statements. The solution of the differential equation

$$\frac{dy}{dx} = a y^q \quad (y(0) = 1) \quad (5.54)$$



**Fig. 5.42** We present for each class of the QSS found, the different central limit theorem behavior observed. A Gaussian (dashed curve) with unitary variance and a  $q$ -Gaussian  $p(x) = Ae_q(-\beta x^2)$  with  $A = 0.66$ ,  $q = 1.5$ , and  $\beta = 1.8$  (full curve) are also reported for comparison. In the inset, a magnification of the central part in linear scale is plotted (from [46]).

is given by

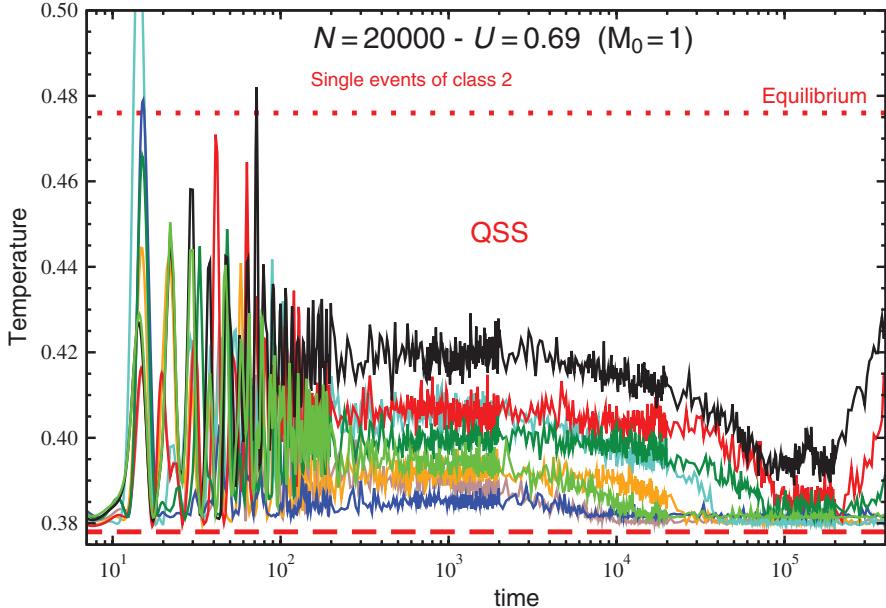
$$y = e_q^{ax}. \quad (5.55)$$

These expressions, respectively, generalize expressions (5.49) and (5.50). As before, we may think of them in three different physical manners, related respectively to the sensitivity to the initial conditions, to the relaxation in phase-space, and, if the system is Hamiltonian, to the distribution of energies at a stationary state. In the first interpretation we reproduce Eq. (5.8). In the second interpretation, we typically expect

$$\Omega(t) = e_{q_{rel}}^{-t/\tau_{q_{rel}}}, \quad (5.56)$$

where  $\tau_{q_{rel}}$  is the relaxation time. Finally, in the third interpretation, we have Eq. (3.207) (with Eq. (3.208)), i.e.,

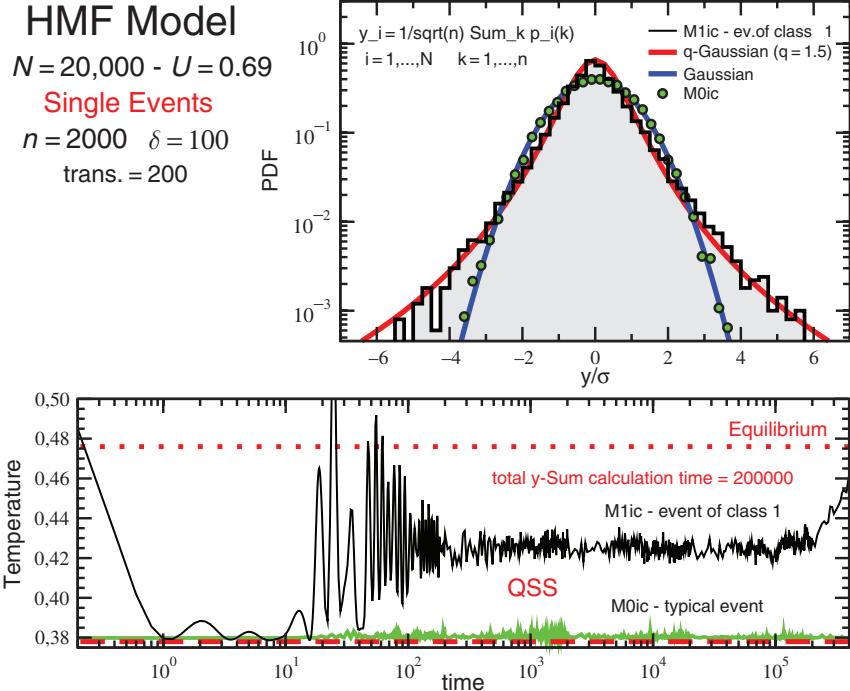
$$Z_{q_{stat}} p_i = e^{-\beta_{q_{stat}} E_i}, \quad (5.57)$$



**Fig. 5.43** Different events of class 2 are plotted for the case  $N = 20,000$ . A large variability is observed for this class, at variance with the other two (from [46]).

where  $Z_{qstat} \equiv \sum_{j=1}^W e^{-\beta_{qstat} E_j}$  is the partition function. The various interpretations are summarized in Table 5.2. The set  $(q_{sen}, q_{rel}, q_{stat})$  constitutes what we shall refer to as the *q-triplet* (occasionally referred also to as the *q-triangle*). In the *BG* particular case, we recover  $q_{sen} = q_{rel} = q_{stat} = 1$ . The existence of these three *q*-exponentials characterized by the *q*-triplet was predicted in 2004 [190] and confirmed in 2005 [361]; see Fig. 5.63, where the observations done (through processing the data sent to Earth by the spacecraft Voyager 1) in the solar wind are depicted (more along these lines can be found in [368]).<sup>7</sup>

<sup>7</sup> If we have a triplet  $(x, y, z)$  of real numbers such that one of them, say  $x$ , is the arithmetic average of the other two (i.e.,  $x = \frac{y+z}{2}$ ), and one of the other two, say  $y$ , is the harmonic average of the other two (i.e.,  $y^{-1} = \frac{x^{-1}+z^{-1}}{2}$ ), then, remarkably enough, the third number necessarily is the geometric average of the other two (i.e.,  $z = \sqrt{xy}$ ). If we define now  $\epsilon \equiv 1 - q$ , we have, from [199], that  $(\epsilon_{sen}, \epsilon_{rel}, \epsilon_{stat}) = (3/2, -3, -3/4)$ . By identifying  $(x, y, z) \equiv (\epsilon_{stat}, \epsilon_{rel}, \epsilon_{sen})$ , it can be checked that they satisfy the just mentioned remarkable relationships! [369]. In fact, these relations admit only one degree of freedom. In other words, we can freely choose only one number, say  $x$ ; the other two ( $y$  and  $z$ ) are automatically determined. If  $x \geq 0$ , the solution is  $x = y = z$ ; if  $x < 0$ , the solution is  $x = y/4 = -z/2$ . The set  $(\epsilon_{star}, \epsilon_{rel}, \epsilon_{sen}) = (-3/4, -3, 3/2)$  belongs to this latter case.



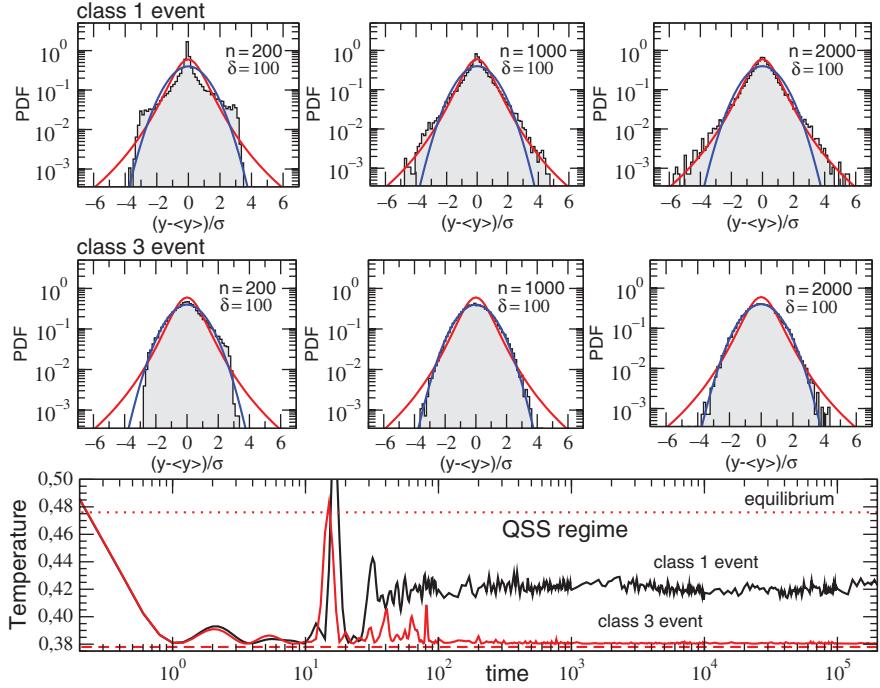
**Fig. 5.44** (a) Comparison of the Central Limit Theorem behavior for the  $u = 0.69$ ,  $N = 20,000$  case with initial magnetization  $m = 1$  and  $m = 0$ . A Gaussian (dashed curve) with unit variance and a  $q$ -Gaussian with  $A = 0.66$ ,  $q = 1.5$ , and  $\beta = 1.8$  (full curve) are also reported for comparison. (b) Temperature time evolutions of the same events shown in panel (a) (from [46]).

## 5.6 Connection with Critical Phenomena

Since it is since long known that systems at criticality (in the sense of standard second order critical phenomena) exhibit a fractal geometry, it is kind of natural to expect that connections would exist between  $q$  and the critical phenomenon: see [353–355]. In particular, an interesting analytical connection has already been established for the Ising ferromagnet, namely [354]

$$q = \frac{1 + \delta}{2}, \quad (5.58)$$

where  $\delta$  is the critical exponent characterizing the dependence, at precisely the critical point, of the order parameter with its thermodynamically conjugate field (e.g.,  $M \sim H^{1/\delta}$ , where  $M$  and  $H$  are, respectively, the magnetization and the external magnetic field).

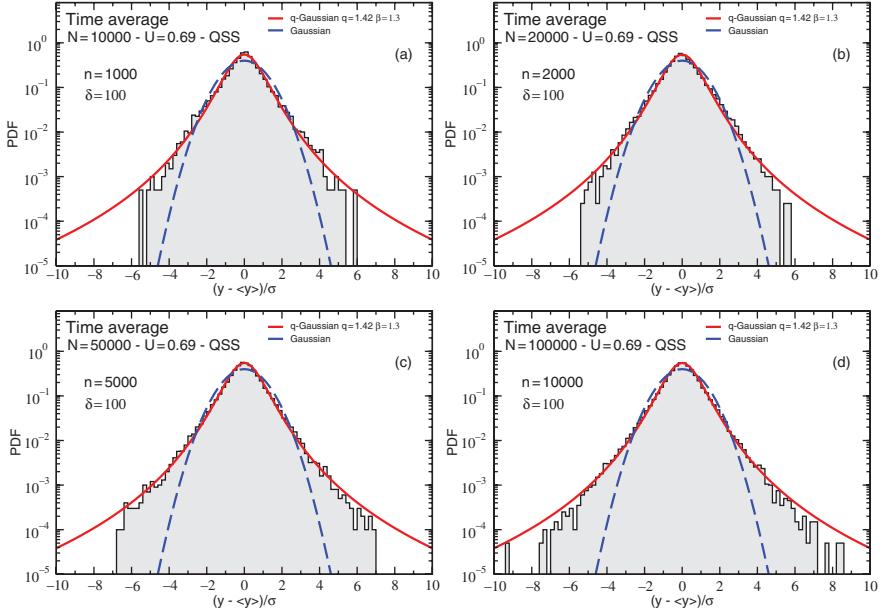


**Fig. 5.45** We show the time evolution of two events with the same  $M_1$  initial conditions, more precisely with  $N=20,000$  at  $U = 0.69$ , but belonging to different classes (1 and 3); the duration along which we are doing the CLT sums is  $n \times \delta$ . The evolution towards the final attractor appears to be a Gaussian for the event of class 3 and a  $q$ -Gaussian-like for the event of class 1. The latter is given by  $G_q(x) = A(1 - (1 - q)\beta x^2)^{1/1-q}$ , with  $q = 1.42 \pm 0.1$ ,  $\beta = 1.3 \pm 0.1$ , and  $A = 0.55$ . Notice that the tails emerge clearly while increasing the number  $n$  of summands. This is also true in the case of the Gaussian, as predicted by the CLT. From [48] (see also [47]).

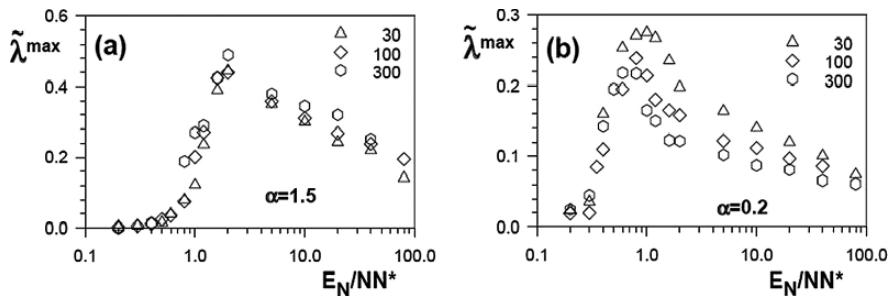
## 5.7 A Conjecture on the Time and Size Dependences of Entropy

We have seen that, for a (not yet fully qualified) large class of systems, there is a special value of  $q$ ,  $q_N$ , such that  $S_{q_N}(N, t) \propto N$  ( $N \rightarrow \infty$ ). This is so for all values of time  $t$ , including  $t \rightarrow \infty$ , if we are describing the system within some *finite* resolution (or some *finite* degree of fine-graining, i.e.,  $\epsilon > 0$ ). We have also seen that, for a (once again not yet fully qualified) large class of systems, there is a special value of  $q$ ,  $q_t$ , such that  $S_{q_t}(N, t) \propto t$  ( $t \rightarrow \infty$ ). This is so for an *infinite* resolution (or *ideally precise* degree of fine-graining, i.e.,  $\epsilon = 0$ ). The scenario is schematically indicated in Fig. 5.64. If this scenario is correct, then we conjecture that  $q_N = q_t \equiv q_{ent}$ , hence, in the  $\epsilon \rightarrow 0$  limit, we would generically have the following form:

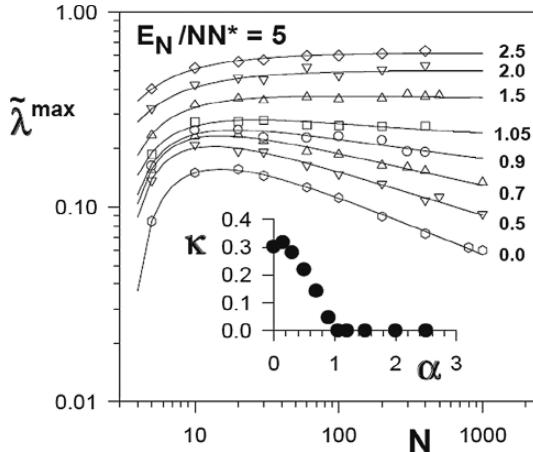
$$S_{q_{ent}} \sim s N t \quad (N \rightarrow \infty; t \rightarrow \infty; s \geq 0). \quad (5.59)$$



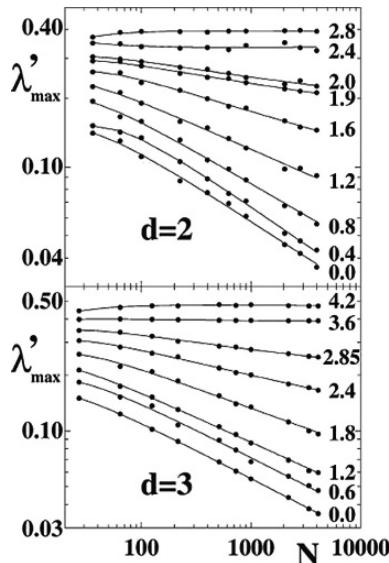
**Fig. 5.46** For  $U = 0.69$  we show the PDFs obtained considering single events of class 1 for the HMF system sizes  $N = 10,000, 20,000, 50,000$  and  $100,000$ , with  $\delta = 100$  and  $n = N/10$ . Again the indications for a  $q$ -Gaussian-like attractor becomes stronger and stronger when sending both  $N$  and  $n$  to infinity. Notice that we consider here a larger scale (compared to that of Fig. 5.45) in the ordinate in order to see in detail the tails of the PDF. The same  $q$ -Gaussian reported in the previous figure, with  $A=0.55$ ,  $q = 1.42 \pm 0.1$ , and  $\beta = 1.3 \pm 0.1$  and obtained by fitting the case with  $N = 100,000$ , is here shown for comparison, together with the standard Gaussian with unitary variance. From [48] (see also [47]).



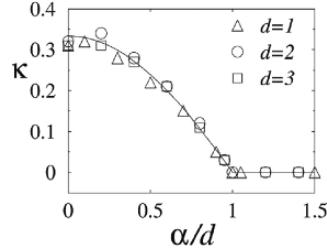
**Fig. 5.47** The  $u \equiv E_N/NN^*$ - dependence of the properly scaled maximal Lyapunov exponent  $\tilde{\lambda}_N^{max}$ , for the  $d = 1$   $\alpha - XY$  model and typical values of  $N$ , for  $\alpha = 1.5$  **(a)** and  $\alpha = 0.2$  **(b)**. As illustrated in Fig. 5.48, the  $N \rightarrow \infty$  limit yields, for high enough values of  $u$  (in fact for  $u > u_c = 0.75, \forall \alpha$ ), a nonvanishing (vanishing) value for  $\tilde{\lambda}_N^{max}$  for  $\alpha \geq 1$  ( $0 \leq \alpha \leq 1$ ) (from [177]).



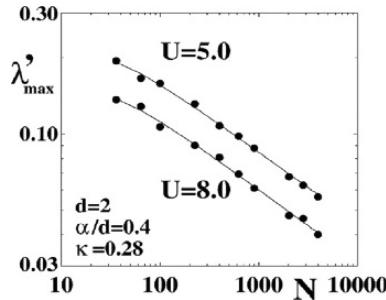
**Fig. 5.48** Log–log plots of  $\tilde{\lambda}_N^{max}$  vs.  $N$  for typical values of  $\alpha$  and  $u = 5$ . The full lines are the best fittings with the heuristic forms  $(a - b/N)/(N^*)^c$ . Consequently,  $\tilde{\lambda}_N^{max} \sim 1/N^{\kappa(\alpha)}$ , where  $\kappa$  is positive for  $0 \leq \alpha < 1$  and vanishes for  $\alpha > 1$ . For  $\alpha = 1$ ,  $\tilde{\lambda}_N^{max}$  is expected to vanish like some power of  $1/\ln N$  (from [177]).



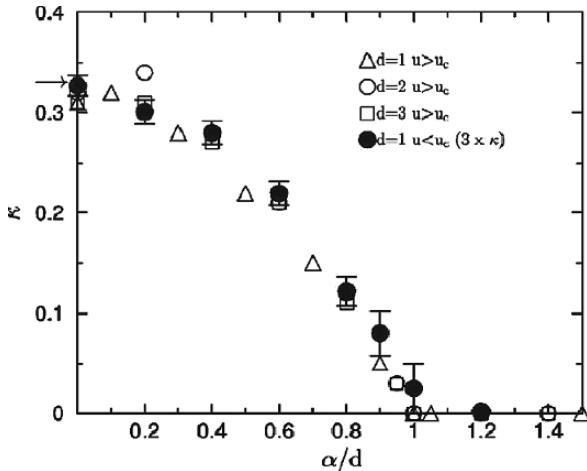
**Fig. 5.49** Log–log plots of  $\tilde{\lambda}_N^{max}$  vs.  $N$  for typical values of  $\alpha$  and  $u = 5$ :  $d = 2$  (top panel) and  $d = 3$  (bottom panel). The full lines are the best fittings with the heuristic forms  $(a - b/N)/(N^*)^c$ . Consequently,  $\tilde{\lambda}_N^{max} \sim 1/N^{\kappa(\alpha,d)}$ , where  $\kappa$  is positive for  $0 \leq \alpha/d < 1$  and vanishes for  $\alpha/d > 1$ . For  $\alpha/d = 1$ ,  $\tilde{\lambda}_N^{max}$  is expected to vanish like some power of  $1/\ln N$  (from [178]).



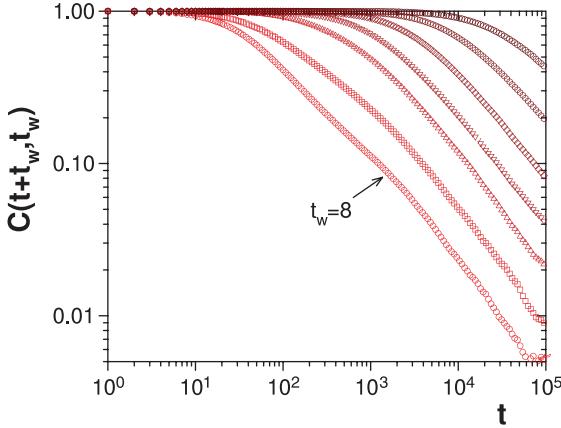
**Fig. 5.50** The exponent  $\kappa$  as a function of  $\alpha/d$  for the  $d = 1, 2, 3$   $\alpha$ -XY model. The points for the  $d = 1$  case are those of the inset of Fig. 5.47. The *solid line* is a guide to the eye consistent with universality. For  $\alpha = 0$  we have  $\kappa(0) = 1/3$  [179] (from [178]).



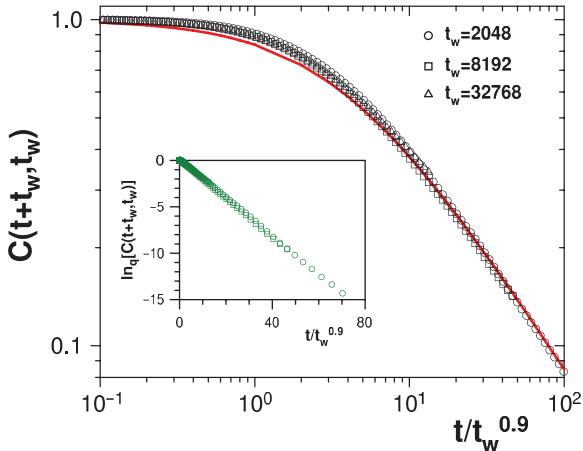
**Fig. 5.51**  $\tilde{\lambda}_N^{\max}(N)$  for the  $(\alpha, d) = (0.8, 2)$  model for two different values of energy density  $u$ . The asymptotic  $N$  behavior, for all values of  $u > u_c$  and  $0 \leq \alpha/d < 1$ , appears to be  $\tilde{\lambda}_N^{\max}(N) \sim A/N^{\kappa(\alpha/d)}$ , where  $A$  decreases from a finite,  $(\alpha, d)$ -dependent, value to zero when  $u$  increases from  $u_c$  to infinity (from [178]).



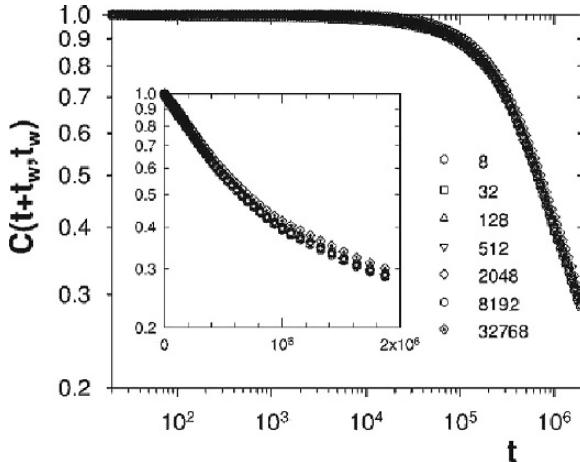
**Fig. 5.52**  $\alpha/d$ -dependance of  $3 \times \kappa_{\text{metastable}}$  (full circles). Open triangles, circles, and squares respectively correspond to  $\kappa_d$  of the  $d = 1, 2, 3$  models [177, 178]. The arrow points to  $1/3$ , value analytically expected [179–181] to be exact for  $\alpha = 0$  and  $u > u_c$  (from [376]).



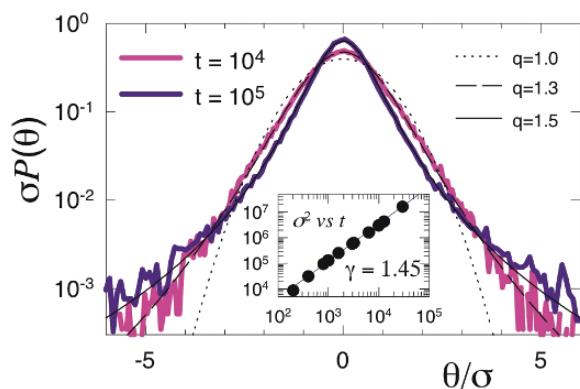
**Fig. 5.53** Normalized two-time auto-correlation function of the state variable  $(\theta, \mathbf{p})$  vs. time, for  $u = 0.69$  (subcritical) and for initial conditions that guarantee that the system will get trapped into a quasi stationary trajectory. Data correspond to averages over 200 of such trajectories. The waiting times are  $t_w = 8 \times 4^n$ , with  $n = 0, \dots, 6$ . The dependence of  $C$  on both times is evident (from [44]).



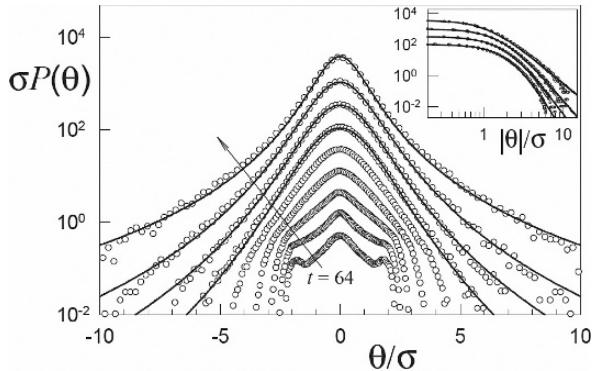
**Fig. 5.54** Auto-correlation function vs. scaled time. The data are the same shown in Fig. 5.53 for the three largest  $t_w$ , but suitably scaling the time coordinate makes the data collapse into a single curve. The red solid line corresponds to  $e^{-0.2t/t_w^{0.9}}$ . Inset:  $\ln_q$ -linear representation of the same data, with  $q = 2.35$ . Linearity indicates  $q$ -exponential behavior (from [44]).



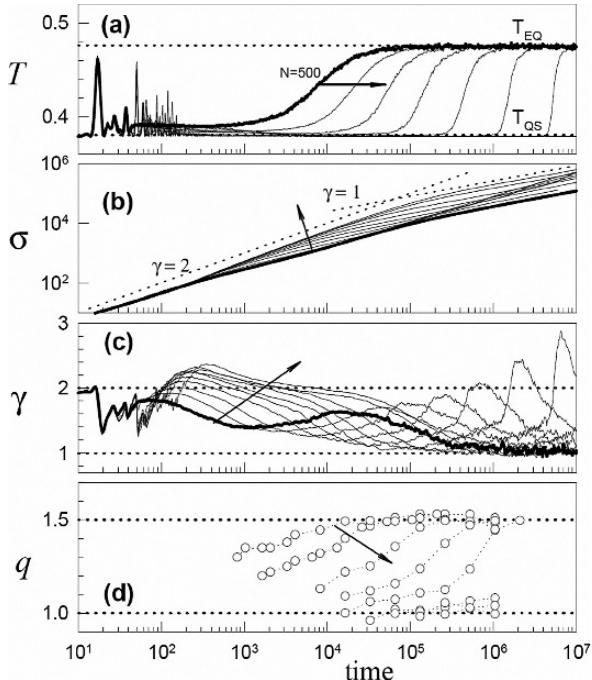
**Fig. 5.55** Auto-correlation function vs. time for  $u = 5$  (supercritical) for  $N = 1000$  and various values of  $t_w$ . The data correspond to an average over 10 trajectories initialized with water-bag configuration. Notice that, as in standard BG systems at thermal equilibrium, there is no aging. *Inset:* Semilog representation of the same data (from [379]).



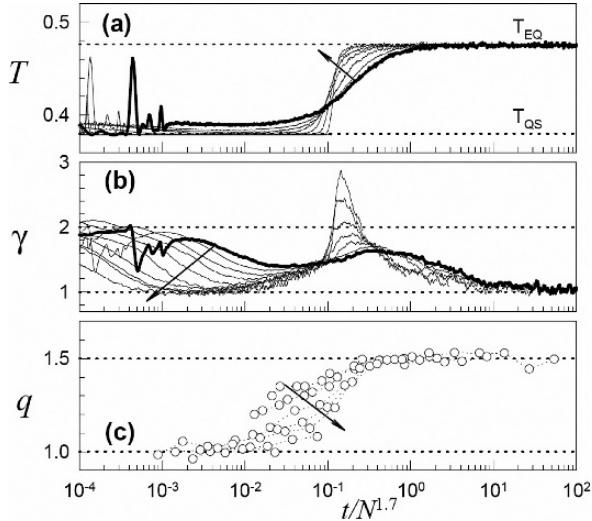
**Fig. 5.56** Histogram of normalized angles at different times of the HMF dynamics. Parameters and initial conditions are the same used in previous figures. Notice that at long times, the histogram is of the  $q$ -Gaussian form. Inset: squared deviation as a function of time. It follows the law  $\sigma^2 \sim t^\gamma$ , with  $\gamma > 1$ , signaling superdiffusion (from [44]).



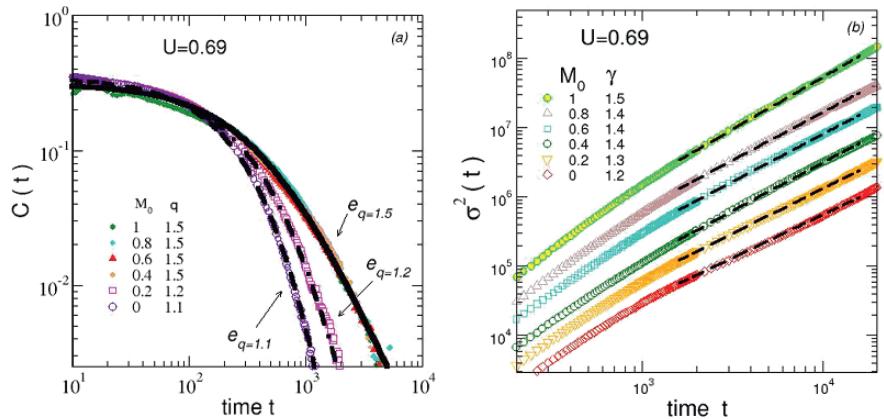
**Fig. 5.57** Angular distribution. From [285].



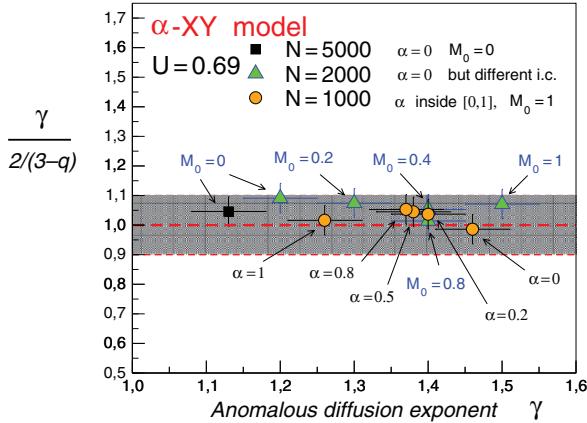
**Fig. 5.58** Time evolution of the temperature (a), variance (b), anomalous diffusion exponent (c), and index  $q$  (d). The persistence of  $q \neq 1$  within the region for which  $T$  has already attained its BG value might be due to extremely slow dynamics (see [274]). From [285].



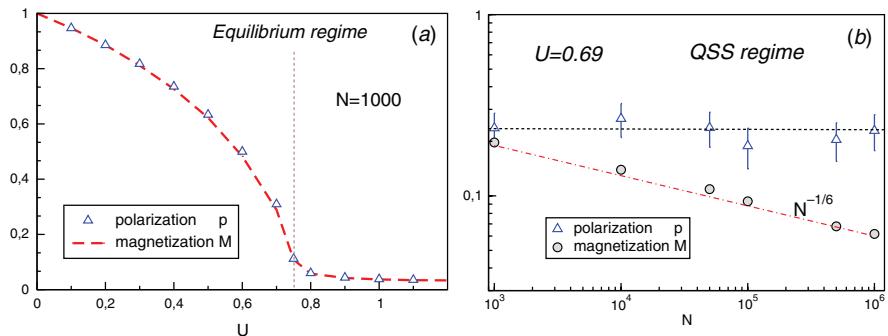
**Fig. 5.59** The same as in Fig. 5.58 but with a  $N$ -scaled time axis. From [285].



**Fig. 5.60** (a) Time evolution of the  $HMF$  velocity autocorrelation functions for  $U = 0.69$ ,  $N = 1000$ , and different initial conditions are nicely reproduced by  $q$ -exponential curves. The entropic index  $q$  used is also reported. (b) Time evolution of the variance of the angular displacement for  $U = 0.69$ ,  $N = 2000$ , and different initial conditions. After an initial ballistic motion, the slope indicates a superdiffusive behavior with an exponent  $\gamma$  greater than 1. This exponent is also reported and indicated by *dashed straight lines*. Anomalous diffusion does not depend in a sensitive way on the size of the system. For both the plots shown, the numerical simulations are averaged over many realizations (from [41]).



**Fig. 5.61** For different system sizes and initial conditions, and for several values of the parameter  $\alpha$  which fixes the range of the interaction of a generalized version of the HMF model [12], the figure illustrates the ratio of the anomalous diffusion exponent  $\gamma$  divided by  $2/(3-q)$  vs.  $\gamma$ . The entropic index  $q$  is extracted from the relaxation of the correlation function (see previous figure). This ratio is always one within the errors of the calculations (from [41]).



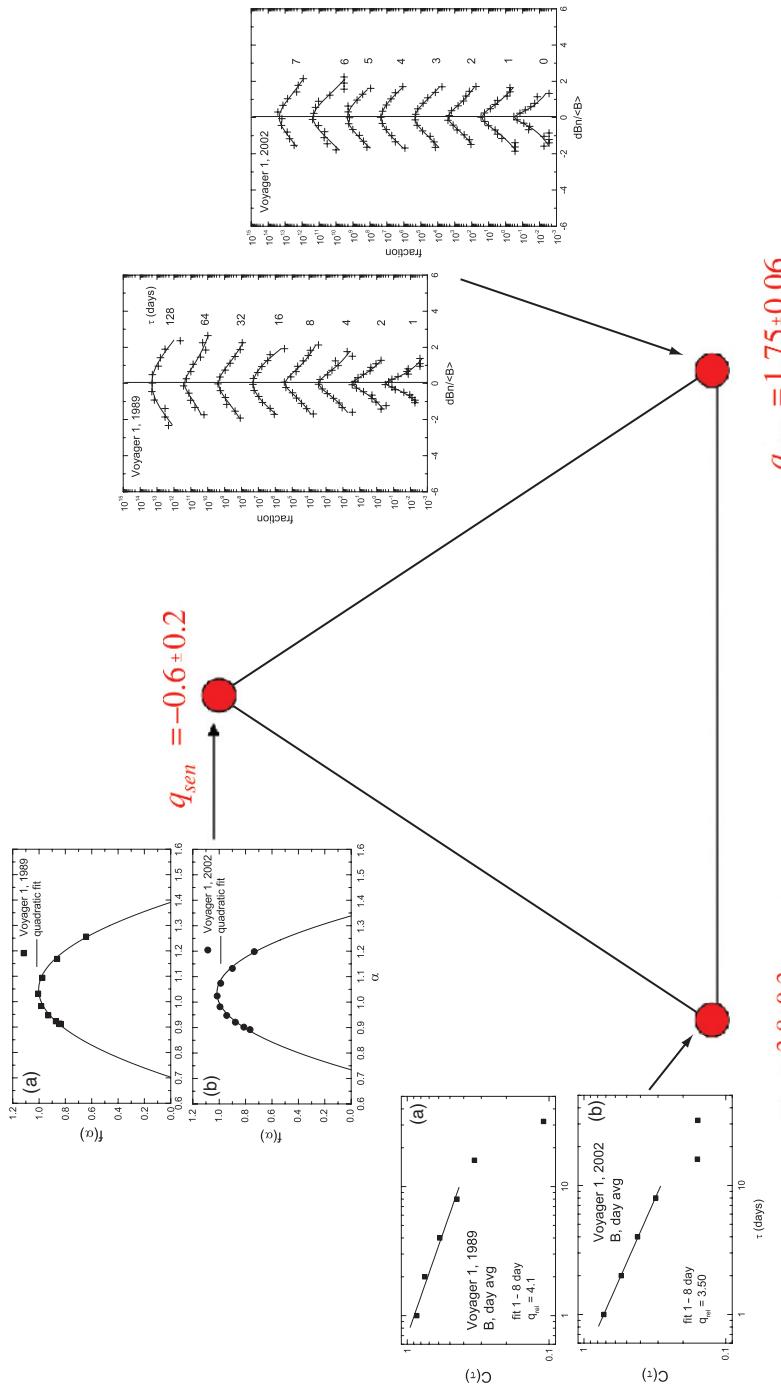
**Fig. 5.62** (a) The magnetization  $M$  and the polarization  $p$  are plotted vs. the energy density for  $N = 10,000$  at equilibrium: the two-order parameters are identical. (b) The same quantities plotted in (a) are here reported vs. the size of the system, but in the metastable *QSS* regime. In this case, increasing the size of the system, the polarization remains constant around a value  $p \sim 0.24$  while the magnetization  $M$  goes to zero as  $N^{-1/6}$  (from [41]).

**Table 5.1** Three possible physical interpretations of Eq. (5.50) within *BG* statistical mechanics

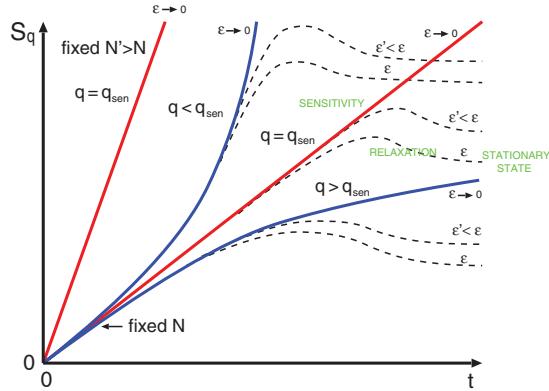
	$x$	$a$	$y(x)$
Equilibrium distribution	$E_i$	$-\beta$	$Z_1 p(E_i) = e^{-\beta E_i}$
Sensitivity to the initial conditions	$t$	$\lambda_1$	$\xi(t) = e^{\lambda_1 t}$
Typical relaxation of observable $O$	$t$	$-1/\tau_1$	$\Omega(t) = e^{-t/\tau_1}$

**Table 5.2** Three possible physical interpretations of Eq. (5.55) within nonextensive statistical mechanics

	$x$	$a$	$y(x)$
Stationary state distribution	$E_i$	$-\beta$	$Z_{q_{stat}} p(E_i) = e^{-\beta E_i}$
Sensitivity to the initial conditions	$t$	$\lambda_{q_{sen}}$	$\xi(t) = e^{\lambda_{q_{sen}} t}$
Typical relaxation of observable $O$	$t$	$-1/\tau_{q_{rel}}$	$\Omega(t) = e^{-t/\tau_{q_{rel}}}$



**Fig. 5.63** The  $q$ -triplet as measured from the magnetic field strength of the solar wind. The three sets of curves correspond to daily averages of the data sent in 1989 (40 AU) and in 2002 (85 AU) by the NASA Voyager 1 spacecraft. See details in [361]. Within the errors bars, these three values have been heuristically approached [199] by the values  $(q_{sen}, q_{rel}, q_{star}) = (-0.5, 4, 7/4)$ .



**Fig. 5.64** Schematic time-dependence of  $S_q$  for various degrees of fine-graining  $\epsilon$ . Instead of  $q_{sen}$ , a better notation would be  $q_{ent}$  (we know that for one-dimensional nonlinear dynamical systems, we typically have  $q_{ent} = q_{sen}$ ). We are disregarding in this scenario the influence of possible averaging over initial conditions that might be necessary or convenient (from [200]).

# Chapter 6

## Generalizing Nonextensive Statistical Mechanics

*Aqui... onde a terra se acaba e o mar começa...*

Luís Vaz de Camões  
Canto Oitavo – LUSÍADAS

We have schematically represented in Fig. 6.1 the various thermostatistical theories that are in principle possible. The present chapter is dedicated to a brief exploration of the *non q-describable region*.

### 6.1 Crossover Statistics

Equations (5.49) (paradigmatic for *BG* statistics) and (5.54) (paradigmatic for nonextensive statistics) can be unified in the following one [282]:

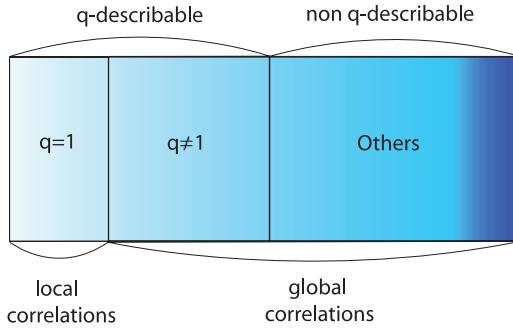
$$\frac{dy}{dx} = -a_1 y - (a_q - a_1) y^q. \quad (6.1)$$

We recover the *BG* equation for  $q = 1$  ( $\forall a_q$ ) or for  $a_q = a_1$  ( $\forall q$ ). We recover the nonextensive equation for  $a_1 = 0$ . The instances of Eq. (6.1) for which  $q$  is a natural number are particular cases of the Bernoulli differential equations [382]. The solution of Eq. (6.1) is given by

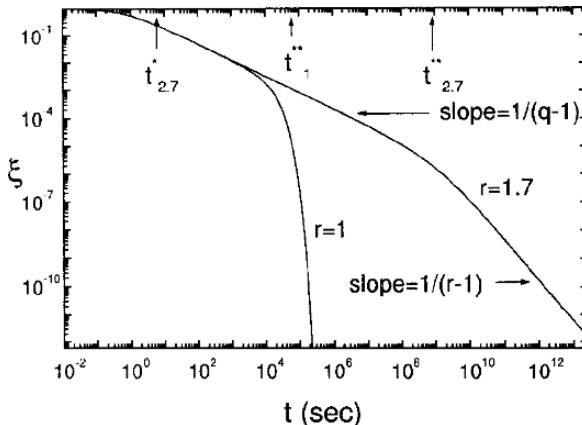
$$y = \frac{1}{\left[1 - \frac{a_q}{a_1} + \frac{a_q}{a_1} e^{(q-1)a_1 x}\right]^{\frac{1}{q-1}}} \quad (x \geq 0). \quad (6.2)$$

It can be straightforwardly verified that it contains, as particular instances, the solutions of Eqs. (5.49) and (5.54). We can also verify that

$$y \sim \begin{cases} 1 - a_q x & \text{if } 0 \leq x << x_q^* \equiv \frac{1}{(q-1)a_q}, \\ \frac{1}{[(q-1)a_q x]^{\frac{1}{q-1}}} & \text{if } x_q^* << x << x_1^{**} \equiv \frac{1}{(q-1)a_1}, \\ \left(\frac{a_1}{a_q}\right)^{\frac{1}{q-1}} e^{-a_1 x} & \text{if } x >> x_1^{**}. \end{cases} \quad (6.3)$$



**Fig. 6.1** Scenario within which nonextensive statistical mechanics is located. At the extreme *left* of the  $q = 1$  region we essentially find the noninteracting systems, such as the ideal gas, and the ideal paramagnet. At the extreme *right* of the  $q = 1$  region, we may find the critical phenomena associated with standard phase transitions [207]. These systems exhibit, at precisely the critical point, collective correlations which bridge with the  $q \neq 1$  systems. At the extreme *right* of the  $q \neq 1$  region, we cross onto a region of what one may consider as very complex systems. For such systems, a statistical mechanics even more general than the nonextensive one might be necessary. Or it just might be impossible to exist. From [200] (see [199] for more details).



**Fig. 6.2** Log–log plot of  $\xi \equiv y$  vs.  $t \equiv x$  for  $q = 2.7$ ,  $a_q = 1$ ,  $a_1 = 10^{-5}$ , and both  $r = 1$  and  $r = 1.7$ . The characteristic values  $t_q^* \equiv x_q^*$  and  $t_r^{**} \equiv x_r^{**}$  are indicated by arrows (the regions corresponding to short-, intermediate-, and long-abscissa values are clearly exhibited). The slope of the intermediate region is  $-1/(q-1)$  (from [282]).

As we see, this solution makes a crossover from a  $q$ -exponential behavior at low values of  $x$ , to an exponential one for high values of  $x$  (see Fig. 6.2). If  $x$  is to be interpreted as an energy (see Tables 5.1 and 5.2), this constitutes a generalization of the  $q$ -statistical weight. It is from this property that this statistics is sometimes referred to as *crossover statistics*.

Equation (6.1) can be further generalized as follows:

$$\frac{dy}{dx} = -a_r y^r - (a_q - a_r) y^q \quad (1 \leq r \leq q). \quad (6.4)$$

The solution of this equation has no *explicit* expression  $y(x)$ , but only  $x(y)$ . This expression appears in terms of two hypergeometric functions [282], and also corresponds to a crossover, namely

$$y \sim \begin{cases} 1 - a_q x & \text{if } 0 \leq x << x_q^* \equiv \frac{1}{(q-1)a_q}, \\ \frac{1}{[(q-1)a_q x]^{\frac{1}{q-1}}} & \text{if } x_q^* << x << x_r^{**} \equiv \frac{[(q-1)a_q]^{\frac{r-1}{q-r}}}{[(r-1)a_r]^{\frac{q-1}{q-r}}}, \\ \frac{1}{[(r-1)a_r x]^{\frac{1}{r-1}}} & \text{if } x >> x_r^{**}. \end{cases} \quad (6.5)$$

Because it exhibits a crossover from a  $q$ -exponential behavior at low  $x$ , to an  $r$ -exponential one at high  $x$  (see Fig. 6.2), it is also referred to as *crossover statistics* in the literature. This type of function has been extremely efficient in fitting a variety of experimental data (see, e.g., [282, 415]).

It should be clear that the generalization of a statistical weight is necessary but not sufficient for having a generalized statistical mechanics. Indeed, the generalization of the entropy is also needed so that the generalized statistical weight can be *deduced* from the entropy through a variational procedure. It is through this path that we can expect to have a smooth matching with thermodynamics itself. In the next section, we further generalize the present approach. We briefly present *spectral statistics* (a straightforward generalization of the crossover statistics), and *Beck–Cohen superstatistics*, which focuses on a possible distribution of parameters such as the direct (or inverse) temperature, assumed to be spatio-temporally fluctuating.

## 6.2 Further Generalizing

The  $q$ -statistical distribution and its generalization, crossover statistics, have been further generalized into *spectral statistics* [383] and Beck–Cohen superstatistics [21, 384, 386]. The exact mathematical connection between spectral and Beck–Cohen statistics is not yet fully clarified. However, as we shall argue later on, indications exist that spectral statistics contains Beck–Cohen statistics as a particular case. Therefore, the logical structure appears to be

$$\begin{aligned} BG \text{ statistics} &\subset q - \text{statistics} \subset \text{crossover statistics} \\ &\subset \text{Beck} - \text{Cohen superstatistics} \subset \text{spectral statistics}. \end{aligned} \quad (6.6)$$

It is worthy to emphasize at this point that we are here focusing only on the (stationary state) probability distributions. This ingredient is necessary but not sufficient for implementing a full statistical mechanical theory. It is also necessary to consistently define an entropy functional which, under appropriate constraints, is optimized precisely by that particular distribution. More than that, one of the

constraints must have an admissible connection with the concept of energy (another, trivial, constraint is of course normalization). These various steps are going to be illustrated in the next subsections.

### 6.2.1 Spectral Statistics

Equation (6.4) can be naturally generalized into

$$\frac{dy}{dx} = - \int d\kappa F(\kappa) y^\kappa, \quad (6.7)$$

where the nonnegative *q-spectral function*  $F(\kappa)$  (QSF) must be integrable, i.e.,  $\int d\kappa F(\kappa)$  must be finite. This (positive) integral does not need to be unity, i.e.,  $F(\kappa)$  is generically unnormalized. The particular case

$$F(\kappa) = a_r \delta(\kappa - r) + (a_q - a_r) \delta(\kappa - q), \quad (6.8)$$

$\delta(x)$  being Dirac's delta distribution, recovers Eq. (6.4). Unless specified otherwise, for simplicity we shall from now on assume that  $F(\kappa)$  is normalized (see in [383] details about how an unnormalized  $F(\kappa)$  can be transformed into a normalized one).

The possible solution of Eq. (6.7) will be noted  $\exp_{\{F\}}(x)$ . In other words,

$$\frac{d \exp_{\{F\}}(x)}{dx} = - \int_{-\infty}^{\infty} d\kappa F(\kappa) [\exp_{\{F\}}(x)]^\kappa. \quad (6.9)$$

By setting  $x = \ln_{\{F\}} y$ , we have

$$\frac{dy}{d[\ln_{\{F\}} y]} = \int_{-\infty}^{+\infty} F(\kappa) y^\kappa d\kappa, \quad (6.10)$$

hence

$$\ln_{\{F\}} x = \int_1^x \left\{ \int_{-\infty}^{+\infty} F(\kappa) u^\kappa d\kappa \right\}^{-1} du \quad (\forall x \in (0, \infty)), \quad (6.11)$$

which is the generic expression of the *inverse function* of  $\exp_{\{F\}}(x)$ .

With this definition we can generalize the entropy  $S_q$  as follows:

$$S_{\{F\}} = \sum_{i=1}^W p_i \ln_{\{F\}} \frac{1}{p_i} \equiv \sum_{i=1}^W s_{\{F\}}. \quad (6.12)$$

At equiprobability (i.e.,  $p_i = 1/W$ ) we have

$$S_{\{F\}} = \int_1^W \left\{ \int_{-\infty}^{+\infty} F(\kappa) u^\kappa d\kappa \right\}^{-1} du. \quad (6.13)$$

The generalized logarithm of Eq. (6.11) appears to be isomorphic to the generalized logarithm introduced recently by Naudts [401] who started from a different perspective.

We can straightforwardly prove that, assuming that  $F(\kappa)$  is normalized, the following properties hold:

$$\ln_{\{F\}} 1 = 0, \quad (6.14)$$

hence

$$\exp_{\{F\}} 0 = 1. \quad (6.15)$$

Also

$$\frac{d}{dx} \ln_{\{F\}} x \Big|_{x=1} = \frac{d}{dx} \exp_{\{F\}} x \Big|_{x=0} = 1, \quad (6.16)$$

as well as *monotonicity*, more precisely

$$\frac{d}{dx} \ln_{\{F\}} x > 0, \quad \forall x \in (0, +\infty), \quad (6.17)$$

and

$$\frac{d}{dx} \exp_{\{F\}} x > 0, \quad \forall x \in \mathcal{A}_{\exp_{\{F\}}}, \quad (6.18)$$

where  $\in \mathcal{A}_{\exp_{\{F\}}}$  is the set of admissible values of  $x$  for the nonnegative  $\exp_{\{F\}} x$  function. When no negative  $q$  contributes (i.e., if  $F(\kappa) = 0, \forall \kappa < 0$ ), then the following properties hold also:

$$\frac{d^2}{dx^2} \ln_{\{F\}} x < 0 \quad (\text{concavity}), \quad (6.19)$$

and

$$\frac{d^2}{dx^2} \exp_{\{F\}} x < 0 \quad (\text{convexity}). \quad (6.20)$$

Analogously, when no positive  $q$  contributes (i.e., if  $F(\kappa) = 0, \forall \kappa > 0$ ), then

$$\frac{d^2}{dx^2} \ln_{\{F\}} x > 0 \quad (\text{convexity}), \quad (6.21)$$

and

$$\frac{d^2}{dx^2} \exp_{\{F\}} x > 0 \quad (\text{concavity}). \quad (6.22)$$

Also, if no  $q$  above unity contributes (i.e., if  $f(\kappa) = 0, \forall \kappa > 1$ ), then

$$\lim_{x \rightarrow +\infty} \ln_{\{F\}} x = +\infty, \quad (6.23)$$

and, if no  $q$  below unity contributes (i.e., if  $f(\kappa) = 0, \forall \kappa < 1$ ), then

$$\lim_{x \rightarrow 0^+} \ln_{\{F\}} x = -\infty. \quad (6.24)$$

Illustrations of  $S_{\{F\}}$  for Gaussian and binary QSFs can be found in [383].

We have seen so far how from a given QSF we can produce the corresponding entropic functional. We will now work in the reverse way: given a specific entropic functional, we will find (if possible) the QSF that produces it. Consider a general entropic functional of the form:

$$S = \sum_{i=1}^W s(p_i), \quad (6.25a)$$

$$s(x) = x \ln_{\{F\}} \frac{1}{x}. \quad (6.25b)$$

We have:

$$\begin{aligned} \ln_{\{F\}} x &= \int_1^x \frac{du}{\int_{-\infty}^{+\infty} F(\kappa) u^\kappa d\kappa} \Leftrightarrow \\ \frac{d}{dx} (\ln_{\{F\}} x) &= \frac{1}{\int_{-\infty}^{+\infty} F(\kappa) x^\kappa d\kappa} \Leftrightarrow \\ \int_{-\infty}^{+\infty} F(\kappa) x^\kappa d\kappa &= \frac{1}{\frac{d}{dx} (\ln_{\{F\}} x)} \Leftrightarrow \\ \int_{-\infty}^{+\infty} F(\kappa) e^{\kappa \ln x} d\kappa &= \frac{1}{\frac{d}{dx} (\ln_{\{F\}} x)}. \end{aligned} \quad (6.26)$$

We set:

$$\omega = -i \ln x. \quad (6.27)$$

Then, from Eq. (6.26), we obtain:

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} F(\kappa) e^{i\omega\kappa} d\kappa = \frac{1}{\sqrt{2\pi}} \cdot \frac{e^{i\omega}}{\frac{d}{d\omega} (\ln_{\{F\}} e^{i\omega})}. \quad (6.28)$$

The LHS of Eq. (6.28) is however nothing but the Fourier transform of  $F$ . Thus, inverting the transform we have:

$$F(\kappa) = \frac{i}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{i\omega(1-\kappa)}}{\frac{d}{d\omega} (\ln_{\{F\}} e^{i\omega})} d\omega. \quad (6.29)$$

Inserting the entropy functional of Eq. (6.12) into Eq. (6.29) we finally get:

$$F(\kappa) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \frac{e^{-i\omega}}{s(e^{-i\omega}) - i \frac{d}{d\omega} [s(e^{-i\omega})]} d\omega. \quad (6.30)$$

Equation (6.30) is quite important. Indeed, it shows that the QSF corresponding to a large class of entropy functionals can be explicitly calculated. It is straightforward to check that for  $s$  given by BG or by nonextensive statistics we get  $F(\kappa) = \delta(\kappa - q)$  as anticipated.

In order to be able to derive the normalized QSF associated with a given entropy, the entropy functional must fulfill the following requirements.

1. It must be possible to write the total entropy  $S$  as a sum of the entropic function  $s$  for each state (Eq. (6.25a)).
2. The function  $s$  must satisfy  $s(1) = 0$ , which is in fact a quite reasonable requirement for an entropy.
3. Furthermore, we must have:

$$\left. \frac{ds(x)}{dx} \right|_{x=1} = -1. \quad (6.31)$$

This condition is equivalent to having the QSF normalized to unity. If we abandon the normalization of the QSF then we can consistently drop this last requirement.

4. The function  $s(x)$  must be defined (or analytically continued) on the unitary circle and it must also be differentiable in the same domain.
5. The integral of Eq. (6.30) must converge.

As a nontrivial illustration, we will now use the present method to find the QSF associated with an exponential entropic form. Let us assume

$$S = \sum_{i=1}^W p_i \left( 1 - e^{\frac{p_i-1}{p_i}} \right), \quad (6.32)$$

hence

$$s(x) = x \left( 1 - e^{-\frac{x-1}{x}} \right). \quad (6.33)$$

It is trivial to see that Eq.(6.33) fulfills all the criteria set above, and we can thus find a normalized QSF for it. Using Eq.(6.30) we get:

$$F(\kappa) = \frac{1}{e} \sum_{n=0}^{\infty} \frac{\delta(\kappa - n)}{n!}. \quad (6.34)$$

Although different, entropy (6.32) has some resemblance with that introduced by Curado [120]. We claim no particular physical justification for the form (6.32). In the present context, it has been chosen uniquely with the purpose of illustrating the mathematical procedure involved in the inverse QSF problem.

### 6.2.2 Beck–Cohen Superstatistics

We may say that Beck–Cohen superstatistics originated essentially from a mathematical remark and its physical interpretation [327, 328]. The basic remark is that there is a simple link, described hereafter, between the  $q$ -exponential function (with  $q \geq 1$ ) and the so-called *Gamma distribution* with  $n$  degrees of freedom. Beck and Cohen [384] start from the standard Boltzmann factor but with  $\beta$  being itself a random variable (whence the name “superstatistics”) due to possible spatial and/or temporal fluctuations. They define

$$P(E) = \int_0^{\infty} d\beta' f(\beta') e^{-\beta'E}, \quad (6.35)$$

where  $f(\beta')$  is a normalized distribution, such that  $P(E)$  also is normalizable under the same conditions as the Boltzmann factor  $e^{-\beta'E}$  itself is. They also define

$$q_{BC} \equiv \frac{\langle (\beta')^2 \rangle}{\langle \beta' \rangle^2} = \frac{\int_0^{\infty} d\beta' (\beta')^2 f(\beta')}{\left[ \int_0^{\infty} d\beta' \beta' f(\beta') \right]^2}, \quad (6.36)$$

where we have introduced *BC* standing for *Beck–Cohen*.

If  $f(\beta') = \delta(\beta' - \beta)$  we obtain Boltzmann weight

$$P(E) = e^{-\beta E}, \quad (6.37)$$

and  $q_{BC} = 1$ .

If  $f(\beta')$  is the Gamma-distribution, i.e.,

$$f(\beta') = \frac{n}{2\beta\Gamma(\frac{n}{2})} \left( \frac{n\beta'}{2\beta} \right)^{n/2-1} \exp\left\{-\frac{n\beta'}{2\beta}\right\} \quad (n = 1, 2, 3, \dots), \quad (6.38)$$

we obtain

$$P(E) = e_q^{-\beta E}, \quad (6.39)$$

and  $q_{BC} = q$ , with

$$q = \frac{n+2}{n} \geq 1. \quad (6.40)$$

Several other examples of  $f(\beta')$  are discussed in [384], and it is eventually established the following important result: all narrowly peaked distributions  $f(\beta')$  behave, in the first nontrivial leading order, as  $q$ -statistics with  $q = q_{BC}$ . Further details and various applications to real systems are now available [21, 385–395] of this theory (which, unless  $f(\beta')$  is deduced from first principles, remains phenomenological).

As we mentioned previously, the above discussion concerns the statistics. More than that is needed to have a statistical mechanical theory, namely it is necessary to introduce an associated generalized entropic functional, as well as an appropriate constraint related to the energy. This program has in fact completely been carried out for superstatistics, and details can be seen in [263, 264, 396]. An interesting point is worthy mentioning: of all admissible  $f(\beta')$ , only Eq. (6.38) yields a stationary-state distribution optimizing the associated entropy within which the Lagrange parameter (usually noted  $\alpha$ ) corresponding to the normalization constraint factorizes from the term containing the  $\beta$  Lagrange parameter. In other words, *of all superstatistics, only  $q$ -statistics admits a partition function on the usual grounds, i.e., depending on  $\beta$  but not on  $\alpha$ .*

Let us conclude this subsection by focusing on the connection of spectral statistics with the Beck–Cohen superstatistics. Quite recently, an entropic functional has been derived that corresponds to superstatistics. This functional is of the form  $S = \sum_i s(p_i)$ , with

$$s(y) = \int_0^y \frac{a + K^{-1}(y)}{1 - \frac{K^{-1}(y)}{E^*}} , \quad (6.41)$$

where

$$K(y) = \frac{P(y)}{\int_0^{+\infty} P(u)du} . \quad (6.42)$$

In Eq. (6.41),  $E^*$  stands for the lowest admissible energy for the system and  $a$  is a Lagrange multiplier. Using Eqs. (6.41) and (6.30) we can in principle get the QSF  $F(\kappa)$  for a given temperature distribution function  $f(\beta')$ . Thus, in principle at least, the various superstatistics can be accommodated into spectral statistics. However, there are certain cases where spectral statistics can go further than superstatistics. For example, it appears that through superstatistics we can, up to now, only produce the nonadditive entropies  $S_q$  for  $q \geq 1$ , while in the spectral formalism we can have them for arbitrary values of  $q$ . This is the reason for which we have written the last logical inclusion in structure (6.6) as it stands there.

**Part III**

**Applications or What for the Theory  
Works**

# Chapter 7

## Thermodynamical and Nonthermodynamical Applications

*Nothing is more practical than a good theory.<sup>1</sup>*

The nature of the present chapter is quite different from all the others of the book. In all its other Chapters we have privileged the presentation and understanding of nonextensive statistical mechanics itself, and of some of its delicate and unusual concepts. In the present chapter, we focus on the concrete and typical applications that are available in the literature, as well as on some connections that have emerged along time with other areas such as quantum chaos, quantum entanglement, random matrices, theory of networks.

The present list is not an exhaustive one. It is aimed mainly to illustrate the specific types of systems that have been handled in one way or another within the nonextensive framework. Some of them are genuine applications of the theory, others are just possible explanations and connections. Whenever the microscopic, or at least the mesoscopic, dynamics of the system is unknown, it is of course impossible to determine  $q$  otherwise than through fitting (as astronomers determine the elliptic eccentricities of the orbits of the planets). This extra difficulty does not exist in *BG* thermostatistics, since the corresponding value trivially is just  $q = 1$ . In the more complex systems addressed in this chapter, all types of situations occur. Sometimes the experimental measurements, or observations, or computational results exist through very many numerical decades with satisfactory precision. In these cases, the correctness of the fitness constitutes already a strong argument favoring the applicability of the nonextensive theory, with its predictions and concepts. Sometimes, we have at our disposal only a few numerical decades and/or not very high precision. It might then be disputable whether the system under focus really belongs to the present frame, or to a somewhat different one. Sometimes, it becomes possible to make precise falsifiable predictions, sometimes not. Sometimes the applications just consist in improved algorithms for optimization, signal analysis, image processing, and similar techniques. In these cases, the quality of the improvement speaks by itself. In all cases, we do achieve a better understanding of the phenomenon, or at least develop some intuition on it.

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<sup>1</sup> Attributed to Lenin.

Before starting with the description of typical applications, let us remind that the knowledge of the microscopic dynamics is *necessary but not sufficient* for the implementation of the entire theory from first principles. Indeed, it is only *in principle* that the microscopic dynamics contains all the ingredients enabling the calculation of the index (or indices)  $q$ . It is still necessary to be able to calculate, in the full phase-space, quantities such as the sensitivity to the initial conditions or the entropy production. This calculation can be extremely hard. But, whenever tractable, then it provides the value(s) of  $q$ . Once  $q$  is known, it becomes possible to implement the thermodynamical steps of the theory. This is to say, we can in principle proceed and calculate the partition function of the system, and, from this, calculate various important thermodynamical quantities such as specific heat, susceptibility, and others. Naturally, the difficulty of this last step of the calculation should not be underestimated. It suffices to remember the formidable mathematical difficulties involved in Onsager's celebrated solution of the square-lattice spin 1/2 Ising ferromagnet. And he only had to deal with *first-neighbor interactions* and *exponential thermal weights*. In a full  $q$ -statistical calculation, we have to deal typically with *interactions at all distances* (or related conditions) and *power-law weights*! This difficulty might explain why we have, up to now, only partial results for the many-body long-range-interacting inertial XY ferromagnet addressed in Section 5.4. This task would be hopeless had we not access to approximate solutions based on variational principles, Green-functions, numerical approaches, and others. As a mathematical exercise, the  $q$ -statistics of simple systems such as the ideal gas and the ideal paramagnet are available in the literature. However, these calculations only provide some mathematical hints with modest physical content. Indeed, thermal equilibrium in the absence of interactions mandates  $q = 1$ . Further, and extremely powerful, hints are also available from the full discussion of simple maps, as shown in Sections 5.1 and 5.2. However, these systems, no matter how useful they might be for various applications, are *nonthermodynamical*. In other words, they do *not* have energy associated, and are therefore useless in order to illustrate the thermostatistical steps of the full calculation, and their connection to thermodynamics itself.

We present next various applications in various areas of knowledge.

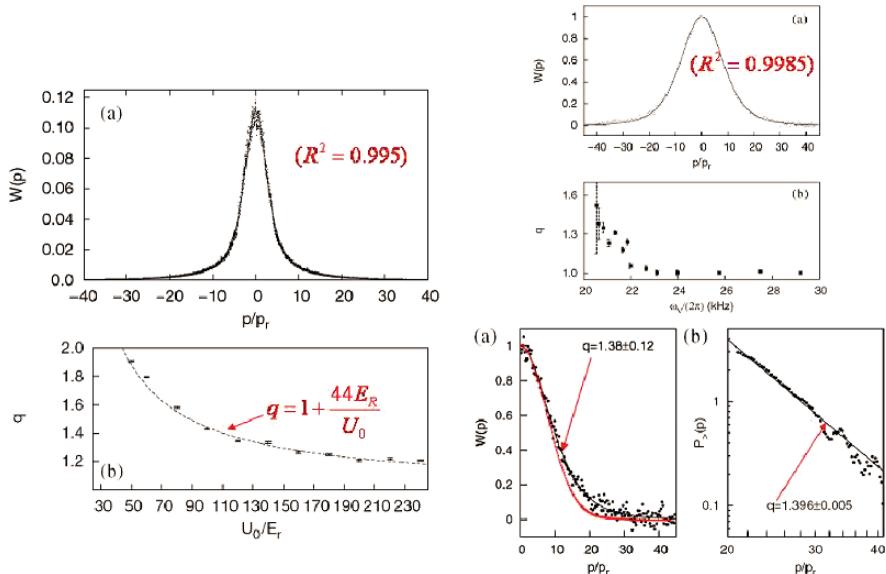
## 7.1 Physics

### 7.1.1 Cold Atoms in Optical Lattices

On the basis of nonextensive statistical mechanical concepts, Lutz predicted in 2003 [460] that cold atoms in dissipative optical lattices would have a  $q$ -Gaussian distribution of velocities, with

$$q = 1 + \frac{44E_R}{U_0}, \quad (7.1)$$

where  $E_R$  and  $U_0$  are, respectively, the *recoil energy* and the *potential depth*. The prediction was impressively verified three years later [461], as shown in Fig. 7.1.

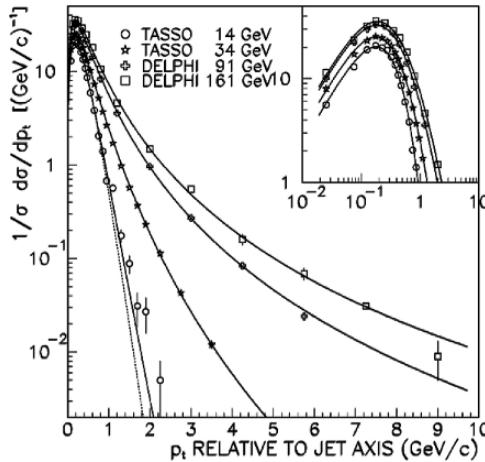


**Fig. 7.1** Computational verification with quantum Monte Carlo (*left panels*), and laboratory verification with  $C_s$  atoms (*right panels*) of Lutz's theory (from [461]).

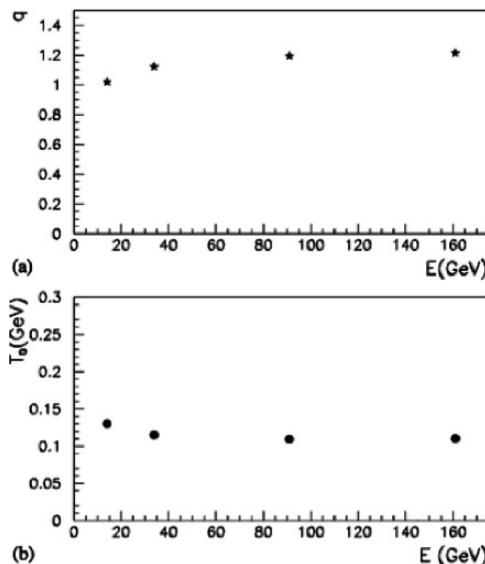
## 7.1.2 High-Energy Physics

### 7.1.2.1 Electron–Positron Annihilation

Electrons and positrons in frontal collisions at high energy typically annihilate and produce a few hadronic jets. The analysis of the transverse momenta of those jets provides interesting physical information related, among others, to the production of mesons. The process can in principle be described in thermostatistical terms, without entering into microscopic details in the realm of Quantum Chromodynamics. Fermi was the pioneer of this type of approach [402], followed by Hagedorn [403]. According to Hagedorn, such high-energy collisions produce excited hadron *fireballs* that reach some kind of *thermal equilibrium*. An important consequence of this approach would be that increasing the collisional energy would *not* change the involved basic masses (that of mesons that are being produced) but it would only increase their number, such as an increase of heat delivery when one boils water does *not* modify the phase-transition temperature, but only increases the amount of liquid that becomes gas. A similar statement was made, a few years later, by Field and Feynman [404]. The use of the Boltzmann weight in the relativistic limit yields [403] a distribution of hadronic transverse momenta which exhibits a reasonably satisfactory agreement with experimental data at relatively low collisional energy, say at 14 GeV (TASSO experiments). But increasing that energy, the temperature (a fitting parameter) did *not* remain constant, as predicted by the theory. This approach was somewhat discredited and abandoned. The idea was revisited in



**Fig. 7.2** Distribution of transverse momenta of the hadronic jets.



**Fig. 7.3** Energy-dependence of the entropic parameter  $q$  and the temperature  $T$ .

2000 by Bediaga, Curado, and Miranda [405], but this time assuming a  $q$ -statistical weight. The results were very satisfactory this time, even for collisional energies up to 161  $GeV$  (DELPHI experiments), as can be seen in Figs. 7.2 and 7.3. The temperature remained virtually constant all the way long, and the agreement of the theoretical curves (which, though conceptually simple, involve nevertheless eight

hypergeometric functions) with the experimental data is quite impressive for the entire range of transverse hadronic momenta. The phenomenological value of  $q$  slightly increases from  $q = 1$  to  $q \simeq 1.2$  (the asymptotic value  $11/9$  has been suggested [406] for the very large energies) when the center-of-mass collisional energy increases from 14 to 161 *Gev*. See [405] for a possible physical origin of this effect.

Many other high-energy multiparticle production processes (from collisions such as  $p\bar{p}$ ,  $Au+Au$ ,  $Cu+Cu$ ,  $Pb+Pb$ , etc.) have been analyzed along related lines [407–414]. The values of  $q$  that emerge (from the BRAHMS, STAR, PHENIX data, for instance) are systematically close to the case discussed above, typically in the range  $1 < q < 1.2$ . The nonzero values of  $q - 1$  are frequently interpreted in terms of sizeable temperature fluctuations that exist during the hadronization process (see [327, 328, 384]).

### 7.1.2.2 Flux of Primary Cosmic Rays

Cosmic rays arrive to Earth within a vast range of energies, up to values close to  $10^{20} \text{ ev}$ . Their associated fluxes vary within impressive 33 orders of magnitude: see Fig. 7.4. This curve includes the so-called “knee” and “ankle,” at intermediate and very high energies, respectively. It turns out that it is possible, without entering into any specific mechanism, to provide [415] an excellent phenomenological description of these data by assuming a crossover between two  $q$ -exponential distribution functions. The two corresponding values of  $q$  are quite close among them, and also close to  $11/9$  ([416]).

### 7.1.2.3 Quantum Scattering of Particles

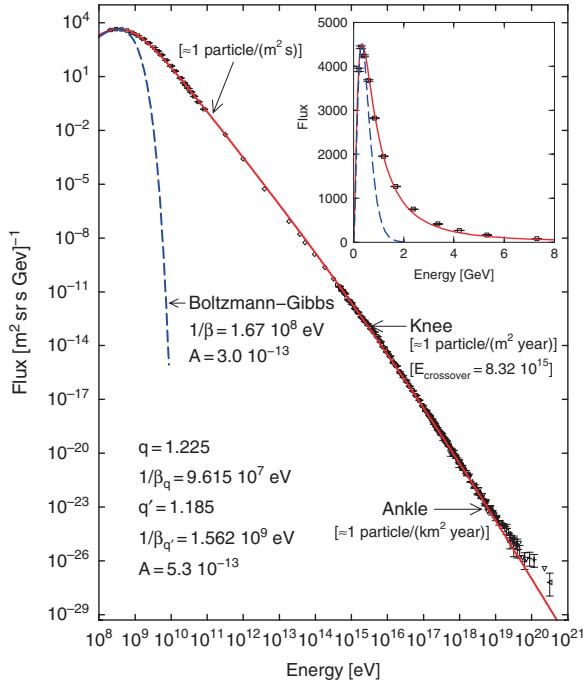
Entropic bounds for scattering of spinless particles (e.g., pions) by a nucleus have been established and tested [417–420] with available experimental results for phase shifts. Typical results involving  $^4He$ ,  $^{12}C$ ,  $^{16}O$ , and  $^{40}Ca$  nuclei are exhibited in Fig. 7.5. Along this line, a conjugation relation naturally emerges for two relevant entropic indices, noted  $q$  and  $\bar{q}$  (see details in [419, 420]). This relation is given by

$$\frac{1}{q} + \frac{1}{\bar{q}} = 2, \quad (7.2)$$

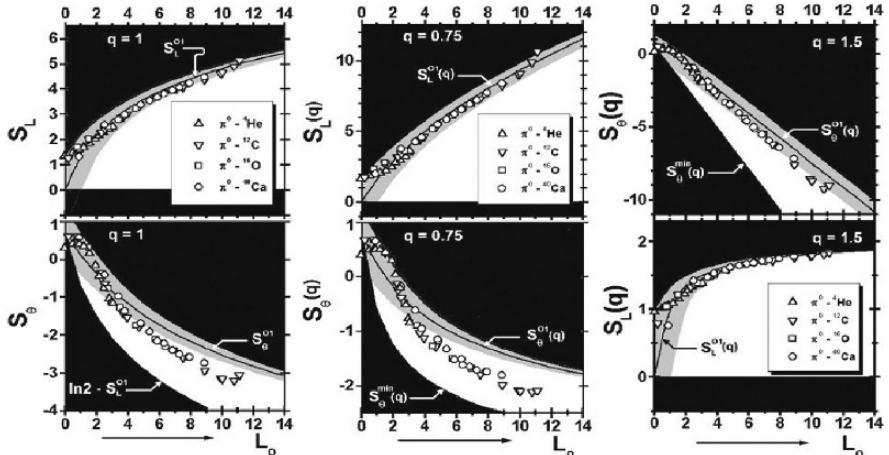
which can equivalently be written as

$$\bar{q} = \mu\nu\mu(q), \quad (7.3)$$

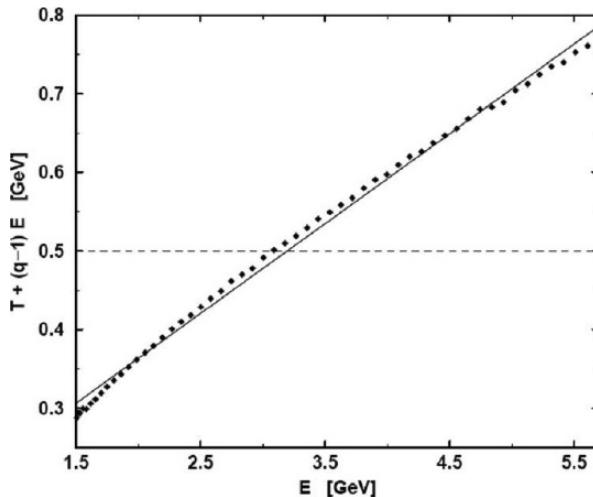
where the multiplicative and additive dualities  $\mu$  and  $\nu$  are those defined in Eqs. (4.39) and (4.40), respectively. A deeper understanding of this intriguing connection would be welcome.



**Fig. 7.4** Fluxes of cosmic rays. The red curve comes from a crossover statistics (see [415]).



**Fig. 7.5** Experimental tests, with data of scattering of pions by various nuclei ( ${}^4\text{He}$ ,  ${}^{12}\text{C}$ ,  ${}^{16}\text{O}$  and  ${}^{40}\text{Ca}$ ), of the theoretically allowed bands (grey regions) of the angular entropy ( $S_\theta$ ) and the angle-momentum entropy ( $S_L$ ) for  $q = 1$ ,  $q = 0.75$ , and  $q = 1.5$  (from [418]).



**Fig. 7.6** The dashed and continuous straight lines correspond to a phenomenological  $q$ -statistical approach with  $q = 1$  and  $q = 1.114$ , respectively. The dots have been obtained from a quantum calculation (from [421]).

#### 7.1.2.4 Diffusion of Charm Quark

A preliminary analysis of the diffusion of a charm quark in a thermal quark-gluon plasma is available [421]. A direct quantum mechanical calculation and a phenomenological theory based on  $q$ -statistics are compared in Fig. 7.6. The two calculations roughly coincide for  $q = 1.114$ , whereas the discrepancy is considerable if  $q = 1$  is adopted instead. Further microscopic dynamical (and surely nontrivial!) studies are certainly necessary in order to understand why the specific value  $q = 1.114$  provides a good first approximation, and why, even for this value, a small but visible systematic discrepancy is observed.

As one more admissible application in the area of high-energy physics, let us mention that a detailed literature exists advancing a possible connection between the solar neutrino problem and nonextensive statistics. Indeed, by now the well-established neutrino oscillations do not totally explain, in some cases, the discrepancy exist's between the theoretical predictions based on the *Standard Solar Model* and the neutrino fluxes measured on Earth. Therefore, some other contributions might be there. It is proposed [422–424] that they come from the fact that most probably the solar plasma is not in thermal equilibrium, but in a kind of stationary state instead, where nonextensive phenomena (basically due to strong spatial-temporal correlations) could be present and relevant.

#### 7.1.3 Turbulence

Quite an effort has been dedicated to understanding the ubiquitous connections of nonextensive statistics with turbulence. This includes lattice-Boltzmann models [425, 426], defect turbulence [427], rotations in oceanic flows [428], air turbulence

in airports [389, 429, 430], turbulence at the level of the trees of the Amazon forest, [431, 432], turbulent Couette–Taylor flow and related situations [433, 439–443], Lagrangian turbulence [444], two-dimensional turbulence in pure electron plasma [445, 446], the so-called one-dimensional “turbulence” [447, 448], among others. Criticism has also been advanced [449]. For several of the experimental situations that have been studied,  $q$ -statistics appears to be a quite good approximation. However, for some experiments, further improvement becomes possible (see, for instance, [389]) whenever many experimental decades are accessible to measurement.

Naturally, we do not intend here to exhaustively review the subject, and the reader is referred to the above literature for details. In what follows we have selected instead only a few of those studies, with the aim of characterizing the types of approaches that have been developed.

### 7.1.3.1 Lattice-Boltzmann Models for Fluids

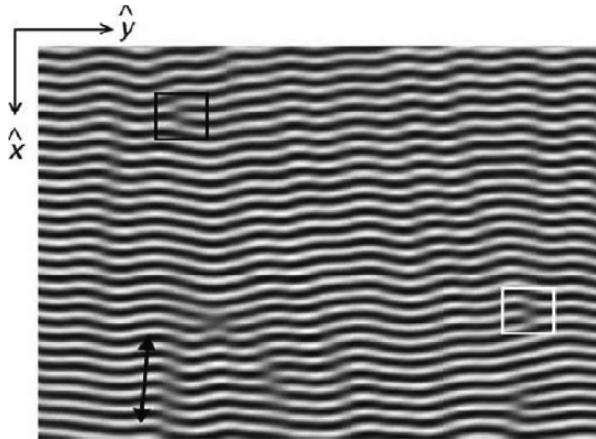
The incompressible Navier–Stokes equation has been considered [425] on a discretized  $D$ -dimensional Bravais lattice of coordination number  $b$ . It is further assumed that there is a single value for the particle mass, and also for speed. The basic requirement for the lattice-Boltzmann model is to be *Galilean-invariant* (i.e., invariant under change of inertial reference frame), like the Navier–Stokes equation itself. It has been proved [425] that an H-theorem is satisfied for a trace-form entropy (i.e., of the form  $S(\{p_i\}) = \sum_i^W f(p_i)$ ) only if it has the form of  $S_q$  with

$$q = 1 - \frac{2}{D}. \quad (7.4)$$

Therefore,  $q < 1$  in all cases ( $q > 0$  if  $D > 2$ , and  $q < 0$  if  $D < 2$ ), and approaches unity from below in the  $D \rightarrow \infty$  limit. This study has been generalized by allowing multiple masses and multiple speeds. Galilean invariance once again mandates [426] an entropy of the form of  $S_q$ , with a unique value of  $q$  determined by a transcendental equation involving the dimension and symmetry properties of the Bravais lattice as well as the multiple values of the masses and of the speeds. Of course, Eq. (7.4) is recovered for the particular case of single mass and single speed.

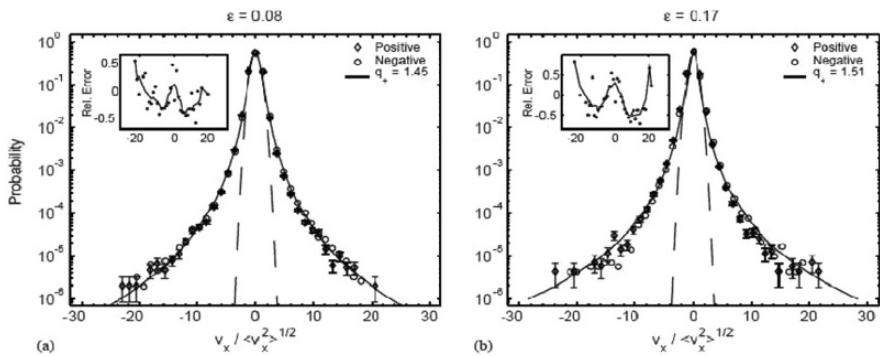
### 7.1.3.2 Defect Turbulence

Experiments have been done [427] in a convection cell which is heated from below and cooled from above, and which is tilted a certain angle with respect to gravity. In such circumstances, defects spontaneously appear in the undulations of the fluid: see Fig. 7.7. The distribution of velocities of these defects as well as their diffusion has been measured: see Figs. 7.8 and 7.9, respectively. The experimental condition is characterized by the *dimensionless driving parameter*  $\epsilon \equiv \frac{\Delta T}{\Delta T_c} - 1 \geq 0$ , where  $\Delta T$  is the temperature difference maintained between bottom and top of the cell, and  $\Delta T_c$  is a characteristic temperature difference of the system. Under many different experimental conditions (in particular, many values of  $\epsilon$ ), it was found that

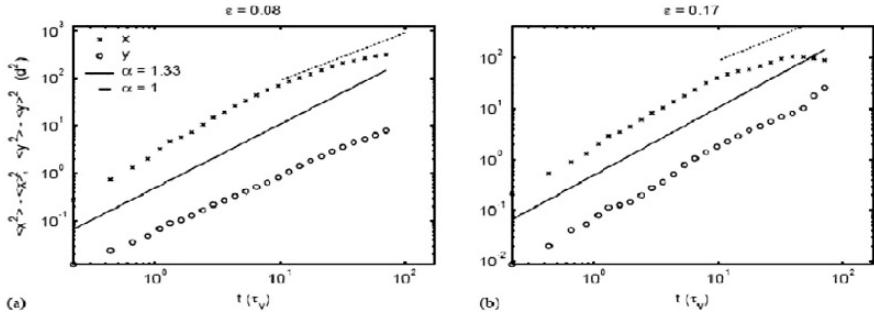


**Fig. 7.7** Example shadowgraph image of undulation chaos in fluid (compressed  $CO_2$  with Prandtl number  $Pr = v/\kappa \simeq 1$ , where  $v$  is the *kinematic viscosity* and  $\kappa$  is the *coefficient of thermal expansion*) heated from below and cooled from above, inclined by an angle of  $30^\circ$ . The dimensionless driving parameter is  $\epsilon = 0.08$ . The black (white) box encloses a positive (negative) defect. The convection cell has a thickness  $d = (388 \pm 2) \mu\text{m}$  and dimensions  $100d \times 203d$ , of which only a central  $51d \times 63d$  region was used for analysis (from [427]).

the distribution of velocities is, along six decades, a  $q$ -Gaussian with  $q \simeq 1.5$ , as illustrated in Fig. 7.8. Furthermore, superdiffusion was observed with a diffusion exponent  $\alpha \simeq 4/3$ , as illustrated in Fig. 7.9. These values satisfy the prediction (4.16) (with the notation change  $\mu \equiv \alpha$ ). Similar results are to be expected [427] for phenomena such as electroconvection in liquid crystals, nonlinear optics, and auto-catalytic chemical reactions.



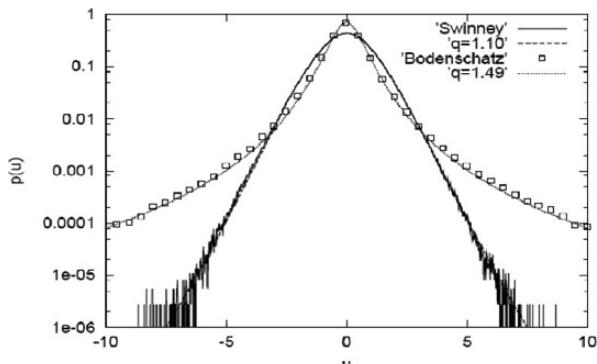
**Fig. 7.8** Transverse velocity ( $v_x$ ) distributions for  $\epsilon = 0.08$  (a) and  $\epsilon = 0.17$  (b) for positive and negative defects, rescaled to unit variance. Solid lines are  $q$ -Gaussian fittings ( $q$  being the only fitting parameter) for positive defects. Dashed lines represent a unit variance Gaussian. Insets: Relative errors [ $p_{\text{experiment}} - p_{\text{theory}}]/p_{\text{theory}}$  for positive defects (from [427]).



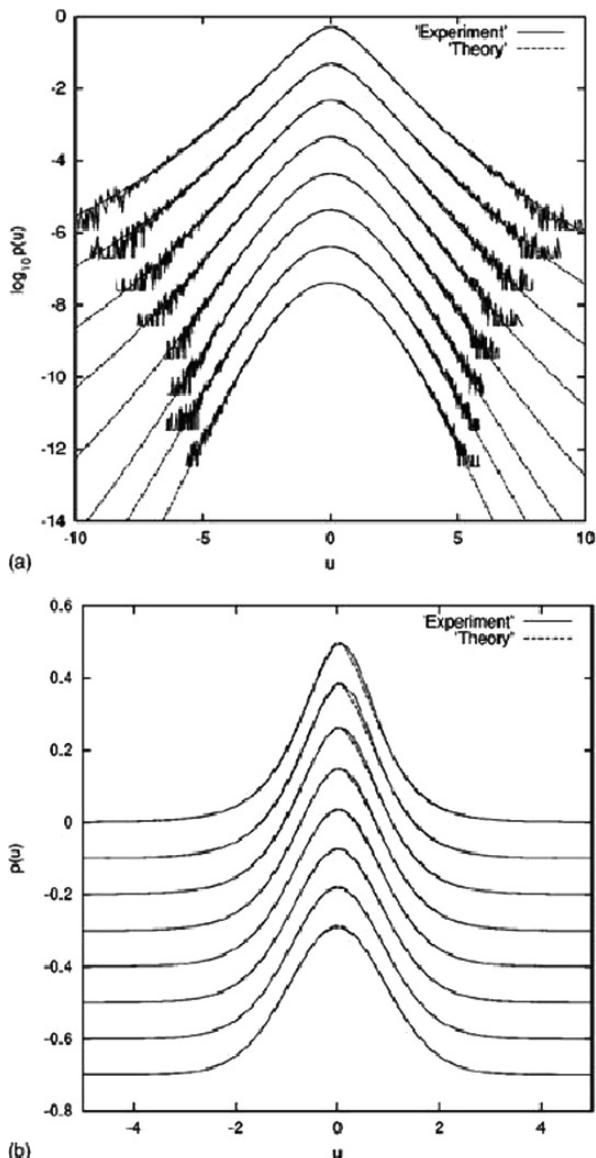
**Fig. 7.9** Time evolution of the second moments of position trajectories in  $x$  and  $y$ . Solid line is the diffusive behavior predicted by Eq. (4.16) with  $q = 3/2$ , i.e.,  $\alpha = 4/3$ ; dotted line corresponds to normal diffusion ( $q = 1$ ). Fits to the data give values of  $\alpha$  in the range 1.16–1.5, depending on the region being fit (from [427]).

### 7.1.3.3 Couette–Taylor Flow

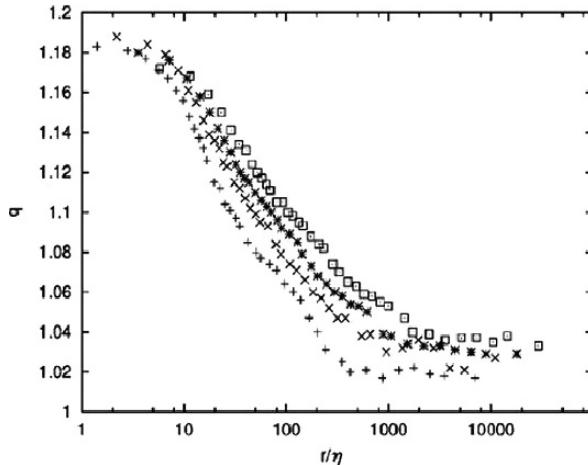
Lagrangian and Eulerian experiments have been done of fluid motion within two rotating concentric cylinders, and results for the velocity distributions have been compared with  $q$ -Gaussians. A large literature exists on the subject, but here we only provide a few typical illustrations [328]: see Fig. 7.10. Further details on Eulerian experiments are indicated in Figs. 7.11 and 7.12. Data collapse for the values of  $q$  is possible: see Fig. 7.13. Recent developments suggest that the theory must be somewhat improved in order to match higher precision data: for more details see [389].



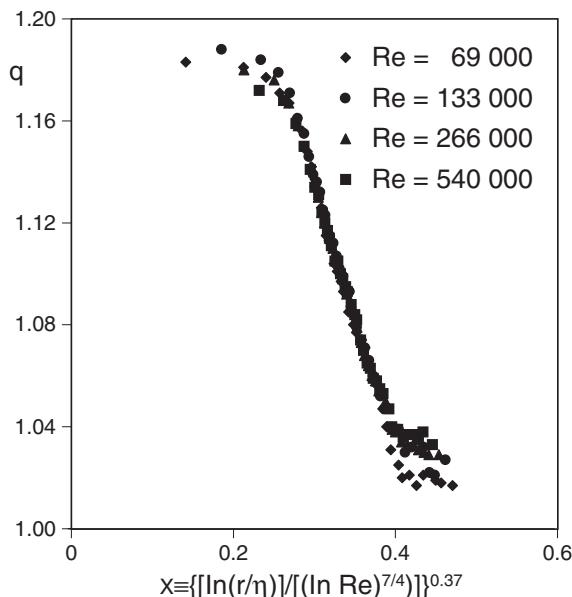
**Fig. 7.10** Histogram of horizontal velocity differences as measured and analyzed by Swinney et al. [433], and by Bodenschatz et al. [438] in turbulent Couette–Taylor flow experiments (from [328]).



**Fig. 7.11** Experimentally measured probability distributions of the velocity differences for the Couette–Taylor experiment at Reynolds number  $Re = 540,000$  for typical values of the distance  $r$  are compared with theoretical  $q$ -Gaussians: (a) logarithmic plot; (b) linear plot. The rescaled distances  $r/\eta$  ( $\eta$  is the Kolmogorov length scale) are, from top to bottom, 11.6, 23.1, 46.2, 92.5, 208, 399, 830, and 14,400. For better visibility, each distribution in (a) is shifted by  $-1$  unit along the  $y$  axis, and each distribution in (b) is shifted by  $-0.1$  unit along the  $y$  axis (from [433]).



**Fig. 7.12** Values of  $q$  used in Fig. 7.11. The Reynolds numbers are, from bottom to top, 69,000, 133,000, 266,000 and 540,000 (from [433]).



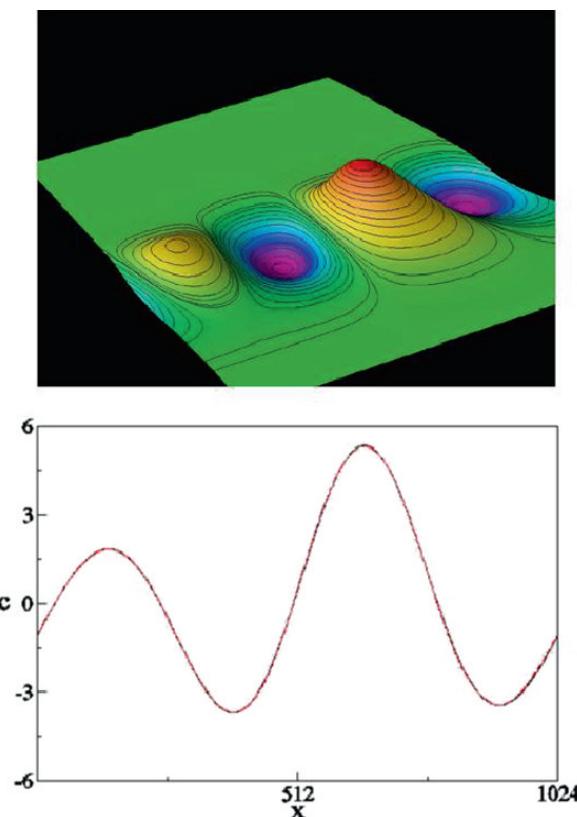
**Fig. 7.13** Same data as in Fig. 7.12. The variable in the abscissa was heuristically found. The variable  $[\ln(r/\eta)]/[(\ln Re)^{7/4}]$  leads to data collapse of the central region; the exponent 0.37 makes the data-collapsed region to become roughly a straight line. These features remain unexplained until now (from [434]).

### 7.1.4 Fingering

When two miscible liquids are pushed one into the other one, it is frequently observed *fingering* (e.g., viscous fingering) [435–437]. By computationally solving an appropriate generalized diffusion equation, this phenomenon has been put into evidence computationally: see Fig. 7.14.

### 7.1.5 Granular Matter

Granular matter systems provide many interesting applications (see, for instance [450–452]). They involve inelastic collisions between the particles.



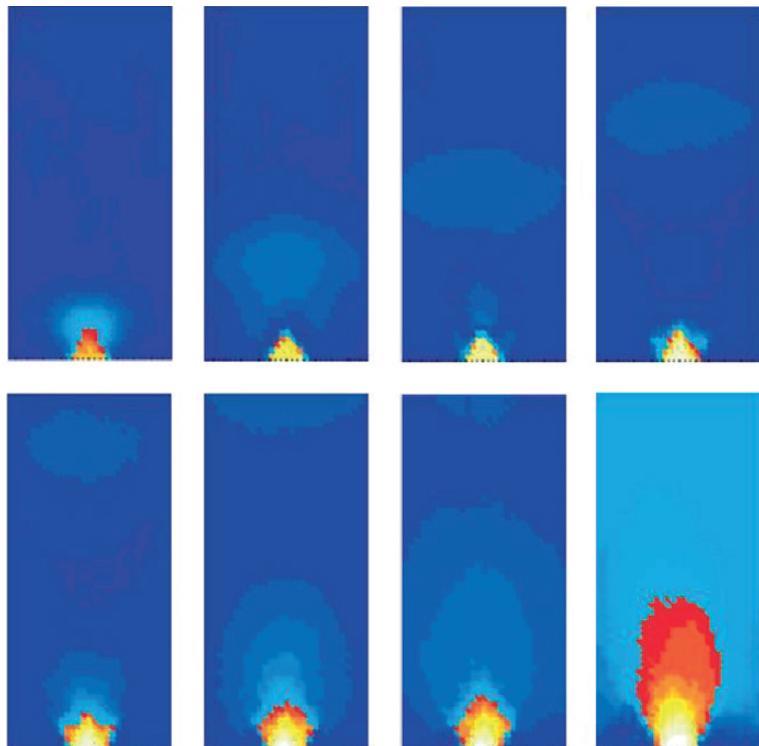
**Fig. 7.14** *Top:* Concentration fluctuations field in the onset of fingering between two miscible liquids showing landscape of  $q$ -Gaussian “hills and wells” (highest positive values are red; highest negative values are magenta). From [435,437]. These structures identify the existence of precursors to the fingering phenomenon as they develop before any fingering pattern can be seen. *Bottom:* Section plane cut through the hills and wells. The *dashed line* is made from junctions (at the successive inflection points) of  $q$ -Gaussian branches.

### 7.1.5.1 Inelastic Maxwell Models

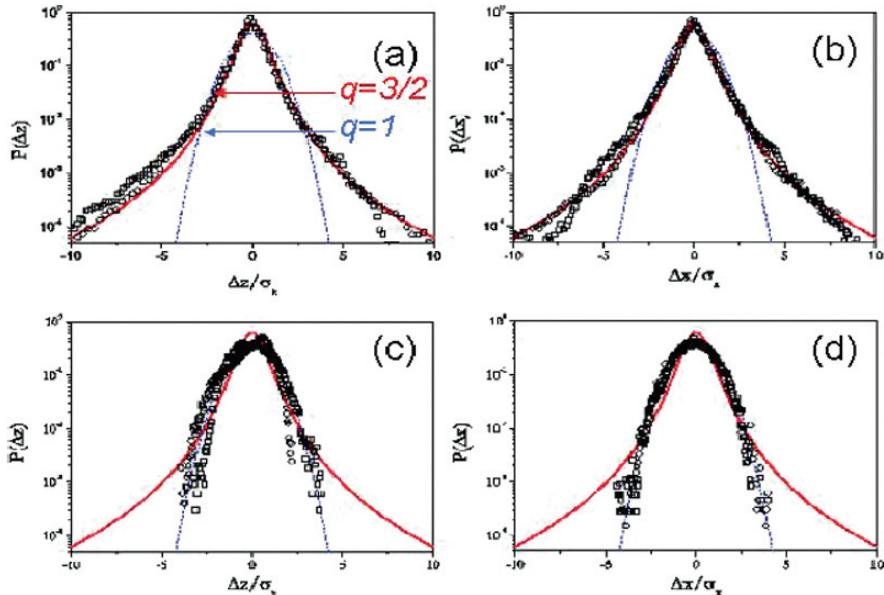
In some simple models, such as the so-called inelastic Maxwell models, analytic calculations can be performed (e.g., in [453]). The velocity distribution that is obtained, from the microscopic dynamics of the system of cooling experiments, for a spatially uniform gas whose temperature is monotonically decreasing with time is given by (see [450] and references therein) following asymptotic (i.e.,  $t \rightarrow \infty$ ) distribution

$$P(v, t) = \frac{2}{\pi v_0(t)} \frac{1}{\left[1 + \frac{v^2}{(v_0(t))^2}\right]^2}, \quad (7.5)$$

with  $v_0(t) = v_0(0) e^{-\lambda(r)t}$ ,  $\lambda(r)$  being a function of the *restitution coefficient*  $r$  of the inelastic collisions (with  $\lambda(1) = 0$ ). Equation (7.5) precisely corresponds to a  $q$ -Gaussian with  $q = 3/2$ .



**Fig. 7.15** Average vertical velocity profile inside the silo for an aperture  $11d$  ( $d$  is the diameter of the grains) in eight different stages of its evolution. Time increases from left to right and from top to bottom. In the last one – corresponding to the fully developed flow – a grain on top has fallen a distance equivalent to twice its diameter  $d$ . Note the existence of a bounded region in the velocity profile that travels in the vertical direction (from [451,452]).



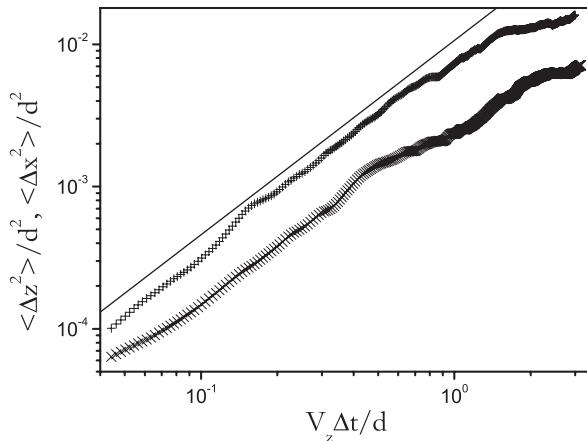
**Fig. 7.16** The vertical ((a) and (c)) and horizontal ((b) and (d)) displacement normalized distributions approach a  $q$ -Gaussian with  $q \simeq 1.5$  in the *intermediate regime* ((a) and (b)), and a Gaussian in the *fully developed regime* ((c) and (d)). The symbols indicate the silo aperture: circles for  $3.8d$  and squares for  $11d$ . The blue (red) solid line is a Gaussian ( $q$ -Gaussian with  $q = 3/2$ ) (from [451, 452]).

### 7.1.5.2 Silo Drainage

Computational simulations have been recently done [451, 452] for the discharge of granular matter out of the bottom of a vertical silo: see Fig. 7.15. Although the outcome precision of the simulations is not very high, our interest in these experiments lies on the fact that they seem to provide one more verification of the predicted scaling (4.16): see Figs. 7.16 and 7.17.

### 7.1.6 Condensed Matter Physics

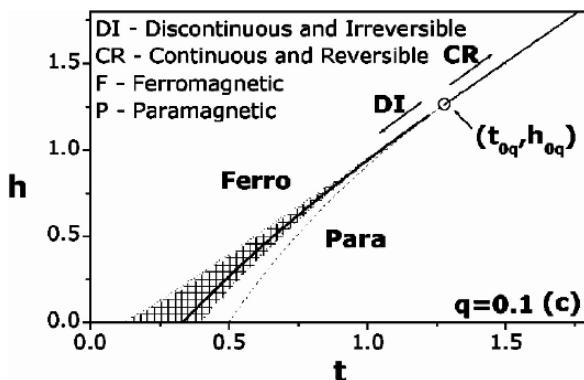
Manganites are a family of magnetic materials having “exotic” magnetic and electric properties (such as giant magnetoresistance), as well as ferro-paramagnetic first- and second-order phase transitions. Their theoretical approach has considerable difficulties. Several papers by the same group, [454–459] among others, have adopted a phenomenological approach based on  $q$ -statistics, using the index  $q$  as a tunable fitting parameter to reflect the consequences of the well-known fractal nature (at the level of microstructures) of the family. The attempt has been successful in substances such as  $La_{0.60}Y_{0.07}Ca_{0.33}MnO_3$  as can be judged from say Figs. 7.18, 7.19, 7.20, 7.21, and 7.22. The deep understanding of this fact on microscopic or mesoscopic grounds remains, nevertheless, an open question. Especially if



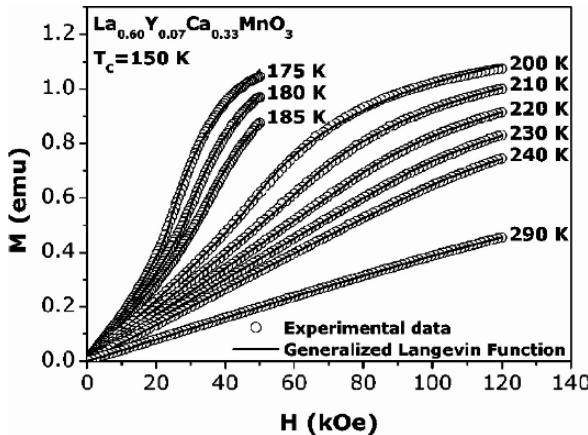
**Fig. 7.17** Time evolution of the second moments at the intermediate regime for a silo aperture  $3.8d$ . The straight line indicates a slope  $\gamma = 4/3$  (from [451,452]).

one takes into account that many other attempts exist in the literature which exhibit only partial success in spite of the fact that they frequently involve several fitting parameters [456].

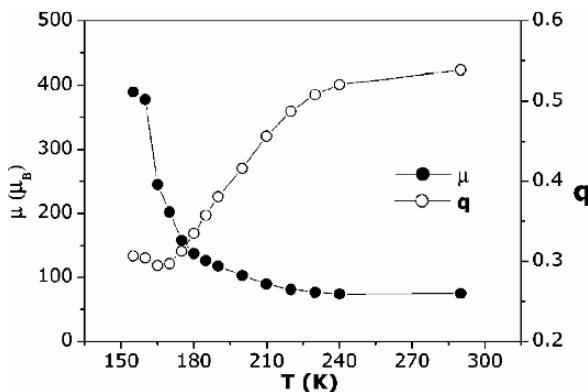
Figure 7.18 shows a typical temperature-magnetic field diagram as obtained for  $q = 0.1$ . In Fig. 7.19 a comparison is done between theoretical and experimental equations of states. The temperature-dependent parameters of the theory ( $q$  and  $\mu$ ) are indicated in Fig. 7.20. Using these phenomenological curves, Figs. 7.21 and 7.22 are obtained, *with no further fitting parameters at all*.



**Fig. 7.18** Results from the theoretical model. Projection of the phase diagram in the  $h - t$  plane, for  $q = 0.1$ . Above certain values of field  $h \geq h_{0q}$ , and temperature  $t \geq t_{0q}$ , the transition becomes continuous (from [456]).



**Fig. 7.19** Measured (open circles) and theoretical (solid lines) magnetic moment as a function of magnetic field, for several values of temperature above  $T_c = 150 \text{ K}$  (from [456]).

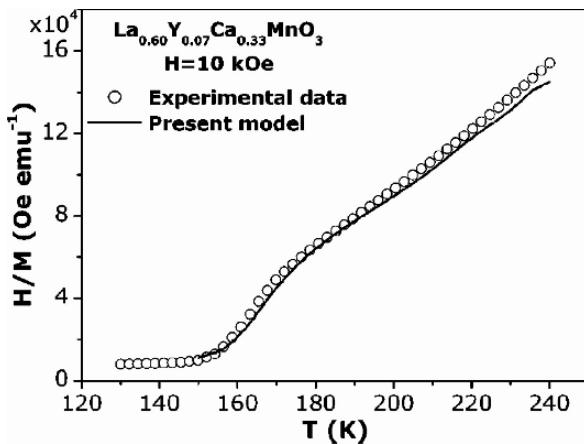


**Fig. 7.20** Temperature dependence of the fitting parameters  $q$  and  $\mu$  (from [456]).

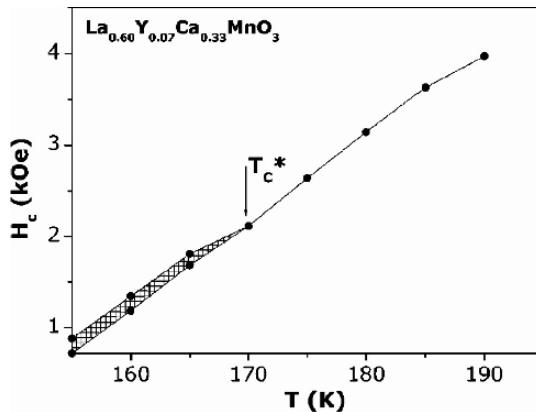
### 7.1.7 Plasma

Anomalous diffusion and distribution of displacements have been measured in dusty two-dimensional  $\text{Ar}$  plasma [462]. The results are respectively exhibited in Figs. 7.23 and 7.24. The numerical values for the anomalous diffusion exponent  $\alpha$  and for  $q$  are indicated in Fig. 7.25. From these, by plainly averaging  $\alpha$ , we obtain an intriguingly precise verification of prediction (4.16) (with the notation change  $\mu \equiv \alpha$ ): see Fig. 7.26.

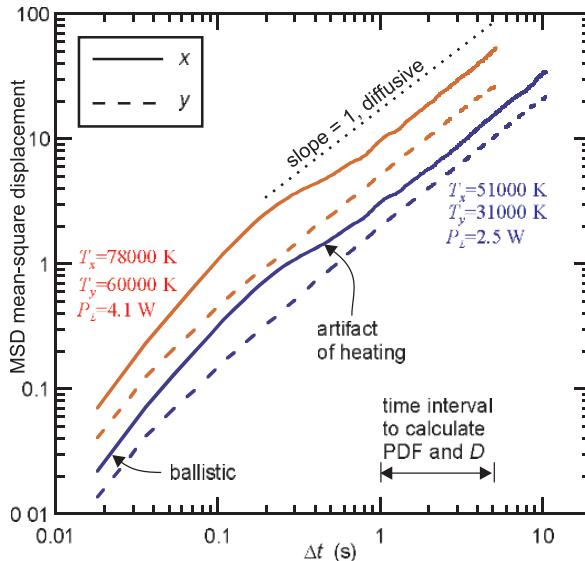
As previously mentioned, several other applications of  $q$ -statistics are available in the literature concerning plasmas, e.g., turbulent pure electron plasma [445, 446]. See also [463–480, 513].



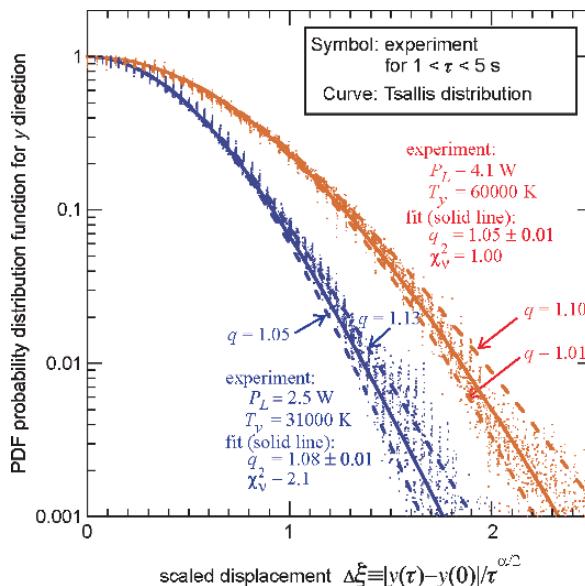
**Fig. 7.21** Measured (open circles) and theoretical (solid line) values of the quantity  $H/M$  vs.  $T$ . The solid line in this plot does not include any fitting parameters, and was calculated using only the fitting parameters of Fig. 7.19 (from [456]).



**Fig. 7.22** The linear temperature dependence, for  $T > T_c^*$ , of the characteristic field  $H_c$ , which corresponds to the inflection point of the experimental  $M$  vs.  $H$  curves, measured in  $\text{La}_{0.60}\text{Y}_{0.07}\text{Ca}_{0.33}\text{MnO}_3$ . For  $T < T_c < T_c^*$  the hysteresis is indicated by the shaded area. The similarity between this experimental plot and the theoretical one, shown in Fig. 7.18, is striking (from [456]).



**Fig. 7.23** Time evolution of the second moment of the displacements at two different sets of temperatures, namely at  $(T_x, T_y) = (78000\text{ K}, 60000\text{ K})$ , and  $(T_x, T_y) = (51000\text{ K}, 31000\text{ K})$ . The data in Fig. 7.25 have been obtained from such measurements. From [462].



**Fig. 7.24** Probability distributions associated with  $y$ -displacements. The present best fittings correspond to  $q$ -Gaussians with  $q = 1.05$  ( $q = 1.08$ ) for  $T_y = 60,000$  ( $T_y = 31,000$ ) (from [462]).

TABLE I: The measure  $\bar{q}$  of non-extensivity indicates non-Gaussian statistics. Mean diffusion exponent  $\bar{\alpha}_y$  (and p-value for testing the null hypothesis that there is no superdiffusion) indicates superdiffusion.

	time	temperature range $T_y$ ( $10^3$ K)		
		10 – 20	20 – 40	40 – 60
$\bar{q}$	$1 < \tau < 5$	$1.20 \pm 0.09$	$1.11 \pm 0.06$	$1.05 \pm 0.02$
$\bar{\alpha}_y$	$1 < \Delta t < 5$	$1.052 \pm 0.019$	$1.059 \pm 0.011$	$1.009 \pm 0.011$
P		0.007	$2 \times 10^{-5}$	0.210
$\bar{\alpha}_y$	$5 < \Delta t < 9$	$1.088 \pm 0.048$	$1.082 \pm 0.040$	
P		0.042	0.038	
$\bar{\alpha}_y$	$9 < \Delta t < 13$	$1.146 \pm 0.062$		
P		0.028		
$\bar{\alpha}_y$	$13 < \Delta t < 17$	$1.183 \pm 0.064$		
P		0.006		

$\alpha_{average}$	1.117	1.070	1.009
$\frac{\alpha_{average}(3-q)}{2}$	1.005	1.011	0.984

Fig. 7.25 The Table is from [462]. The lower box has been calculated from the data of the above Table.

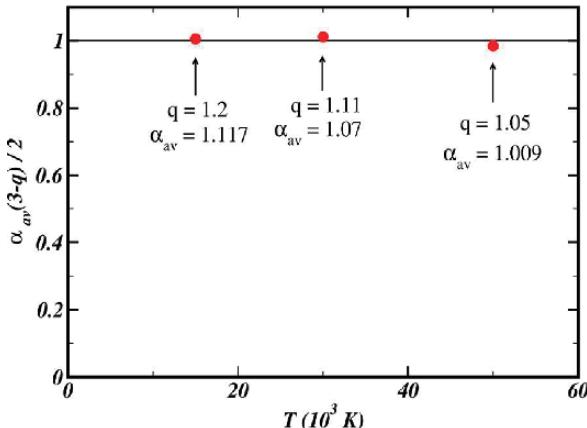


Fig. 7.26 Constructed from the data in the lower box of Fig. 7.25. As we see,  $q$  approaches unity when the temperature increases (we have plotted the mid point of the temperature intervals indicated in the Table of Fig. 7.25). For these average values of  $\alpha_{average}$ , the prediction (4.16) ( $\mu \equiv \alpha$ ) is satisfied within an overall error bar of 1.6% (intriguingly small, in fact, if we take into account that we are using average values for  $\alpha$ ; compare with Fig. 5.61, where the error bar is 10%).

## 7.1.8 Astrophysics

### 7.1.8.1 Self-Gravitating Systems

A vast literature explores the possible connections of  $q$ -statistics with self-gravitating systems and related astrophysical phenomena. The first such connection was established in 1993 by Plastino and Plastino [217].<sup>2</sup> It provided a possible way out for an old gravitational difficulty, namely the impossibility of existence of a self-gravitating system such that its total mass, total energy, and total entropy are all three simultaneously *finite*. Within a Vlasov–Poisson polytropic description of a Newtonian self-gravitating system (i.e.,  $D = 3$ ), a connection was put forward between the polytropic index  $n$  and the entropic index  $q$ , namely (see [481,482] and references therein)

$$\frac{1}{1-q} = n - \frac{1}{2}. \quad (7.6)$$

The limit  $n \rightarrow \infty$  (hence  $q = 1$ ) recovers the isothermal sphere case (responsible for the paradox mentioned previously);  $n = 5$  (hence  $q_c = 7/9$ , where the subindex  $c$  stands for *critical*) corresponds to the so-called Schuster sphere; for  $n < 5$  (hence  $q < q_c = 7/9$ ), simultaneous finiteness of mass, energy, and entropy naturally emerges. Equation (7.6) can be generalized to the  $D$ -dimensional Vlasov–Poisson problem, and the following result is obtained [481]

$$\frac{1}{1-q} = n - \frac{D-2}{2}. \quad (7.7)$$

The critical case corresponds to the Schuster  $D$ -dimensional sphere, for which

$$n = \frac{D+2}{D-2}. \quad (7.8)$$

Replacing this expression into Eq. (7.7), we obtain

$$q_c(D) = \frac{8 - (D-2)^2}{8 - (D-2)^2 + 2(D-2)}. \quad (7.9)$$

We see that  $q_c$  decreases below unity when  $D$  increases above  $D = 2$ . The fact that the limiting case  $q_c = 1$  occurs at  $D = 2$  is quite natural. Indeed, the  $D$ -dimensional gravitational potential energy decays, for  $D > 2$ , as  $-1/r^{D-2}$  with distance  $r$ . Consequently, the dimension below which BG statistical mechanics can be legitimately used is precisely  $D = 2$ .

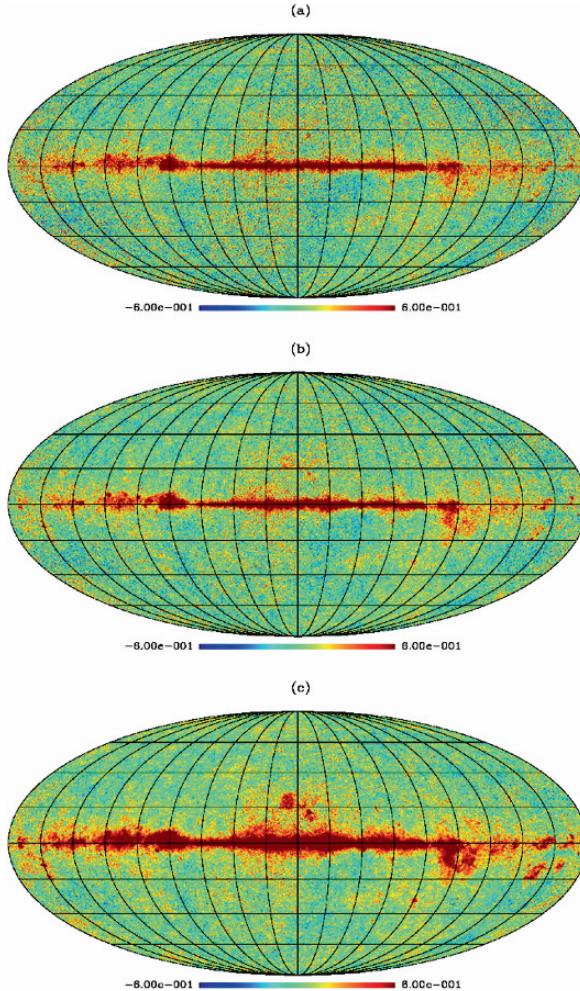
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<sup>2</sup> This contribution constitutes in fact a historical landmark in nonextensive statistical mechanics. Indeed, it was the very first connection of the present theory with *any* concrete physical system.

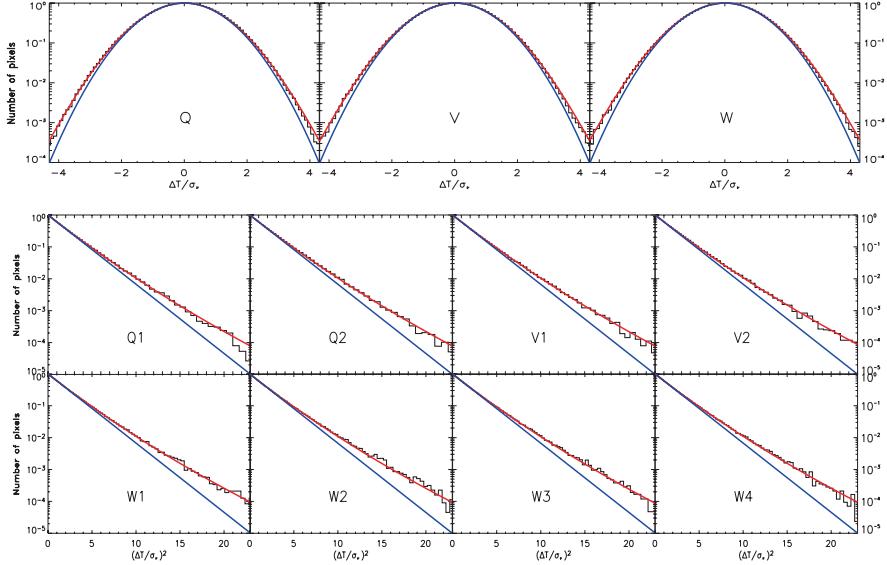
Many more contributions along these and other lines concerning galaxies, black holes, cosmology can be found in the literature [321, 464, 483–538].

### 7.1.8.2 Temperature Fluctuations of the Cosmic Microwave Background Radiation

The  $q$ -Gaussians are used since many decades in astrophysics with no deep theoretical justification [300]. They are called  $\kappa$ -distributions, and are written as follows:



**Fig. 7.27** The WMAP1 (WMAP with one-year data) CMBR temperature fluctuations maps, denoted by (a) W (93.5 GHz), (b) V (60.8 GHz), and (c) Q (40.7 GHz). To enhance the effect of the cosmic temperature fluctuations over the galaxy foregrounds, in these plots we consider only those pixels with  $\Delta T \in [-0.6, 0.6]$  mK. Data from the area contaminated by the Galaxy emissions are usually excluded from the statistical analysis, and, for the regions investigated, the whole range of temperatures measured by WMAP is considered.



**Fig. 7.28** *Top:* Fits to the (positive and negative) WMAP3 (WMAP with three-year data) CMB temperature fluctuations data, corresponding to the Q, V, and W co-added maps (after the Kp0 cut-sky), in the NUMBER OF PIXELS vs.  $\Delta T/\sigma_\nu$  plots. We show the  $\chi^2$  best-fits: Gaussian distribution (blue curve) with  $\sigma_Q = 104 \mu\text{K}$ ,  $\sigma_V = 118 \mu\text{K}$ , and  $\sigma_W = 131 \mu\text{K}$ , respectively, and each nonextensive distribution (red curve)  $P_q$  with  $q = 1.04$ . *Bottom:* Similar analysis, but now with the eight DA WMAP3 maps (Q1, ..., W4) after applying the Kp0 mask. We plotted the NUMBER OF PIXELS vs.  $(\Delta T/\sigma_\nu)^2$  to enhance the non-Gaussian behavior. To avoid possible unremoved Galactic foregrounds, we consider only the negative temperature fluctuations. Again, we show the  $\chi^2$  best-fits: Gaussian distribution (blue curve) and nonextensive distribution (red curve)  $P_q$ , now with  $q = 1.04 \pm 0.01$  (from [539]).

$$f(v) \propto \frac{1}{\left(1 + \frac{v^2}{\kappa v_0^2}\right)^{\kappa+1}}. \quad (7.10)$$

With the notation changes  $\kappa = (2 - q)/(q - 1)$  and  $1/(\kappa v_0^2) = (q - 1)\beta$ , we immediately identify  $e_q^{-\beta v^2}$ . This appears to be the case of the temperature fluctuations, around the value  $T \simeq 2.7 \text{ K}$ , of the cosmic microwave background radiation of the universe: See Figs. 7.27 and 7.28 [539]. Many cosmological theories assume (or imply) this distribution to be Gaussian. As we see in Fig. 7.28, this is not correct, the overall value of the index being  $q = 1.04 \pm 0.01$ . The Gaussian assumption is excluded at a 99% confidence level, and does not constitute more than a first approach to the problem. Moreover, anisotropy is found between the four universe quadrants, the strongest non-Gaussian contribution comes from the South-East universe quadrant, where  $q_{SE} \simeq 1.05$ .

Other astrophysical phenomena might be related with nonextensive concepts as well. Such is the case of solar flares, whose probability distributions of characteristic times appear to be of the  $q$ -exponential form: see [301].

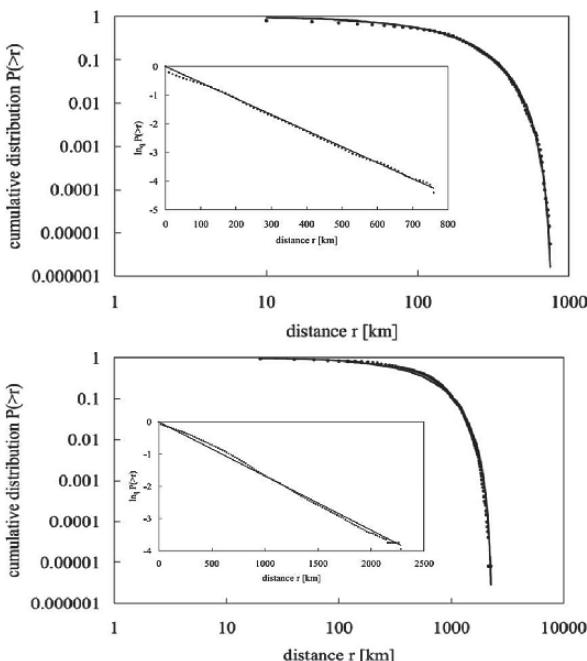
## 7.1.9 Geophysics

### 7.1.9.1 Earthquakes

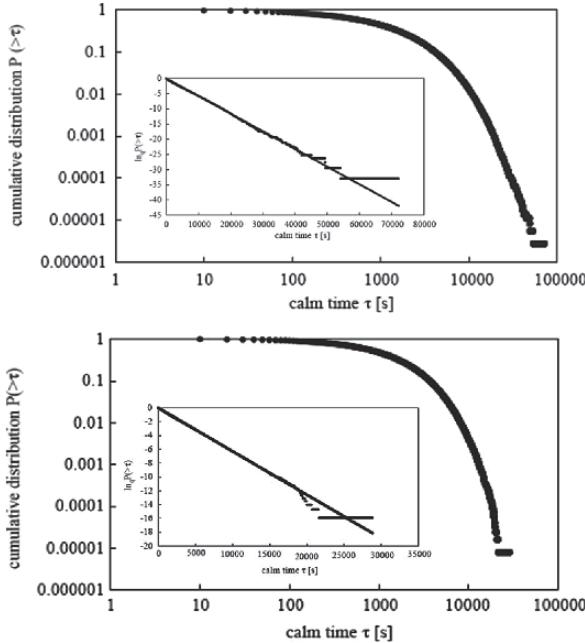
The  $q$ -statistical theory and functional forms have been successfully applied to earthquakes in many occasions [287–291, 380, 381, 540–544].

Successive earthquakes in a given geographic area occur with epicenters distributed in a region just below the Earth surface. We note  $r$  the successive distances (measured in three dimensions). It has been verified [540] that, in California and Japan, this distribution,  $p(r)$ , happens to be well represented (see Fig. 7.29) by a  $q$ -exponential form. More precisely, the corresponding accumulated probability is given by the *Abe–Suzuki distance law*

$$P(>r) = e_q^{-r/r_0} \quad (0 < q < 1; r_0 > 0). \quad (7.11)$$



**Fig. 7.29** Log–Log plots of the cumulative distribution of successive distances in California (top) and Japan (bottom). Dots from the California and Japan catalogs, respectively; continuous curves from Eq. (7.11). Insets: The same in  $q$ -log vs. linear representation (California:  $q = 0.773$ ,  $r_0 = 179$  Km, and the linear regression coefficient  $R = -0.9993$ ; Japan:  $q = 0.747$ ,  $r_0 = 595$  Km, and  $R = -0.9990$ ). For details see [540].



**Fig. 7.30** Log–Log plots of the cumulative distribution of calm-times in California (*top*) and Japan (*bottom*). Dots from the California and Japan catalogs, respectively; continuous curves from Eq. (7.14). *Insets:* The same in  $q$ -log vs. linear representation (California:  $q = 1.13$ ,  $\tau_0 = 1724$  s, and the linear regression coefficient  $R = -0.988$ ; Japan:  $q = 1.05$ ,  $\tau_0 = 1587$  s, and  $R = -0.990$ ). For details see [544].

Consequently

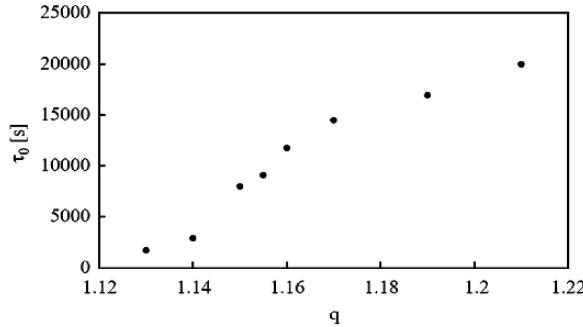
$$p(r) = -\frac{dP(>r)}{dr} = \frac{1}{r_0} e^{-r/[r_0(2-Q)]}, \quad (7.12)$$

with

$$Q \equiv 2 - \frac{1}{q} < q. \quad (7.13)$$

Let us address now a different phenomenon, namely the fact that, between successive earthquakes in a given area of the globe, there are calm-times, noted  $\tau$ , and defined through a fixed threshold  $m_{th}$  for the magnitude. It has been verified [544] that, in California and Japan, the calm-time distribution,  $p(\tau)$ , happens to be well represented (see Fig. 7.30) by a  $q$ -exponential form. More precisely, the corresponding accumulated probability is given by the *Abe–Suzuki time law*

$$P(>\tau) = e_q^{-\tau/\tau_0} \quad (q > 1; \tau_0 > 0). \quad (7.14)$$



**Fig. 7.31** Dependence of  $(q, \tau_0)$  on  $m_{th}$ . Data from the California catalog. From the bottom to the top,  $m_{th} = 0.0, 1.4, 2.0, 2.1, 2.2, 2.3, 2.4, 2.5$ . For further details see [544].

Moreover, the pair  $(q, \tau_0)$  depends in a defined form on the threshold  $m_{th}$ , as indicated in Fig. 7.31.

As another important application to earthquakes let us focus on the *aging* which occurs within the nonstationary regime called *Omori regime*, the set of aftershocks that follow a big event. We introduce the following correlation function:

$$C(n + n_W, n_W) \equiv \frac{\langle t_{n+n_W} t_{n_W} \rangle - \langle t_{n+n_W} \rangle \langle t_{n_W} \rangle}{\sigma_{n+n_W} \sigma_{n_W}}, \quad (7.15)$$

where

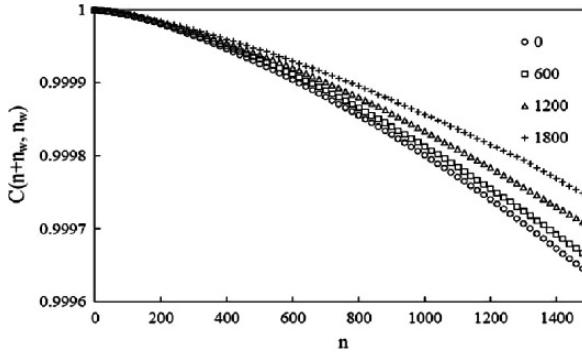
$$\langle t_m \rangle = \frac{1}{N} \sum_{k=0}^{N-1} t_{m+k}, \quad (7.16)$$

$$\langle t_m t_{m'} \rangle = \frac{1}{N} \sum_{k=0}^{N-1} t_{m+k} t_{m'+k}, \quad (7.17)$$

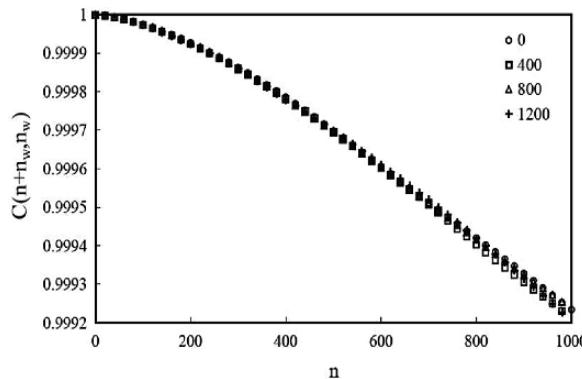
and

$$\sigma_m^2 = \langle t_m^2 \rangle - \langle t_m \rangle^2, \quad (7.18)$$

$N$  being the number of events that are being considered within the Omori regime, and  $t_m$  being the time at which the  $m$ th event occurs;  $m$  is sometimes referred to as *natural time*. By definition,  $C(n_W, n_W) = 1$ . For a stationary state,  $C(n + n_W, n_W)$  depends on the natural time  $n$ , but not on the *waiting natural time*  $n_W$ ; if it also depends on  $n_W$ , the state is necessarily a nonstationary one, and exhibits *aging*, one of the most characteristic features of glassy systems. The correlation function of typical earthquakes in Southern California has been discussed in [541]: see Figs. 7.32 and 7.33 for catalog data, respectively, inside and outside the Omori

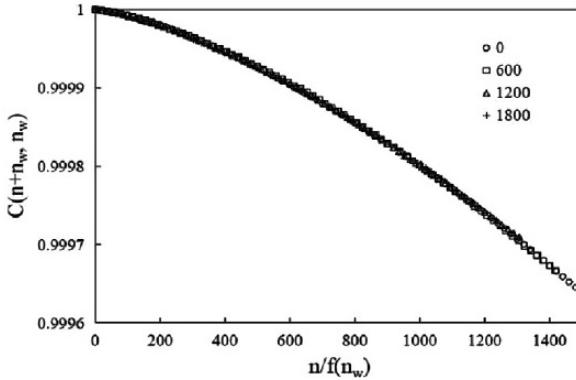


**Fig. 7.32** Dependence of the correlation function on the natural time  $n$  *inside* the Omori regime following a specific event taken from the California catalog. Aging is visible. For further details see [541].

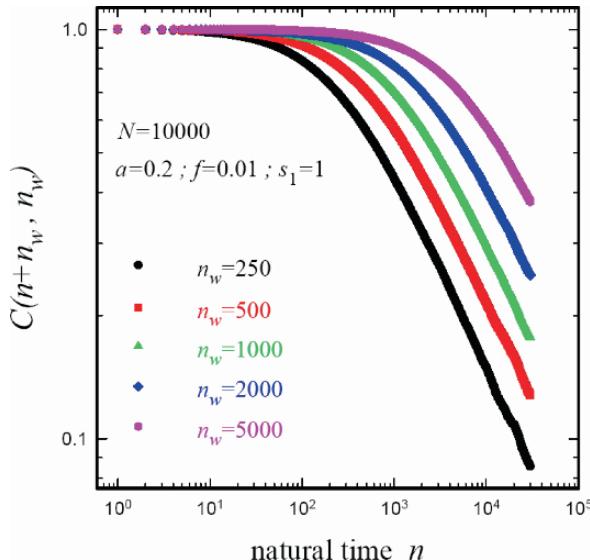


**Fig. 7.33** Dependence of the correlation function on the natural time  $n$  *outside* the Omori regime following a specific event taken from the California catalog. No aging is visible. For further details see [541].

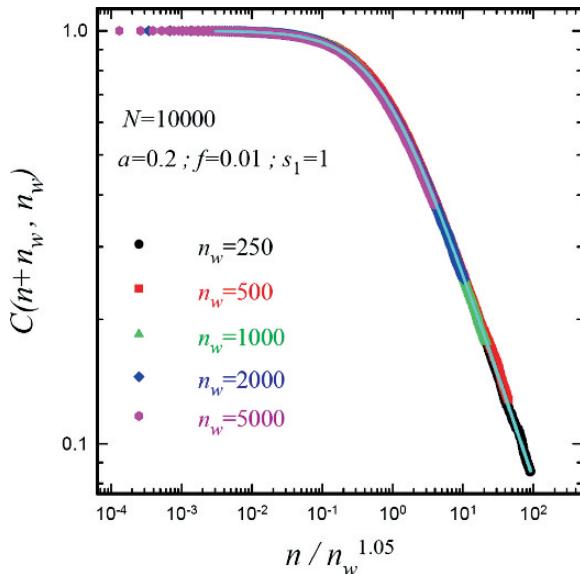
regime. Whenever aging is observed, data collapse can be obtained (see Fig. 7.34) through rescaling, more specifically by using as abscissa  $n/f(n_W)$  instead of  $n$ , where  $f(n_W) = an_W^\gamma + 1$ ,  $a$  and  $\gamma$  being fitting parameters. The connection with  $q$ -statistics comes from the fact that the type of dependence that we observe in Fig. 7.34 appears to be of the  $q$ -exponential form. Let us address this point now. This correlation function has been calculated [380] for a simple mean-field model called the *coherent noise model* (Newman model): the results can be seen in Figs. 7.35, 7.36, and 7.37. Another model for earthquakes has been discussed as well [381], the Olami–Feder–Christensen models. The results for the Newman and the OFC models are respectively  $C(n+n_W, n_W) = e_{2.98}^{-0.7n/n_W^{1.05}}$  and  $C(n+n_W, n_W) = e_{2.9}^{-0.6n/n_W^{1.05}}$ : see Fig. 7.38. Summarizing, both earthquake models that have been considered yield virtually the same result, namely that the rescaled correlation function is of the  $q$ -exponential form with  $q \simeq 2.98$ .



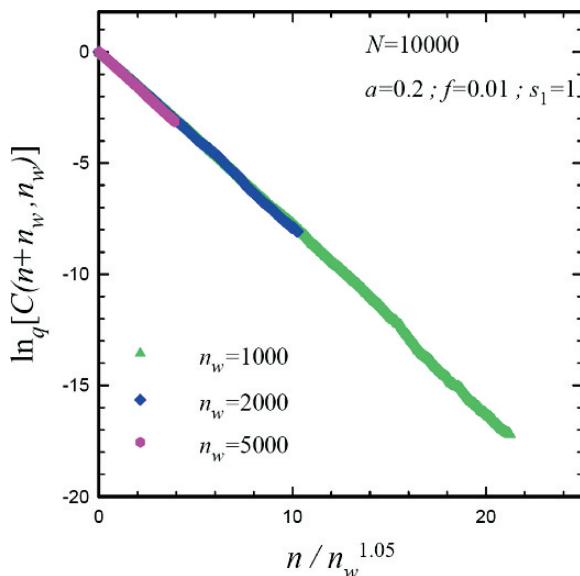
**Fig. 7.34** Dependence of the correlation function on a rescaled natural time  $n/f(n_w)$  *inside* for the same data of Fig. 7.32 with  $f(n_w) = an_w^\gamma + 1$  ( $a = 1.37 \times 10^{-6}$ , and  $\gamma = 1.62$ ). For further details see [541].



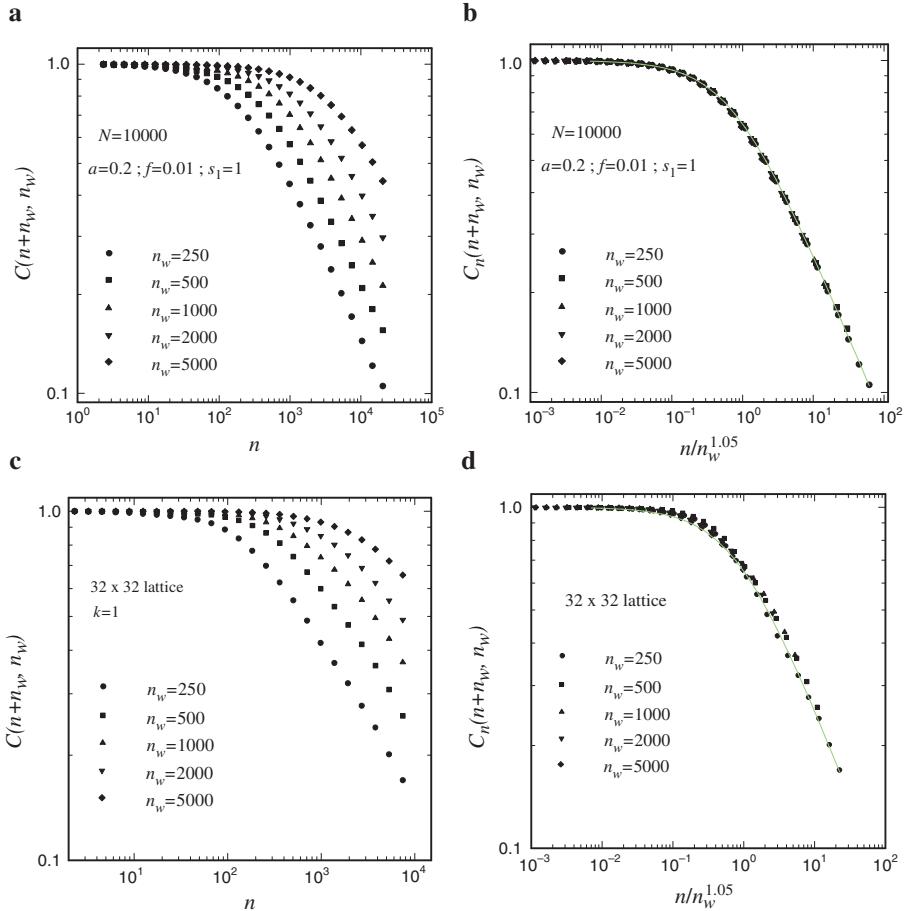
**Fig. 7.35** Event–event correlation functions for different values of the natural waiting time  $n_w$ . The ensemble average (which differs, in fact, from the time average, thus exhibiting the breakdown of ergodicity) is performed over 120,000 numerical runs with different initial conditions (from [543]).



**Fig. 7.36** Data collapse of the same numerical data of Fig. 7.35 in  $\log$  vs.  $\log$  representation (from [543]).



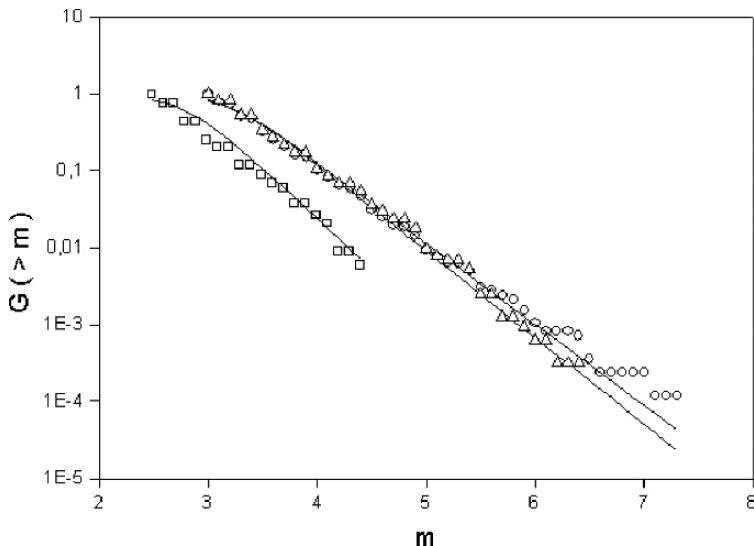
**Fig. 7.37** Data collapse of the same numerical data of Fig. 7.35 in  $q$ -log vs. linear representation. The straight line implies that the scaling function is a  $q$ -exponential with  $q \simeq 2.98$  (from [543]).



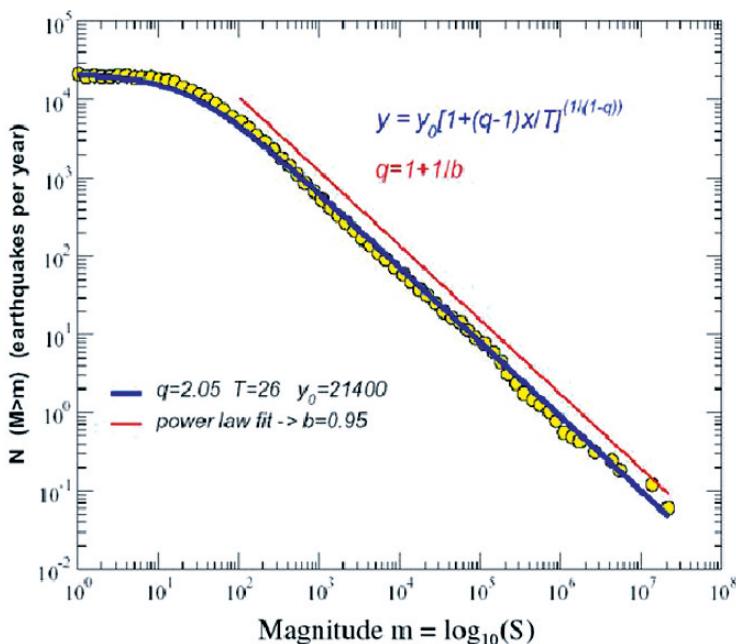
**Fig. 7.38** The collapsed and noncollapsed correlation functions for the Newman model (*top*) and the Olami–Feder–Christensen model (*bottom*) (from [381]).

Let us address now the most classical quantity for earthquakes, namely the probability of having earthquakes of magnitude  $m$  (*Gutenberg–Richter law*). A nontrivial result (generalizing in fact the classical Gutenberg–Richter law) has been analytically obtained [542] along this line for the cumulative probability  $G(> m)$  involving two parameters,  $q$  and  $a$  ( $a$  is the constant of proportionality between the released relative energy  $\epsilon$  and the linear dimension  $r$  of the fragments of the fault plates). These results are much in line with those presented in Figs. 7.39 and 7.40.

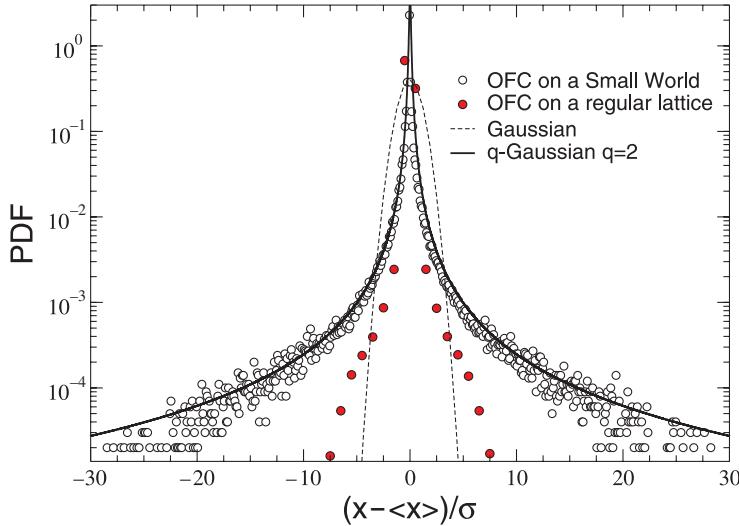
Finally, let us focus on the histograms of the avalanche size differences (*returns*, as such quantities are called in finance). These have been focused in [855, 856]. In particular, such probability distributions have been calculated in a dissipative Olami–Feder–Christensen model (Fig. 7.41), and also for real earthquakes (Fig. 7.42). The results for the OFC model have been calculated in both a



**Fig. 7.39** Cumulative probability for having earthquakes with magnitude above  $m$  (exceedence). California (circles, over 10,000 earthquakes,  $q = 1.65$ ,  $a = 5.73 \times 10^{-6}$ ), Iberian Peninsula (triangles, 3000 earthquakes,  $q = 1.64$ ,  $a = 3.37 \times 10^{-6}$ ), and Andalusian region (squares, 300 earthquakes,  $q = 1.60$ ,  $a = 3 \times 10^{-5}$ ). For further details see [542].



**Fig. 7.40** Cumulative number of earthquakes with magnitude above  $m$  per year. The dots are from the California catalog (for further details see [545]), and correspond to 335,076 earthquakes. The blue curve is a  $q$ -exponential with  $q = 2.05$ .



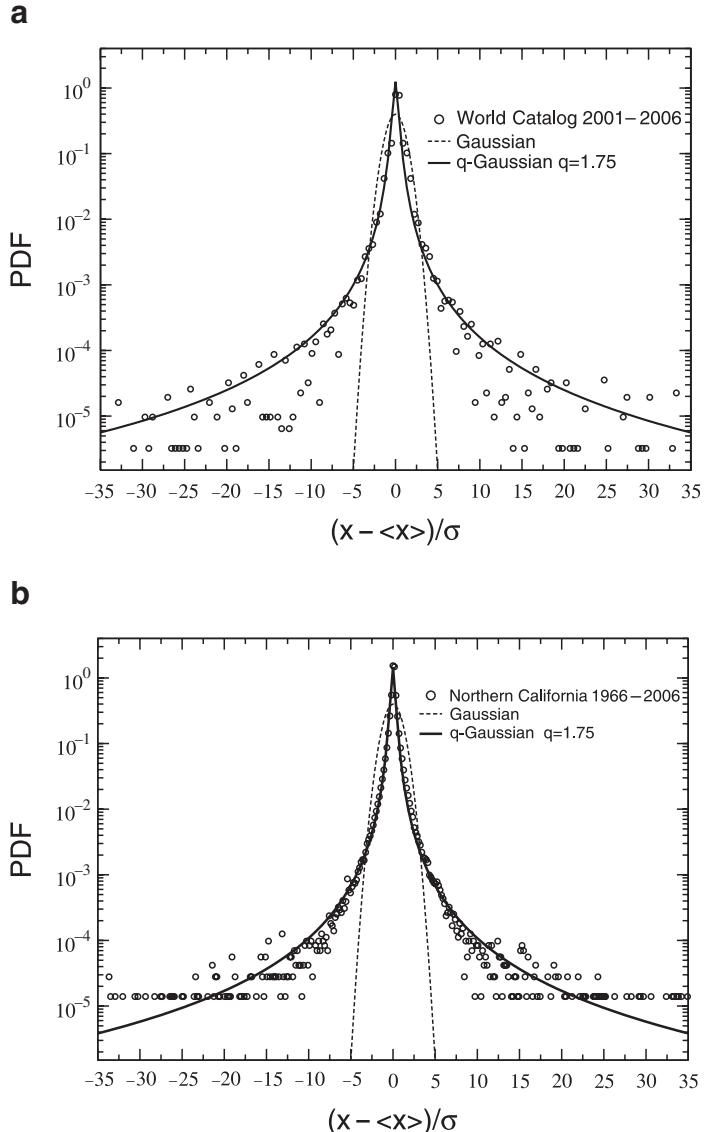
**Fig. 7.41** Probability distribution of the avalanche size differences (returns)  $x(t) = S(t+1) - S(t)$  for the OFC model on a small-world topology (critical state, *open circles*) and on a regular lattice (noncritical state, *full circles*). For comparison, a Gaussian and a  $q$ -Gaussian (with  $q = 2$ ) are indicated as well. All the curves have been normalized so as to have unit area. For further details see [855].

small-world lattice (referred to as the *critical case*) and a regular lattice (referred to as the *noncritical case*). The conclusion is highly interesting: at criticality  $q$ -Gaussian-like distributions are obtained, whereas something close to a Gaussian on top of another (larger) Gaussian is obtained out of criticality.<sup>3</sup>

The (analytic) connection between the various  $qs$  that have been presented here for earthquakes remains an open worthwhile question.<sup>4</sup>

<sup>3</sup> This fact is quite suggestive on quite different experimental grounds. Indeed, the velocity distribution of cold atoms in dissipative optical lattices has been measured by at least two different groups, namely in [857] and in [461]. The latter obtained a  $q$ -Gaussian velocity distribution (see Fig. 2(a) in [461]). The former, however, obtained a double-Gaussian distribution (see Fig. 11(a) in [857]). The reason for such a discrepancy is, to the best of our knowledge, not yet understood. A possibility could be that in the latter experiment, the apparatus is at “criticality,” whereas in the former experiment it might be slightly out of it. The point surely is worthy of further clarification.

<sup>4</sup> Along this line, some hint might be obtained from the following observation. Series corresponding to thirteen earthquakes have been analyzed in [291]. It is claimed that the cumulative distribution of the distances between the epicenters of successive events is well fitted by a  $qs$ -exponential (where  $s$  stands for *spatial*); analogously, the cumulative distribution of the time intervals between successive events was also well fitted by a  $qt$ -exponential (where  $t$  stands for *temporal*). From the data corresponding to the set of 13 earthquakes (see Table 3 of [291]), we can calculate  $qs = 0.73 \pm 0.09$ ,  $qt = 1.32 \pm 0.08$ , and  $qs + qt = 2.05 \pm 0.07$ . If the distances and times between successive events were independent, we should obtain, for the standard deviation of  $qs + qt$ , roughly  $0.08 + 0.07 \simeq 0.17$ . Since the data yield 0.07 instead of 0.17, correlation is present, which suggests  $qs + qt \simeq 2$  for each earthquake.



**Fig. 7.42** The same as in Fig. 7.41 but for real earthquakes. *Left:* From the World catalog. *Right:* From the Northern California catalog. For comparison, a Gaussian and a  $q$ -Gaussian have indicated as well. Both fittings provided  $q = 1.75 \pm 0.15$ . For further details see [855]).

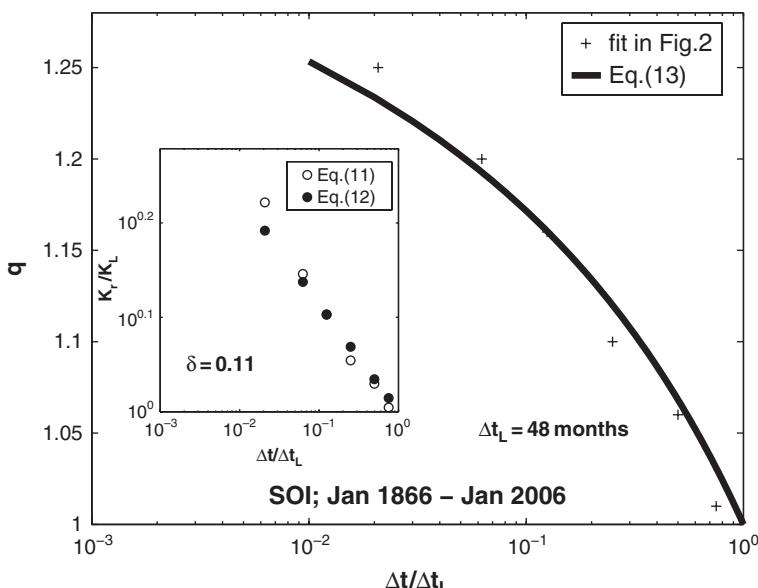
### 7.1.9.2 El Niño

The *Southern Oscillation Index* (SOI) corresponds to the daily registration of the oceanic temperature (including appropriate pressure corrections) at a fixed point of the Earth. Histograms can be constructed by using values separated by a fixed time lag. They are well fitted by  $q$ -Gaussians with  $q$  depending on the time lag [292, 293]. See Figs. 7.43 and 7.44. Like for financial returns, the index  $q$  gradually approaches unity (i.e., Gaussian distribution) when the time lag increases, which corresponds of course to an increasing loss of time correlation of the successive values of the signal. A micro- or meso-scopic theory interprets the results exhibited in Figs. 7.43 and 7.44 would of course be welcome.

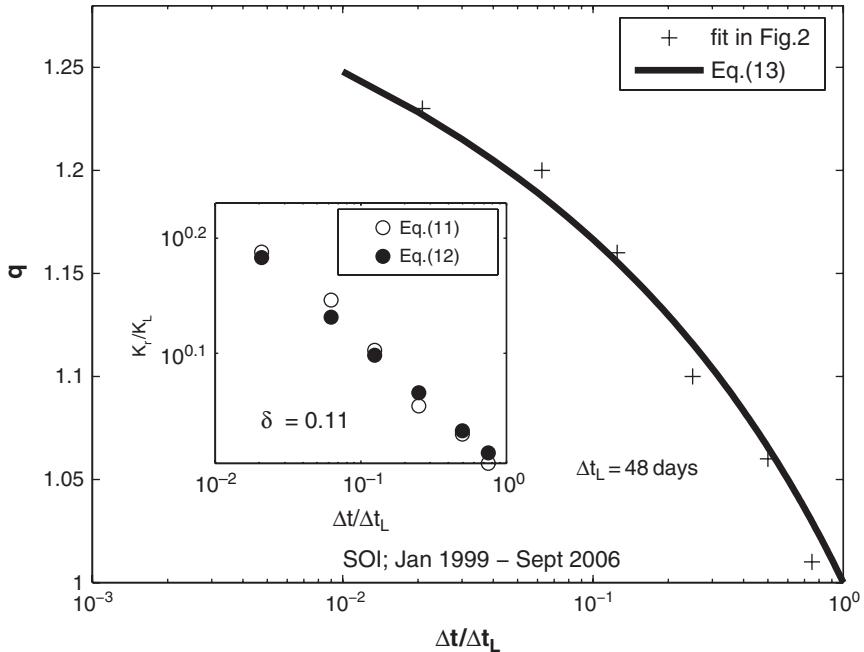
Further geophysical applications, e.g., to clouds [294], the Stromboli volcano [295], geological faults [295], are available in the literature as well.

### 7.1.10 Quantum Chaos

The quantum kicked top (QKT) is a paradigmatic system showing quantum chaos. In its regular regime, the overlap function  $O$  behaves roughly constant with time, and, in the strongly chaotic regime, it decreases exponentially with time before the emergence of quantum interference effects. It is therefore possible that, precisely in the frontier between both regions, the exponential time dependence of the overlap



**Fig. 7.43** Dependence of  $q$  on the (conveniently rescaled) time lag for the SOI. The data correspond to the Jan 1866–Jan 2006 period. See [292] for further details.



**Fig. 7.44** Dependence of  $q$  on the (conveniently rescaled) time lag for the SOI. The data correspond to the Jan 1999–Sept 2006 period. See [293] for further details.

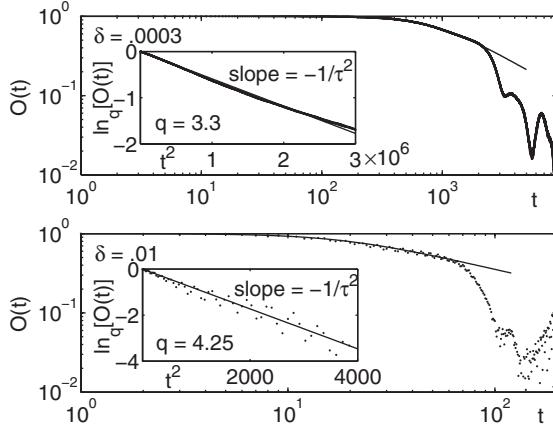
function be replaced by a  $q$ -exponential form. This conjecture has indeed been verified numerically [546, 547], as can be seen in Figs. 7.45, 7.46, and 7.47.

### 7.1.11 Quantum Entanglement

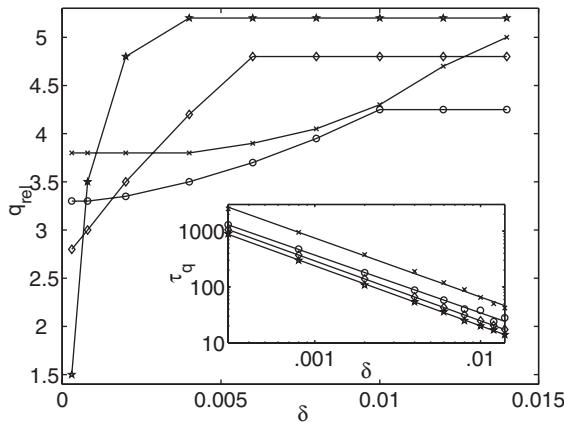
A considerable effort has been dedicated to the connections between generalized entropic forms and the location of the critical frontier which has separable states on one side and quantum entangled ones on the other one. A remarkably simple, and sometimes quite performant, criterium based on the conditional form of the entropy  $S_q$  was advanced by Abe and Rajagopal in [548]. For some systems, this procedure enabled the exact calculation of the separable-entangled separatrix. Such is the case illustrated in Fig. 7.48 (from [549]). An entire literature exists in fact exploring this and related questions [114, 550–571].

### 7.1.12 Random Matrices

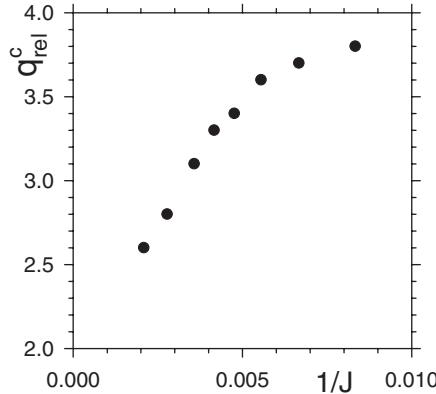
The standard Gaussian ensembles of random matrices can be alternatively obtained by maximizing the Boltzmann–Gibbs–von Neumann entropy under appropriate constraints. By optimizing instead the entropy  $S_q$  it is possible to  $q$ -generalize such



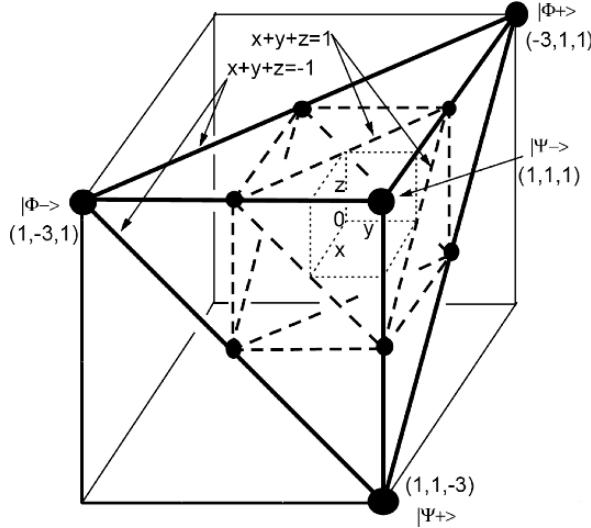
**Fig. 7.45** Overlap vs. time for an initial angular momentum coherent state located at the border between regular and chaotic zones of the QKT of spin 240 and  $\alpha = 3$ . This region, the edge of quantum chaos, shows the expected power law decrease in overlap. The top figure is for a perturbation strength in the weak perturbation regime,  $\delta = 0.0003$  and the bottom figure is for a perturbation strength of  $\delta = 0.01$ , within the FGR regime. On the log-log plot the power law decay region, from about 600–2500 in the weak perturbation regime and 20–70 in the FGR regime, is linear. We can fit the decrease in overlap with the expression  $[1 + (q_{rel} - 1)(t/\tau_{q_{rel}})^2]^{1/(1-q_{rel})}$  where, in the weak perturbation regime, the entropic index  $q_{rel} = 3.3$  and  $\tau_{q_{rel}} = 1300$  and in the FGR regime  $q_{rel} = 4.25$  and  $\tau_{q_{rel}} = 34$ . The insets of both figures show  $\ln_{q_{rel}} O \equiv (O^{1-q_{rel}} - 1)/(1-q_{rel})$  vs.  $t^2$ ; since  $\ln_q x$  is the inverse function of  $e_q^x \equiv [1 + (1 - q) x]^{\frac{1}{1-q}}$ , this produces a straight line with a slope  $-1/\tau_{q_{rel}}^2$  (also plotted) (from [547]).



**Fig. 7.46** Values of  $q_{rel}$  and  $\tau_q$  (inset) for  $J = 120$  (x), 240 (circles), 360 (diamonds), and 480 (stars).  $q_{rel}$  remains constant for perturbation strengths below the critical perturbation and above the saturation perturbation. In between  $q_{rel}$  increases with a rate dependent on  $J$ . The values of  $q_{rel}^c$ ,  $q_{rel}^s$ ,  $\delta_c$ , and  $\delta_s$  can be seen in the figure. In addition the rate of growth of  $q_{rel}$  with increased perturbation strength can be seen. The inset shows a log-log plot of the value of  $\tau_q$  vs.  $\delta$  for the above values of  $J$ . The data can be fit with a lines of slope  $-1.06$ ,  $-1.03$ ,  $-1.07$ , and  $-1.08$  for  $J = 120$ , 240, 360, and 480 (top to bottom) (from [547]).



**Fig. 7.47** Values of  $q_{rel}^c$  vs.  $1/J$ . These are determined by exploring a number of perturbations much less than  $\delta_c$ . We note that  $q_{rel}^c$  of the  $J = 480$  QKT is larger than  $q_{rel}$  reported in Fig. 7.46. It is unclear why in this instance the value of  $q_{rel}$  decreases with increased perturbation strength (from [547]).



**Fig. 7.48** The physical space of the mixed state considered in the present paper is the tetrahedron determined by the four big circles. Every big circle and its three neighboring small circles determine a region (small tetrahedron) where no separability is possible. The four small tetrahedra delimit a central octahedron where the system is separable. The  $x + y + z = 1$  plane (dashed) generalizes the  $x_c = 1/3$  Peres criterion, and plays the role of a critical surface. The entanglement “order parameter”  $\eta \equiv 1/q_J$  is zero inside the central octahedron, and continuously increases when we approach the four vertices of the big tetrahedron, where  $\eta = 1$  (from [549]).

ensembles. This has been done in [572] and elsewhere [573–577], and interesting generalizations of the *semi-circle law* for the eigenvalue density, and of *Wigner's surmise* for the level-spacing distribution are obtained. The index  $q$  determines the degree of confinement, in such a way that  $q \leq 1$  corresponds to strong localization and  $q > 1$  corresponds to weak localization.

## 7.2 Chemistry

### 7.2.1 Generalized Arrhenius Law and Anomalous Diffusion

The *Arrhenius law* plays a fundamental role in chemistry. It has been interestingly generalized in [578].

Let us consider the following nonlinear Fokker–Planck equation

$$\begin{aligned} \frac{\partial \rho(x, t)}{\partial t} &= \frac{\partial}{\partial x} \left[ \frac{\partial U(x)}{\partial x} \rho(x, t) \right] + D \frac{\partial^2 [\rho(x, t)]^{2-q}}{\partial x^2} \\ &= \frac{\partial}{\partial x} \left[ \frac{\partial U(x)}{\partial x} \rho(x, t) \right] + (2 - q) D \frac{\partial}{\partial x} \left\{ [\rho(x, t)]^{1-q} \frac{\partial \rho(x, t)}{\partial x} \right\} \quad (7.19) \\ &[q \in \mathbb{R}; (2 - q)D > 0; t \geq 0], \end{aligned}$$

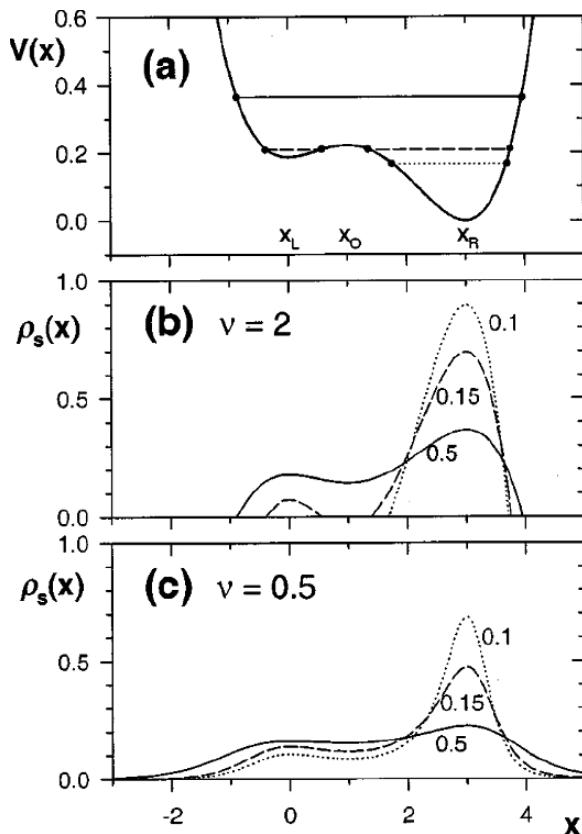
with

$$\int dx \rho(x, t) = 1, \quad \forall t, \quad (7.20)$$

$U(x)$  being a potential whose global minimal value is  $U_0$ . The stationary solution is given by

$$\rho_s(x) \equiv \lim_{t \rightarrow \infty} \rho(x, t) = \frac{e^{-\beta V(x)}}{Z}, \quad (7.21)$$

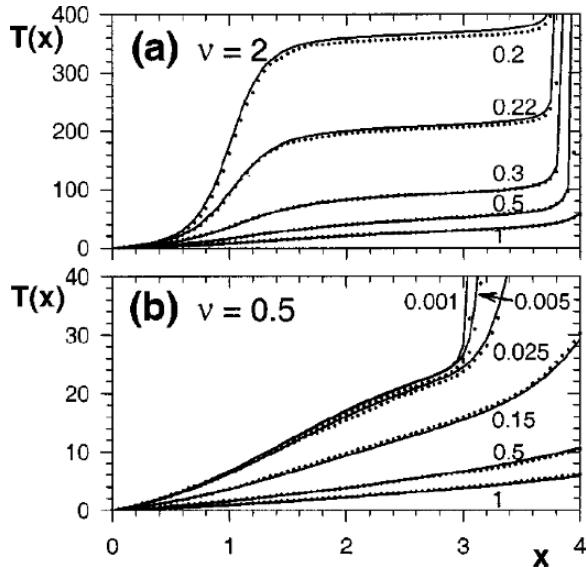
with  $V(x) \equiv U(x) - U_0$ ,  $\beta = \frac{Z^{1-q}}{(2-q)D}$ ,  $Z$  being a positive normalization constant. See Fig. 7.49. By using the associated Ito–Langevin equation one can consider a large amount of stochastic trajectories each of them starting at  $x_L$ . We note  $T(x) \equiv T(x_L \rightarrow x)$  the average time for the *first passage* to a value larger than  $x$ , with  $x \geq x_L$ : see Fig. 7.50. In particular, we can focus on the *escape time*  $T \equiv T(x_R)$ : see Fig. 7.51.



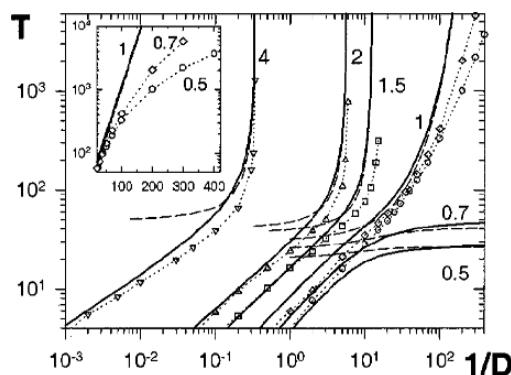
**Fig. 7.49** (a) Dimensionless double well potential  $V(x) = ax^4 + bx^3 + cx^2 + d$ , with  $a = 1/48$ ,  $b = -1/9$ ,  $c = 1/8$ ,  $d = 3/16$ . The left (local) minimum occurs at  $x = x_L = 0$ ; the right (global) minimum occurs at  $x = x_R = 3$ ; the central maximum occurs at  $x = x_0 = 1$ . The stationary distribution is shown for  $\rho = 2$  (b) and  $\rho = 0.5$  (c), for typical values of  $D$ , as indicated in the figure;  $q = 2 - \rho$ . For  $q \geq 1$  the full phase-space is covered by power-law tails. For  $q < 1$  a cutoff restricts the attainable space. Observe in (b) that, as  $D$  decreases, the motion becomes more confined until only the neighborhood of the deepest valley is allowed. The horizontal lines in (a) represent the cutoff condition  $V(x) = 1/\beta$ , which defines the allowed regions for  $q = 0$  and the same values of  $D$  as in (b). All quantities are dimensionless (from [578]).

### 7.2.2 Lattice Lotka–Volterra Model for Chemical Reactions and Growth

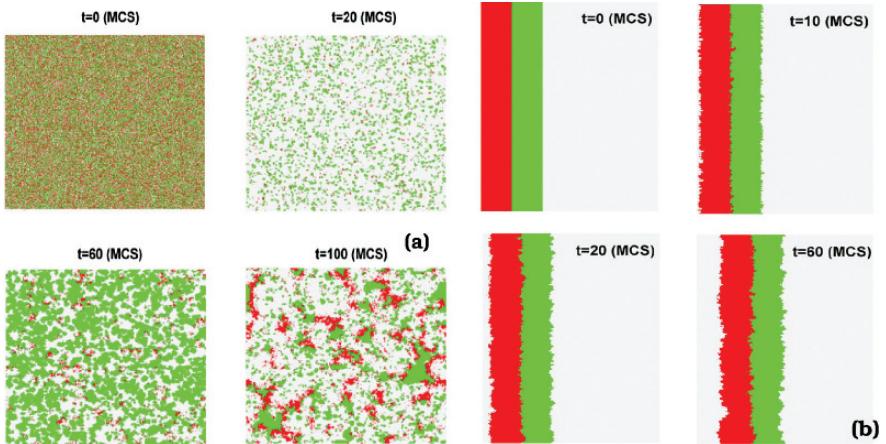
The *lattice Lotka–Volterra* (LLV) model is a paradigmatic one for two-constituent chemical reactions, growth, prey-predator, kinetics, and other phenomena. Its mean-field approximation (classical Lotka–Volterra model) is conservative, but its exact microscopic dynamics is not. A large literature is devoted to its study. Here we focus on the time dependence of its configurational entropy by following [579, 580]: see Figs. 7.52, 7.53, 7.54, 7.55, 7.56, and 7.57, where the red and green colors indicate



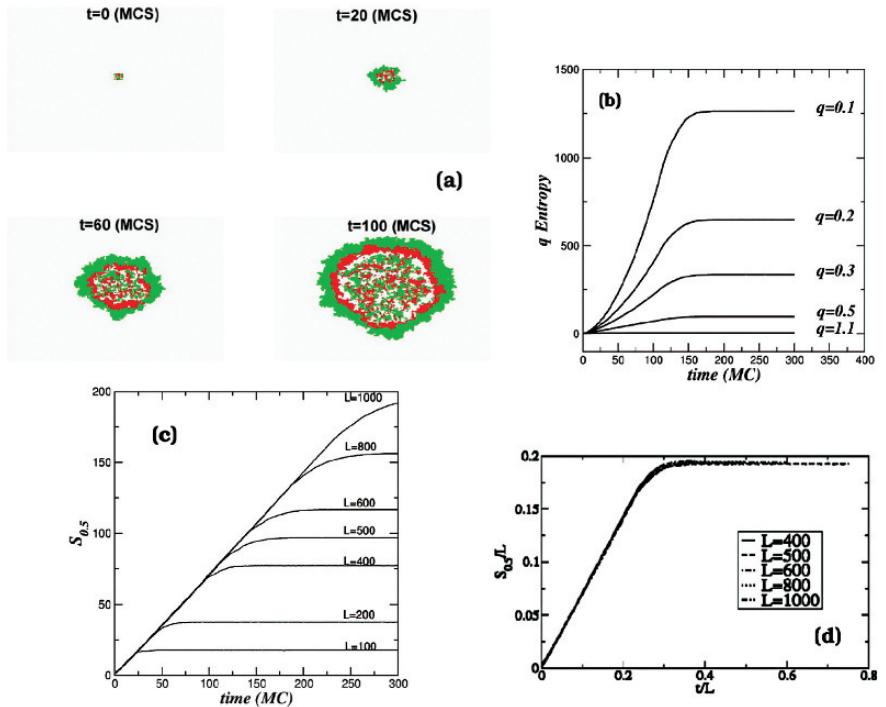
**Fig. 7.50**  $T(x)$  for typical values of  $D$  (indicated in the figure) for  $v = 2 - q = 2$  (a), and  $v = 2 - q = 0.5$  (b). Circles correspond to numerical experiments (mean values over 1000 realizations), and full lines to the analytical predictions of the theory (from [578]).



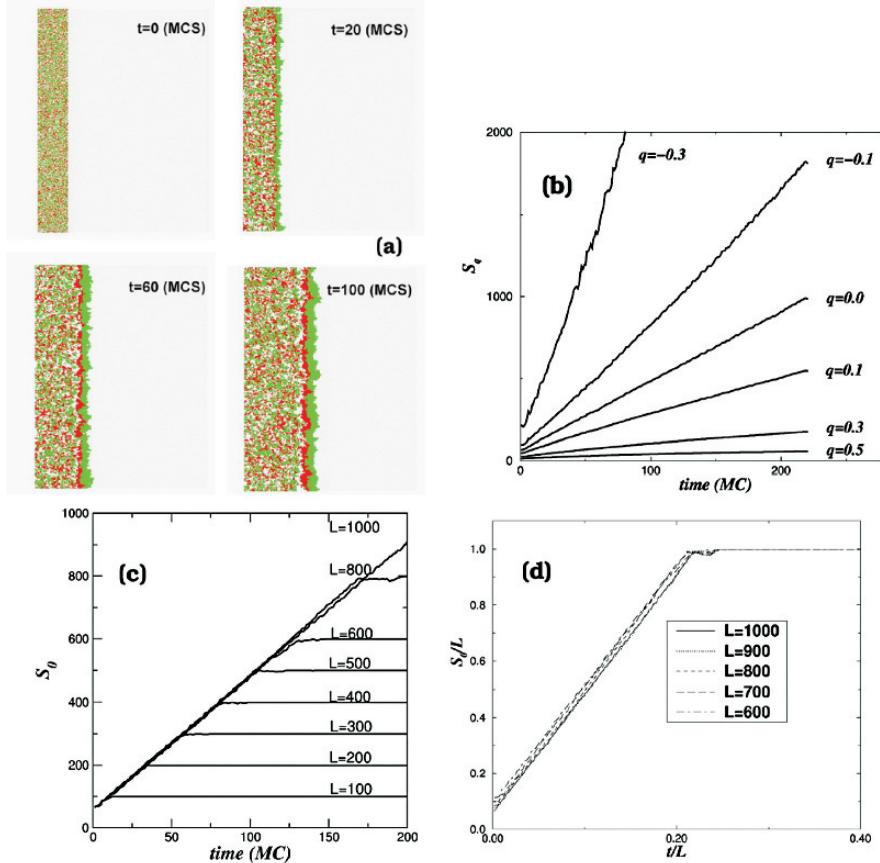
**Fig. 7.51** Escape time  $T$  as a function of  $1/D$  for typical values of  $v = 2 - q > 0$  (as indicated in the figure). Full lines are analytical results of the theory. Dashed lines correspond to the analytical low- $D$  approximation. Symbols correspond to the initial condition where all the particles (at least 1000) are injected at the same time at  $x_L$ . Dotted lines are guides for symbols. Inset: Detail (semi-log) of the low- $D$  region for  $v = 2 - q \leq 1$ . The particular case  $v = q = 1$  recovers Arrhenius law and normal diffusion (from [578]).



**Fig. 7.52**  $d = 2$  (a) and  $d = 1$  (b) time evolution of typical initial conditions. In (a) we observe the spontaneous tendency towards clusterization.  $MCS$  stands for *Monte Carlo steps* (from [579]).



**Fig. 7.53** Time evolution for initial conditions very localized (isotropically) in a  $L \times L$  square lattice (from [579]).

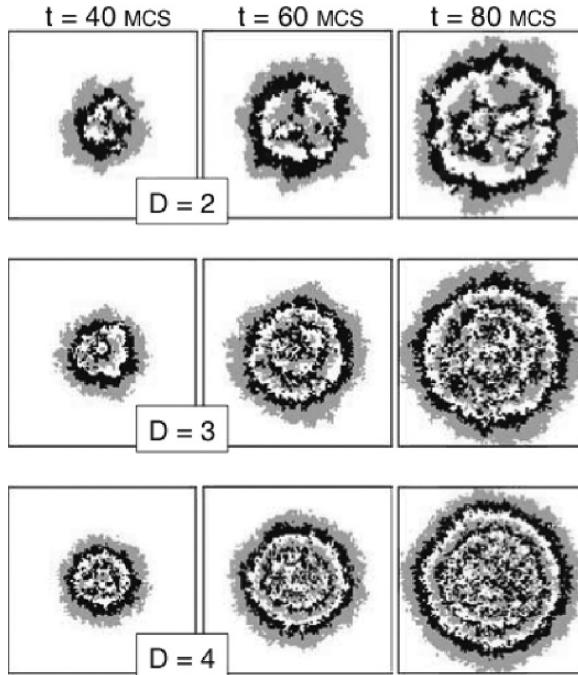


**Fig. 7.54** Time evolution for initial conditions very localized within a  $L$ -sized strip in a  $L \times L$  square lattice (from [579]).

the two constituents, and the white color indicates that the cell is empty. The entropy  $S_q$  of the  $D$ -dimensional model with very localized initial conditions asymptotically increases *linearly with time* only for

$$q = 1 - \frac{1}{D}. \quad (7.22)$$

This is, essentially, a kind of trivial consequence of the fact that the number  $W$  of possibilities increases as the available  $D$ -dimensional hypervolume, i.e.,  $W \propto t^D$ . Consequently, if we consider the simplest case, namely equal probabilities,  $S_q = \ln_q W \sim W^{1-q}/(1-q) \propto t^{(1-q)D}$ . Then, in order to have  $S_q \propto t$ , Eq. (7.22) must be satisfied. This equation is, in fact, but the particular case of Eq. (3.120) with  $\rho = D$ . Let us also note that the possibly nontrivial entropic effects associated



**Fig. 7.55** Snapshots of the dynamics for  $D = 2, 3, 4$ . The  $D = 2$  snapshots correspond to the square lattice itself. The  $D = 3, 4$  snapshots correspond to a two-dimensional section of the  $D$ -dimensional lattice (from [580]).

with the roughness of the overall contour of the system and of its internal evolving clusters remain to be studied.

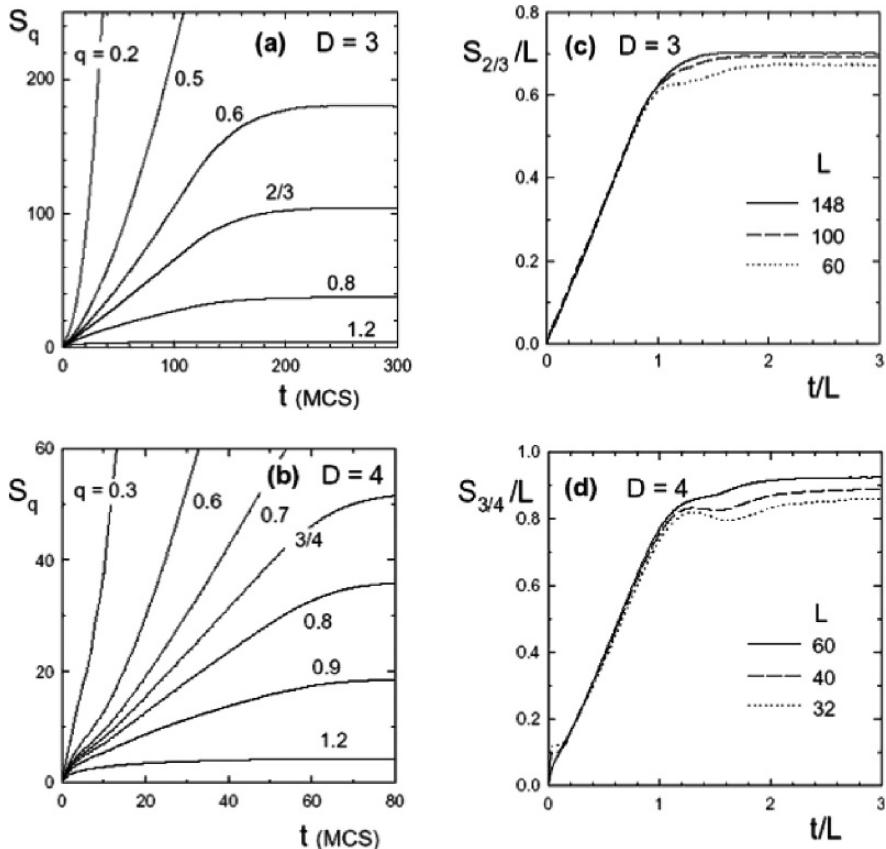
### 7.2.3 Re-Association in Folded Proteins

Re-association of *CO* molecules in heme-proteins has been experimentally studied, and the results are discussed in [282]. See Figs. 7.58 and 7.59. The rate  $\xi$  of non-re-associated molecules was proposed in the literature to be given by

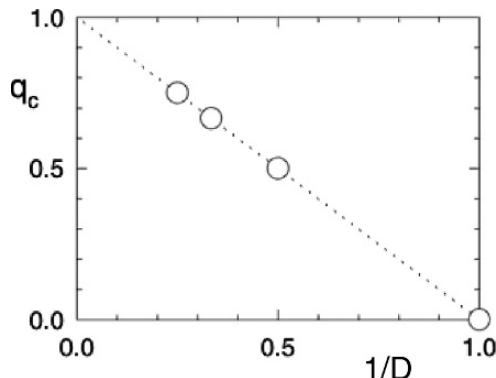
$$\xi \equiv \frac{N(t)}{N(0)} = \frac{1}{(1 + t/t_0)^n}. \quad (7.23)$$

But, with the identifications  $n \equiv 1/(q - 1)$  and  $1/t_0 \equiv (q - 1)/\tau$ , this equation can be rewritten as

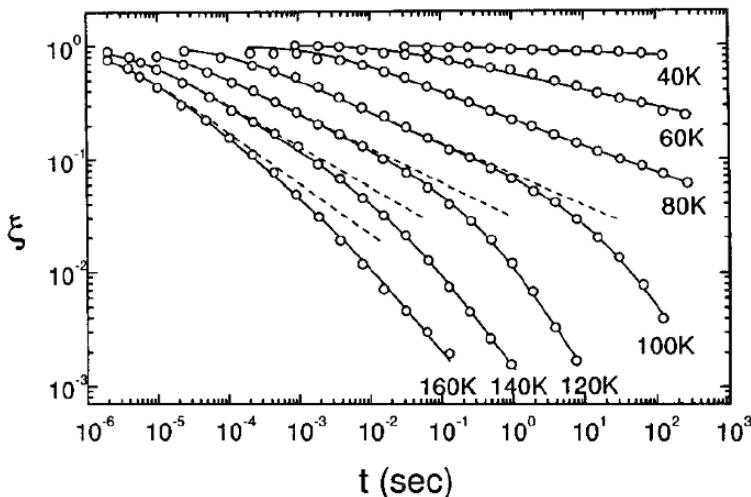
$$\xi = e_q^{-t/\tau}. \quad (7.24)$$



**Fig. 7.56** Time evolution of  $S_q$  for the  $D = 3, 4$  models. The entropy is calculated over the entire phase-space of the  $D$ -dimensional system, and *not* of its two-dimensional sections, such as those shown in Fig. 7.55 (from [580]).



**Fig. 7.57** Dependence of  $q_c$  on dimensionality. Equation (7.22) is thus numerically verified (from [580]).



**Fig. 7.58** Log-log plot of the time evolution of  $\xi \equiv N(t)/N(0)$  associated with  $MbCO$  in glycerol-water. The dots are the experimental data (Figs. 2a and 14 of [283]). The dashed lines indicate the fittings with Eq. (7.23) with the same  $n(T) \equiv 1/[q(T) - 1]$  used in [283]. The full lines correspond to our best present fittings, with the same  $n(T)$  used in [283], and  $r(T)$ ,  $a_q(T)$ , and  $a_r(T)$  as shown in Fig. 7.59 (from [282]).

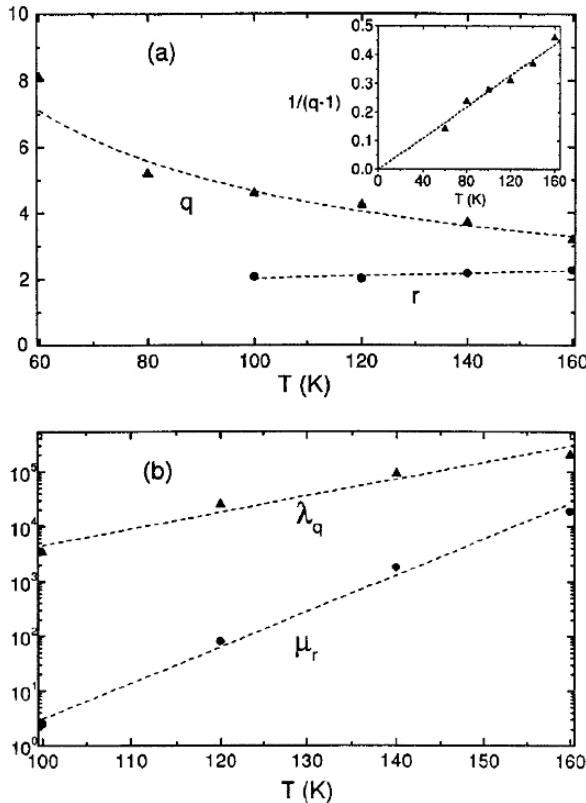
#### 7.2.4 Ground State Energy of the Chemical Elements (Mendeleev's Table) and of Doped Fullerenes

There is nothing more basic in modern chemistry than Mendeleev's Table of elements. However, its standard implementation makes no reference at all to a very basic quantity, namely the energy of the ground state of each specific element. This has been recently addressed in [581]. The outcome is quite astonishing. The ground-state energy of the free atom (as calculated by a performant ab-initio Hartree-Fock method) has been heuristically found to be given, from the hydrogen to the lawrencium, by

$$E = E_H e^{Z \cdot 2.4333(Z-1)}_{0.58145}, \quad (7.25)$$

where  $E_H = -13.60534$  ev, and  $Z$  is the atomic number of the element. See Figs. 7.60 and 7.61.

The ground-state energy of doped fullerenes (as calculated now through a density functional theory method) has also been addressed in [581]. The doping atoms that have been studied are the covalent atoms  ${}^6C$ ,  ${}^7N$ ,  ${}^8O$ ,  ${}^9F$ ,  ${}^{14}Si$ ,  ${}^{615}P$ ,  ${}^{16}S$ ,  ${}^{17}Cl$ , and  ${}^{35}Br$ , and the transition metals  ${}^{21}Sc$ ,  ${}^{22}Ti$ ,  ${}^{23}V$ ,  ${}^{24}Cr$ ,  ${}^{25}Mn$ ,  ${}^{26}Fe$ ,  ${}^{27}Co$ ,  ${}^{28}Ni$ , and  ${}^{29}Cu$ . Discounting the energy of pure fullerene  $C_{60}$  (i.e., without doping), which is 62.21 Kev, the energies are given by precisely (!) the same Eq. (7.25) by substituting  $E_H$  by  $E_{FUL} = -14.98$  ev: see Fig. 7.62.



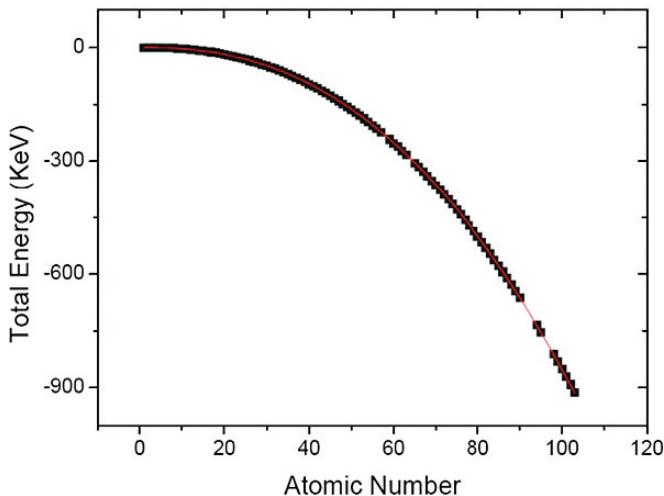
**Fig. 7.59** The temperature dependences of  $(q, r)$  (a), and of  $(\lambda_q, \mu_r)$ , used to fit the experimental data of Fig. 7.58. Inset of (a):  $T$ -dependence of  $n(T) \equiv 1/(q - 1)$  (from Fig. 15 of [283]) (from [282]).

Summarizing, for both Mendeleev Table and doped fullerenes, the ground-state total energies (calculated respectively by ab-initio Hartree–Fock and Functional Density Theory methods) are described (with all presently available precision) by one and the same equation, namely the  $q$ -exponential form (7.25)! The deep understanding of these two results constitutes, in our opinion, a fantastic challenge in the chemical science. The derivation of the nontrivial index  $q = 0.58145$  from first principles would be more than expected. It would, among others, reveal whether there is a deep connection with nonextensivity, or whether it is just a coincidence.

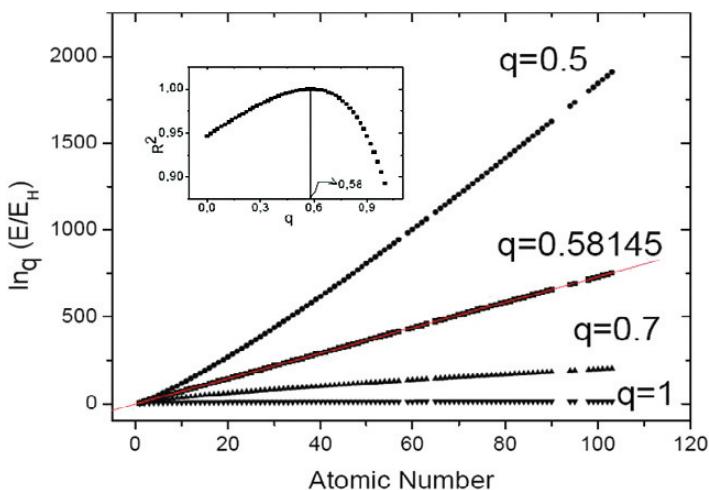
### 7.3 Economics

A sensible amount of papers have used  $q$ -statistical concepts to discuss and/or extend various financial and economical quantities, such as distributions of returns, distributions of stock volumes, Black–Scholes equation, volatility “smile”, pricing, risk aversion in economic transactions, and various others [582–622].

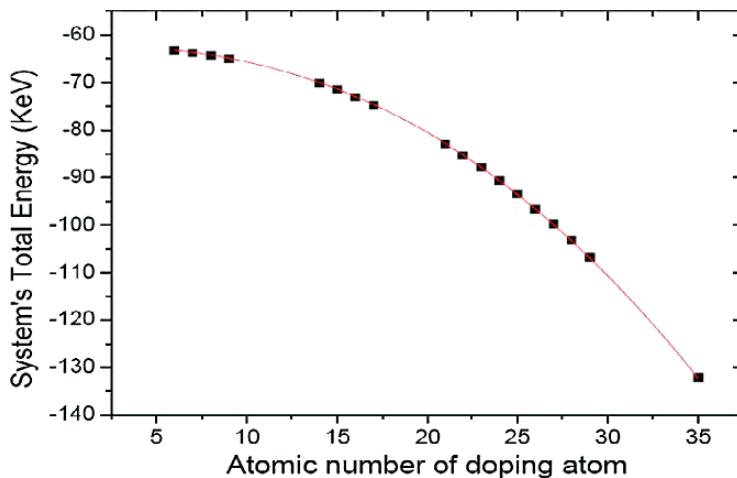
Some typical results are shown in Figs. 7.63, 7.64, 7.65, 7.66, 7.67, 7.68, 7.69, 7.70, and 7.71.



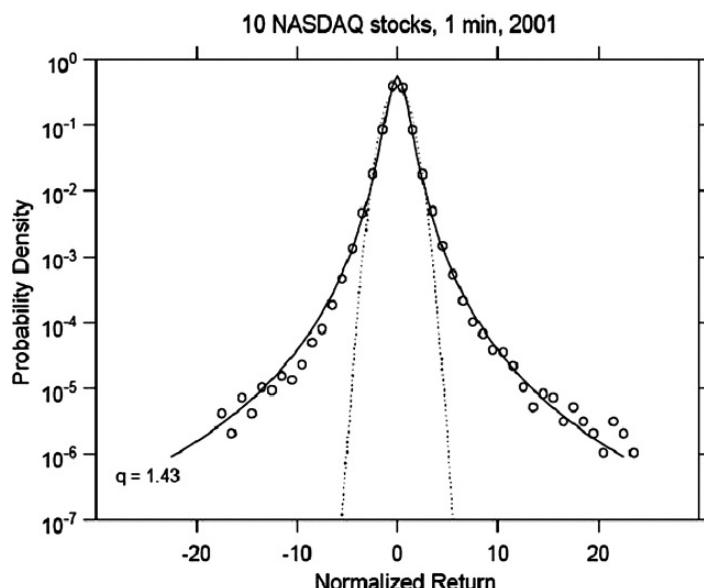
**Fig. 7.60** Ground-state energy of the free atom (as calculated by a Hartree–Fock method) as a function of the atomic number  $Z$ . It runs from hydrogen to lawrencium. The red line has been calculated with Eq. (7.25) (from [581]).



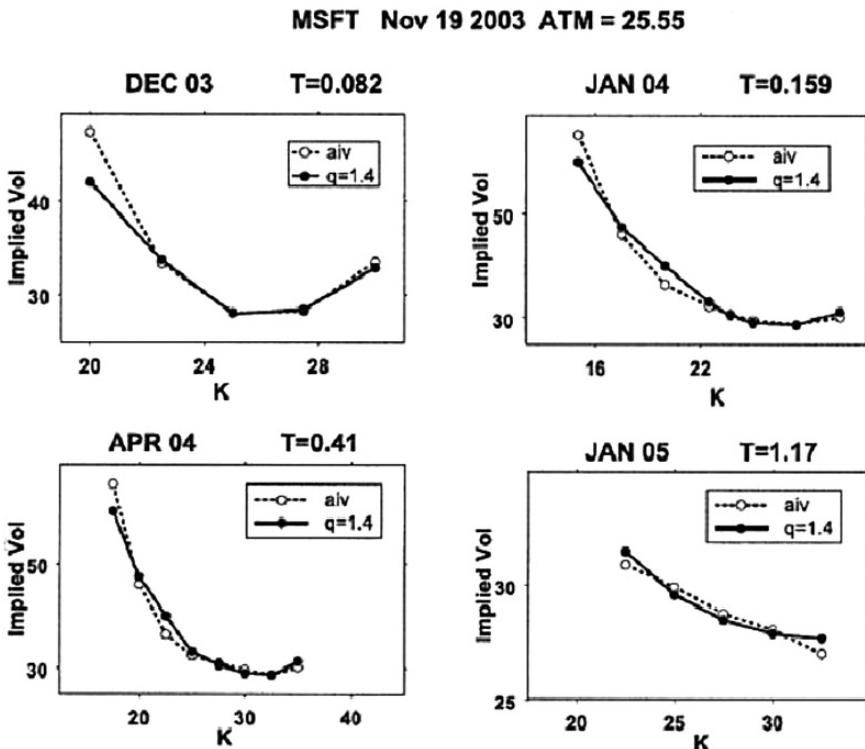
**Fig. 7.61** The same as in Fig. 7.60 in  $q$ -log vs. linear representation. *Inset:* Linear regression coefficient as a function of  $q$ . The maximum is attained at  $q = 0.58145$ , and its value is  $R^2 = 1$  (with six-digit precision!) (from [581]).



**Fig. 7.62** Ground-state energy of the doped fullerenes after discounting the energy of pure fullerene (as all calculated by a Functional Density Theory method) as a function of the atomic number  $Z$ . It runs from  $^6C$  to  $^{29}Cu$ . The red line has been calculated with Eq. (7.25) by replacing  $E_H$  by  $E_{FUL} = -14.98$  ev. Its  $q$ -log vs. linear representation yields once again  $R^2 = 1$  with six-digit precision! (from [581]).



**Fig. 7.63** Distributions of log returns over 1 minute intervals for 10 high-volume stocks. Solid line:  $q$ -Gaussian with  $q = 1.43$ . Dashed line: Gaussian (from [583]).



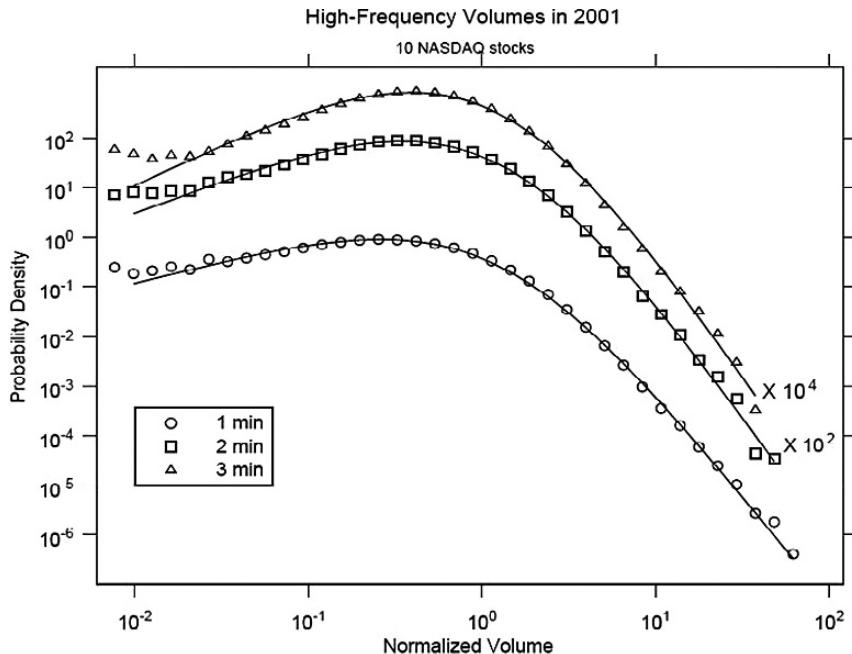
**Fig. 7.64** Quantitative comparison between the skewed implied volatilities obtained from a set of Microsoft options traded on November 19, 2003, and the theoretical model with  $q = 1.4$ , which fits well the returns distribution of the underlying stock (from [594]).

## 7.4 Computer Sciences

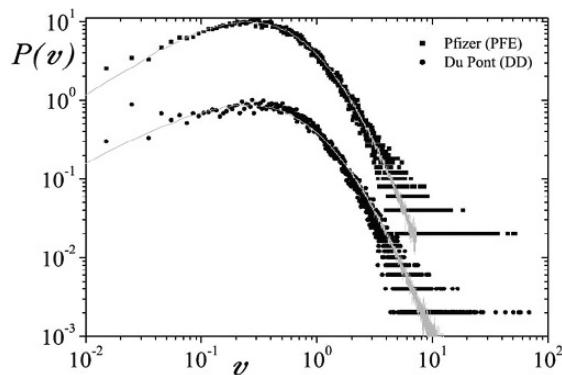
### 7.4.1 Optimization Algorithms

Global optimization consists in numerically finding a global minimum of a given (not necessarily convex) cost/energy function, defined in a continuous  $D$ -dimensional space. Such algorithms have a plethora of useful applications. A well-known classical procedure, referred to as the *Boltzmann machine*, is the so-called *Simulated Annealing*, introduced in 1983 [623], which visits phase-space with a Gaussian distribution. A few years later, a faster procedure, referred to as the *Cauchy machine* because it visits phase-space using a Cauchy–Lorentz distribution, was introduced [624]. Finally, inspired by  $q$ -statistics, an algorithm was introduced [625, 626], named *Generalized Simulated Annealing* (GSA), which recovers the two just mentioned ones as particular cases.

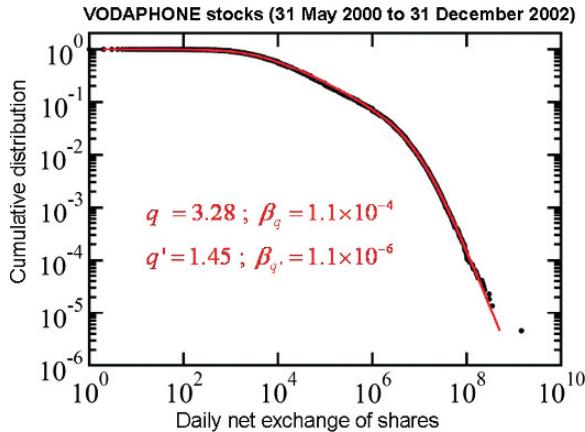
GSA consists, like the Boltzmann and Cauchy machines, of two algorithms that are to be used with alternation. These are the *Visiting algorithm* and the *Acceptance*



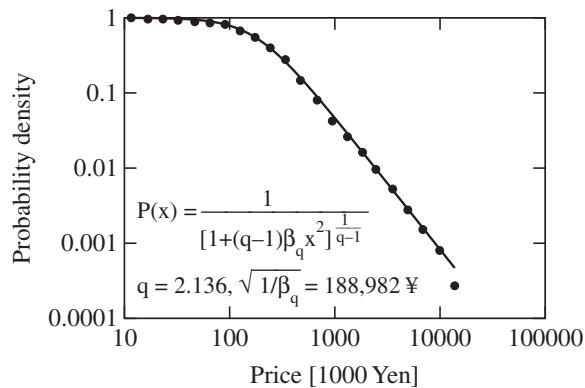
**Fig. 7.65** Probability density of volumes of 10 high-capitalization stocks in NASDAQ, compared to the theoretical curves  $p(v) = \frac{1}{Z} \left(\frac{v}{\theta}\right)^\lambda e_q^{-v/\theta}$  with  $\lambda, \theta > 0, q > 1$ , and the normalization constant  $Z > 0$  (full lines). See details in [592].



**Fig. 7.66** Probability density of volumes of two specific stocks, compared to stochastic results following essentially  $p(v) = \frac{1}{Z} \left(\frac{v}{\theta}\right)^\lambda e_q^{-v/\theta}$  with  $\lambda, \theta > 0, q > 1$ , and the normalization constant  $Z > 0$  (full lines). See details in [606].

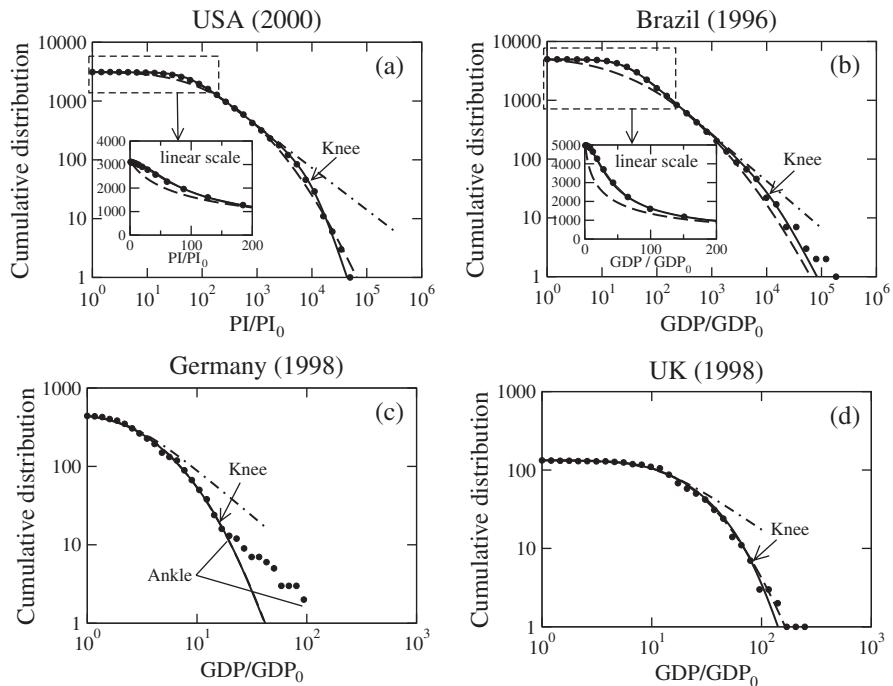


**Fig. 7.67** Cumulative distribution of the daily net exchange of shares (between all pairs of two institutions), at the London Stock Exchange (*Block market*). Data from I.I. Zovko; fitting by E.P. Borges [using the analytic form (in red) emerging within *crossover statistics*; see Eq. (6.4)]; unpublished (2005).

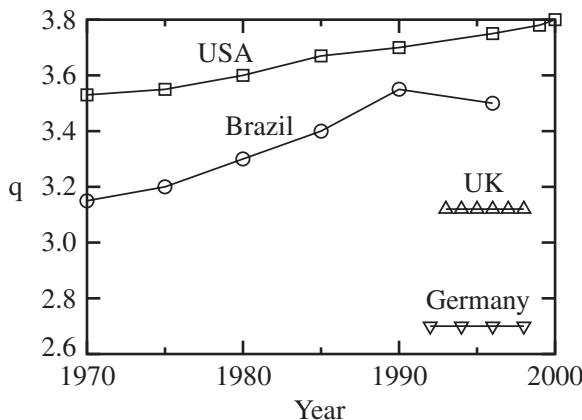


**Fig. 7.68** Cumulative distribution of the land prices in Japan. Data from [586]; fitting by E.P. Borges (2003).

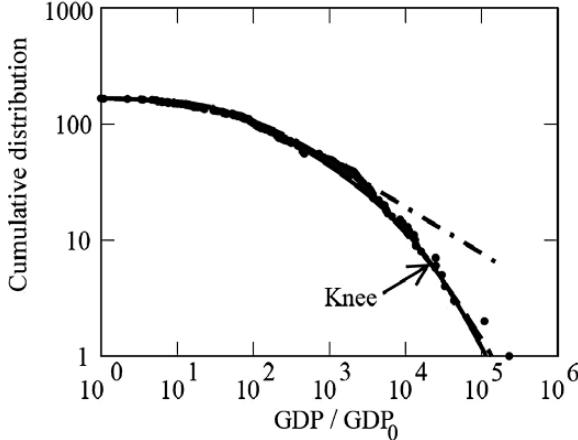
algorithm. The visiting algorithm is based on an exploration of phase-space using a  $q_V$ -Gaussian (instead of using either a Gaussian or a Cauchy distribution), and the acceptance algorithm is based on a  $q_A$ -exponential weight (instead of the Monte Carlo Boltzmann weight). Therefore, a GSA machine is characterized by the pair  $(q_V, q_A)$ . The choice  $(1, 1)$  is the Boltzmann machine, and the choice  $(2, 1)$  is the Cauchy machine. In practice, the most performant values have been shown to be  $q_V > 1$ , slightly below the maximal admissible value for the  $D$ -dimensional problem (for  $D = 1$  the maximal admissible value is  $q_V = 3$ , and a performant value is  $q_V \approx 2.7$ ); for  $D$  dimensions, the maximal admissible value is  $q_V = (D + 2)/D$ ,



**Fig. 7.69** Cumulative distribution of the *scaled total personal income* of the USA *counties* (a), and the *scaled gross domestic product* of the Brazilian (b), German (c), and United Kingdom (d) *counties*. See [596] for further details.



**Fig. 7.70** Time evolution of the index  $q$  for USA (squares), Brazil (circles), United Kingdom (up triangles), and Germany (down triangles). This means that the economic inequalities are larger in USA, then in Brazil, then United Kingdom, and finally Germany. We also see that inequalities are increasing in USA and Brazil, whereas they remain at the same level in United Kingdom and Germany. See [596] for further details.



**Fig. 7.71** Cumulative distribution of the *scaled gross domestic product* of 167 countries around the world for the year 2000;  $q = 3.5$ . See [596] for further details.

and  $q_A < 1$ . A very convenient random number generator following a  $q$ -Gaussian distribution has been recently proposed in [627].

Part of the simulated annealing procedure consists in the *Cooling algorithm*, which determines how the *effective temperature*  $T$  is decreased with time, so that the global minimum is eventually attained within the desired precision. A quick cooling is of course computationally desirable. But not too quick, otherwise the rate of success of ultimately arriving to the real global minimum decreases sensibly. The optimal cooling procedure appears to be given by [625, 626]

$$\frac{T(t)}{T(1)} = \frac{2^{q_V-1} - 1}{(1+t)^{q_V-1} - 1} = \frac{\ln_{q_V}(1/2)}{\ln_{q_V}[1/(t+1)]} \quad (t = 1, 2, 3, \dots), \quad (7.26)$$

where  $T(1)$  is the initial high temperature imposed onto the system. We verify that, for  $q_V = 1$ , we have

$$\frac{T(t)}{T(1)} = \frac{\ln 2}{\ln(1+t)} \quad (t = 1, 2, 3, \dots), \quad (7.27)$$

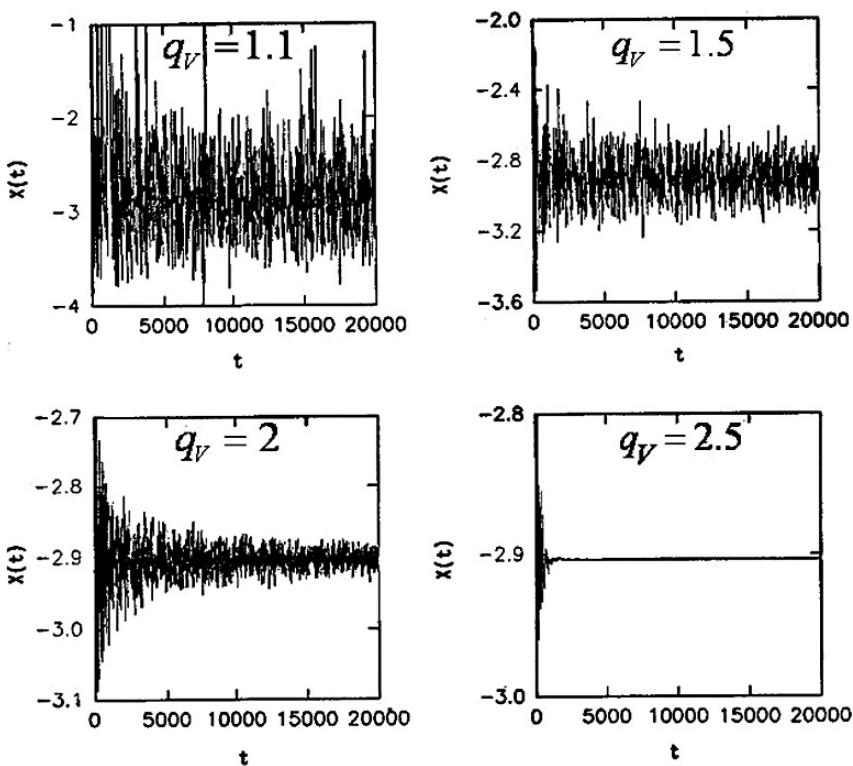
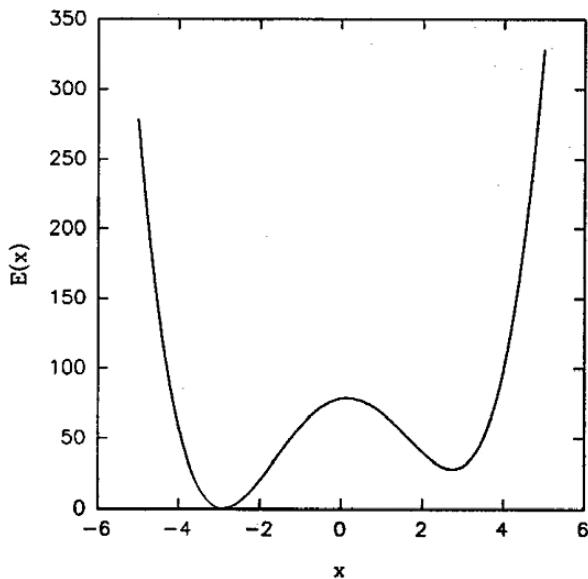
and that, for  $q_V = 2$ , we have

$$\frac{T(t)}{T(1)} = \frac{2}{t} \quad (t = 1, 2, 3, \dots). \quad (7.28)$$

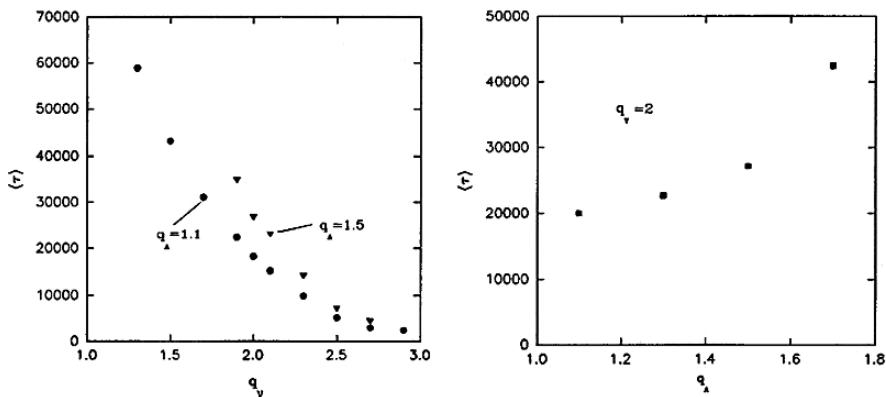
For the  $D = 1$  upper limit, we have  $q_V = 3$ , hence

$$\frac{T(t)}{T(1)} = \frac{3}{(1+t)^2 - 1} \quad (t = 1, 2, 3, \dots). \quad (7.29)$$

**Fig. 7.72** The cost function is given by  $E(x) = x^4 - 16x^2 + 5x + 78.3323$  (from [625]).



**Fig. 7.73** Influence of  $q_V$  on the stochastic time evolution towards the global minimum. The runs start with  $x(1) = 2$  and  $T(1) = 100$ . Further details in [625].



**Fig. 7.74** Influence of  $(q_V, q_A)$  on the average computer time needed for finding the global minimum with a given precision. For the present problem the optimal choice consists in  $q_V \simeq 2.8$  and  $q_A < 1$ . Further details in [625].

We see therefore a strong influence of  $q_V$  on the cooling allowed speed, which can ultimately benefit (decrease) quite strongly the necessary computational time. To test the method, a toy model has been studied. The cost function is shown in Fig. 7.72, and typical runs are shown in Fig. 7.73. The influence of  $(q_V, q_A)$  is depicted in Fig. 7.74.

Another toy model [626] is to use the  $D = 4$  cost function

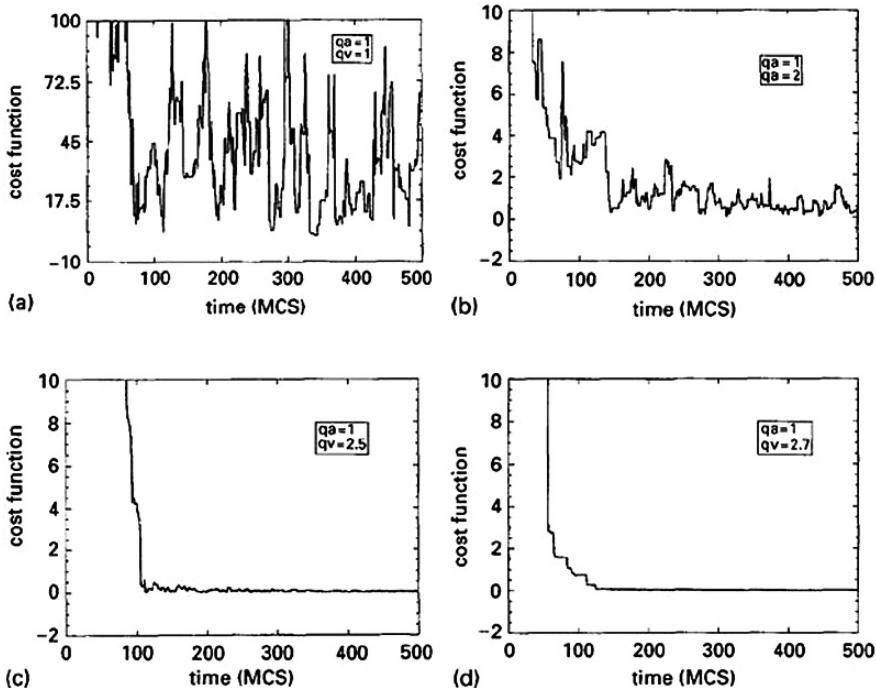
$$E(x_1, x_2, x_3, x_4) = \sum_{i=1}^4 (x_i^2 - 8)^2 + 5 \sum_{i=1}^4 x_i , \quad (7.30)$$

which has 15 *local* minima and one *global* minimum. Typical results can be seen in Figs. 7.75 and 7.76.

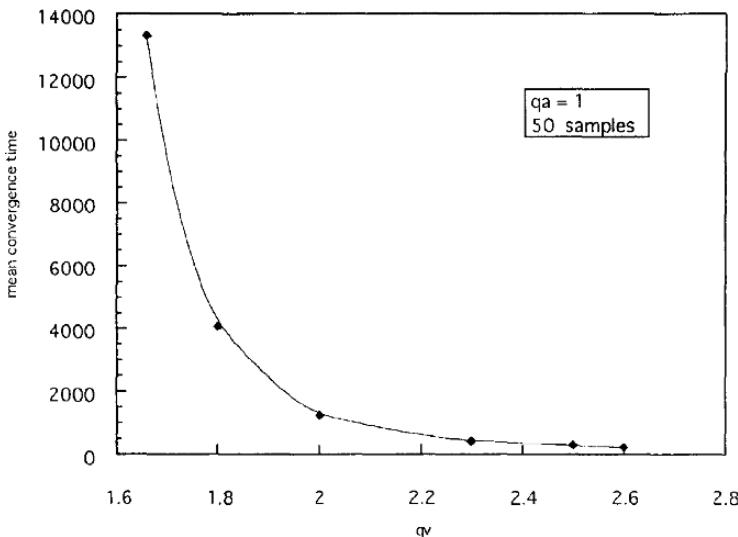
An extension of these ideas has been advanced which leads to a  $q$ -generalization of the so-called *Pivot method* [628, 629]. Typical results are indicated in Figs. 7.77 and 7.78. The first use of the GSA in quantum systems was done in [630]. Since those early times a large number of algorithmic methods have been implemented, for chemical, neural network and other purposes, inspired by  $q$ -statistics [631–640, 642–727].

#### 7.4.2 Analysis of Time Series and Signals

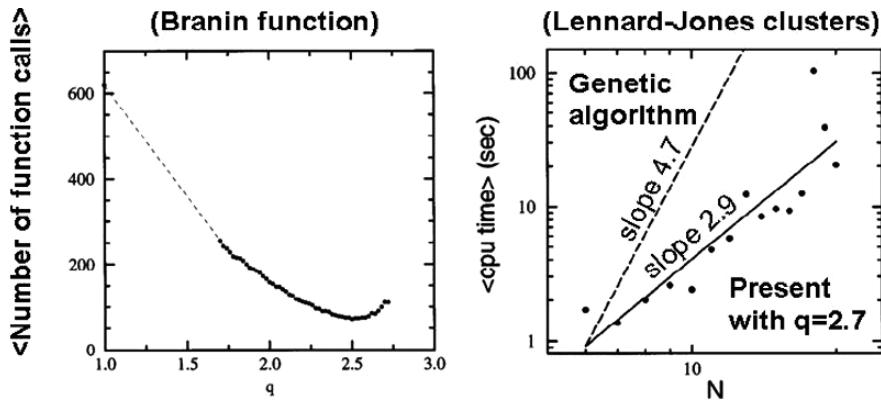
Concepts of  $q$ -statistics have inspired several methods for processing time series and signals, such as electroencephalograms (EEG), electrocardiograms (ECG), and various others. It has been possible to focus on some specific features of epilepsy (in humans and turtles), Alzheimer disease, and other complex circumstances [728–754]. The analysis of the tonic–clonic transition of some types of epilepsy constitutes a



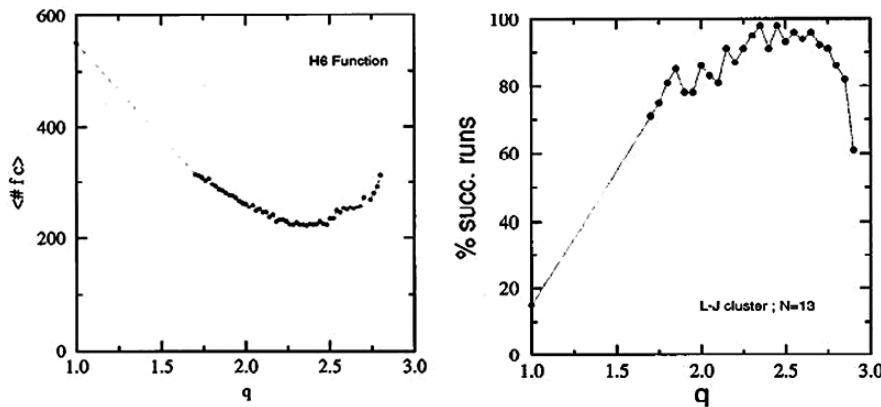
**Fig. 7.75** Typical runs of the GSA algorithm.  $E_t$  vs.  $t$  (MCS) for random initial conditions and  $T(1) = 100$ . Acceptance parameter  $q_A = 1$  and (a)  $q_V = 1$ , (b)  $q_V = 2$ , (c)  $q_V = 2.5$ , and (d)  $q_V = 2.7$  (from [626]).



**Fig. 7.76** Mean convergence time vs.  $q_V$ . The solid line is a guide to the eye. The mean convergence time for  $q_V = 1$  is about 50,000. By taking  $q_V \simeq 2.6$ , there is a gain in computer time of a factor close to 100 (from [626]).

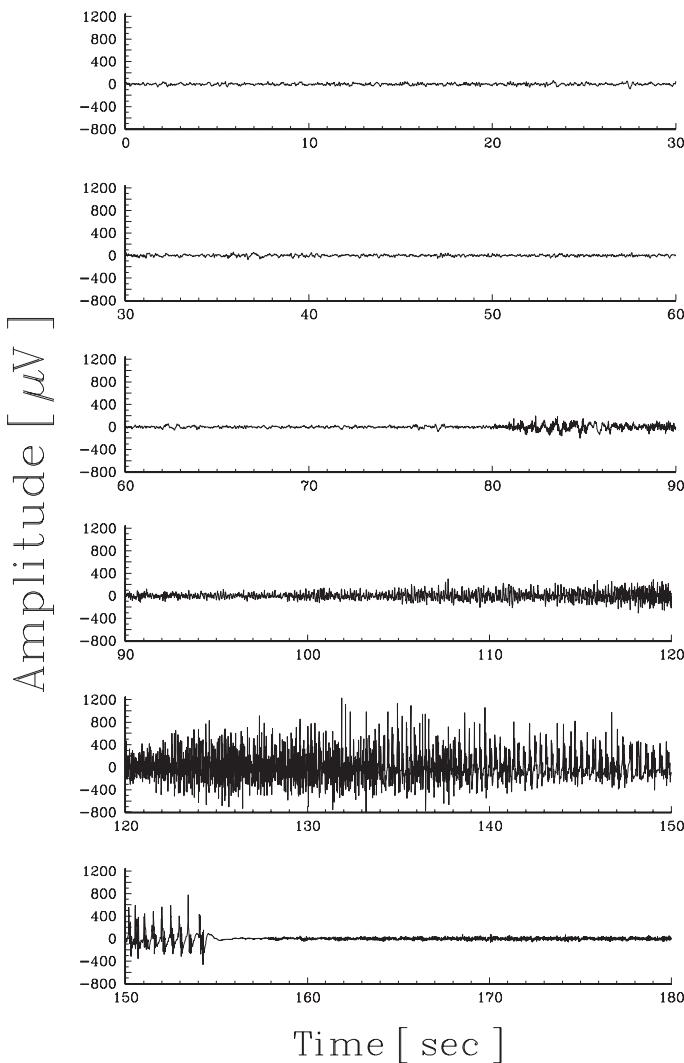


**Fig. 7.77** Typical results of a  $q$ -generalized pivot method. The method is sensibly more performant for  $q > 1$  than for  $q = 1$ , and even more performant than the popular Genetic Algorithm (from [628]).

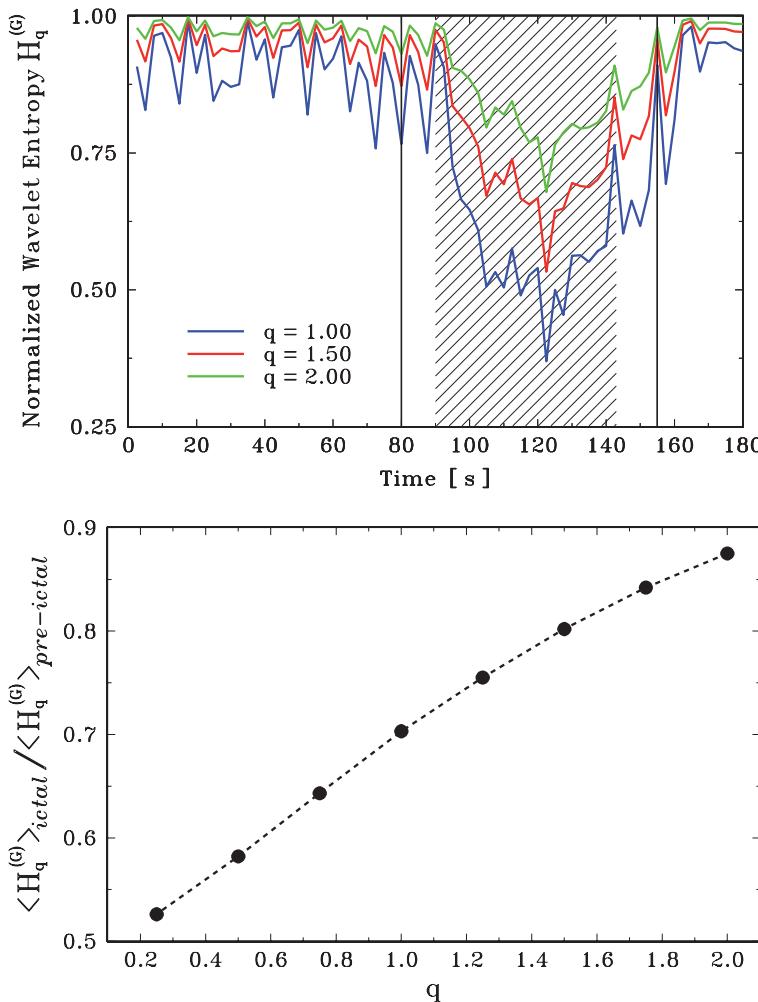


**Fig. 7.78** Typical results of a  $q$ -generalized pivot method. Using  $q > 1$  instead of  $q = 1$  provides a double advantage: the computer time decreases (from 600 to 200 in the left panel), and the success rate (dramatically) increases (from 15 to 95% in the right panel) (from [629]).

typical illustration [744]. The EEG during a crisis can be seen in Fig. 7.79. Nothing very special can be seen in the direct EEG during the body of the crisis which would reveal the moment of the tonic-clonic transition, which clinically is very dramatic. However, as we verify in Fig. 7.80, after appropriate processing the tonic-clonic transition becomes absolutely visible. The discrimination becomes even stronger if  $q < 1$  is used. If no specialized personnel were present at the precise moment of the crisis of the patient, the existence of such a neat peak makes possible the automatic start of computer-controlled administration of appropriate drugs during the emergency.



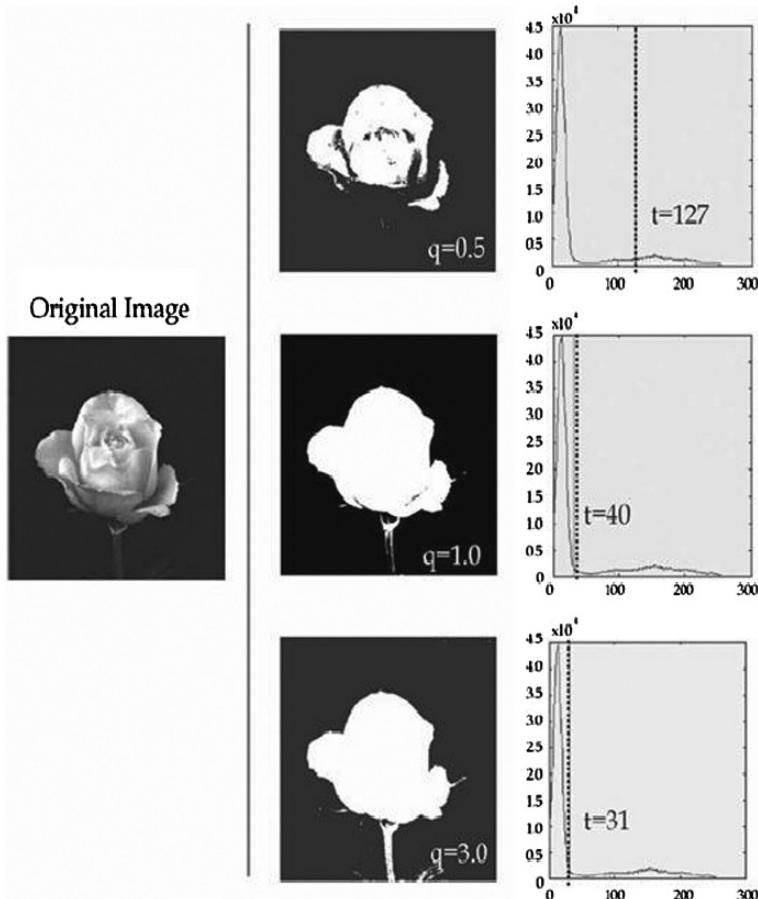
**Fig. 7.79** Electroencephalogram (including the contribution of muscular activity) during an epileptic crisis which starts at 80 s, and ends at 155 s. By direct inspection of the EEG, it is virtually impossible to detect the (clinically dramatic) transition (at 125 s) between the tonic stage and the clonic stage of the patient (from [744]).



**Fig. 7.80** *Top panel:* After processing (of the EEG signal) which includes the use of the entropic functional  $S_q$ , the precise location of the tonic–clonic transition becomes very visible. *Bottom panel:* The effect is even more pronounced for values of  $q$  going below unity (from [744]).

### 7.4.3 Analysis of Images

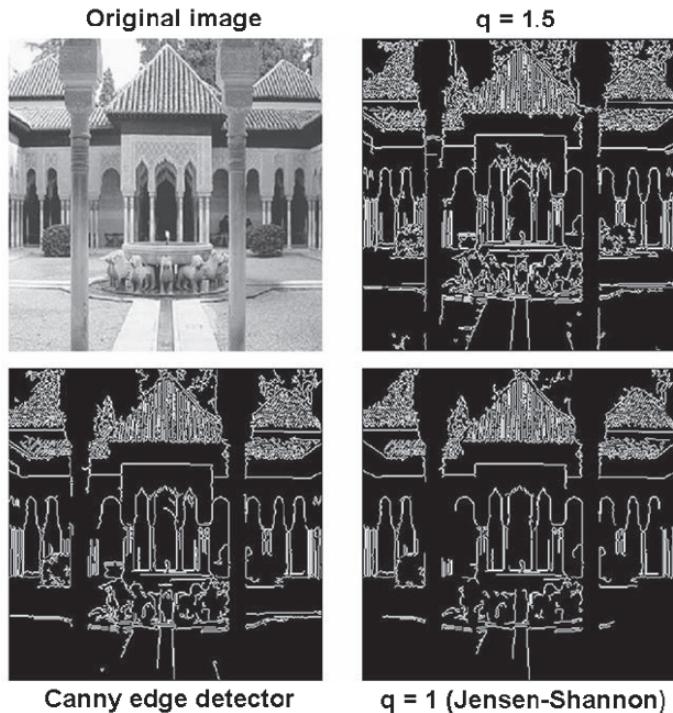
Various applications exist in the literature concerning image processing, such as *segmentation* or *thresholding* (see Fig. 7.81), *edge detection* (see Fig. 7.82), *fusion* (see Fig. 7.83), images for *Magnetic Resonance* and *Computed Tomography* (see Fig. 7.84), *facial expression recognition* (see Fig. 7.85), among others [755–772].



**Fig. 7.81** Segmentation using the entropic functional  $S_q$ . Influence of the index  $q$  in natural images. Further details in [755].

#### 7.4.4 PING Internet Experiment

PING is a quick internet procedure which enables, from a given computer, to check whether any other specific computer is on-line at that moment. There is naturally a time delay (*sparseness time interval*) before the answer arrives. Abe and Suzuki [773] devised an interesting experiment which consisted in automatically repeating the ping instruction many times in order to measure the distribution of the sparseness time interval. The results can be seen in Figs. 7.86 and 7.87. They are relatively well fitted by the expression  $P(>\tau) = e^{-\tau/\tau_0}$ . If we plot the four pairs  $(q, \ln \tau_0)$ , it does not suggest a monotonic *curve*, but rather something which could be closer to a



**Fig. 7.82** Image edge detection using a  $q$ -generalized Jensen–Shannon divergence. The  $q = 1.5$  image shows more details than both the  $q = 1$  image and the Canny edge detector image. Further details in [764].

“cloud,” would we have many such points. But, of course, with only four points it is hard to advance any behavior with some degree of reliability.

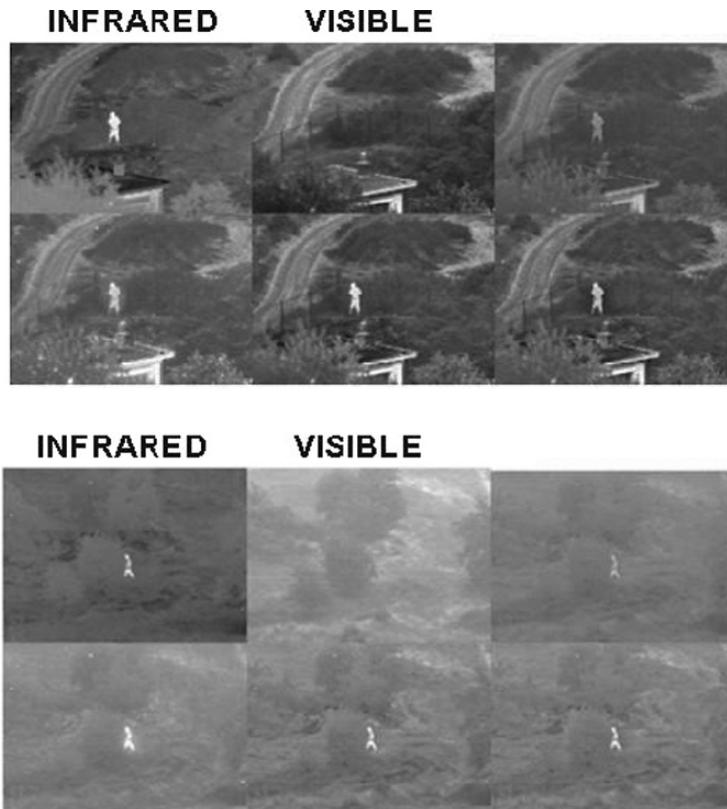
## 7.5 Biosciences

### i. Motion of *Hydra viridissima*

*Hydra viridissima* is a small organism which may live in “dirty” (feeding) water. Experiments are described in [774] which enabled the study of its motion, particularly the measure of the distribution of the velocities and the (anomalous) diffusion. The results are indicated in Figs. 7.88 and 7.89. It turned out that the distribution of velocities is *not* Maxwellian, but rather a  $q$ -Gaussian with  $q \simeq 1.5$ . Also, the diffusion was shown to occur with an exponent  $\gamma \simeq 1.24 \pm 0.1$ . Therefore, the prediction (4.16) is verified within the experimental error bars.

### ii. Ecology

The entropy  $S_q$  has been used to measure ecological diversity and species rarity [775].



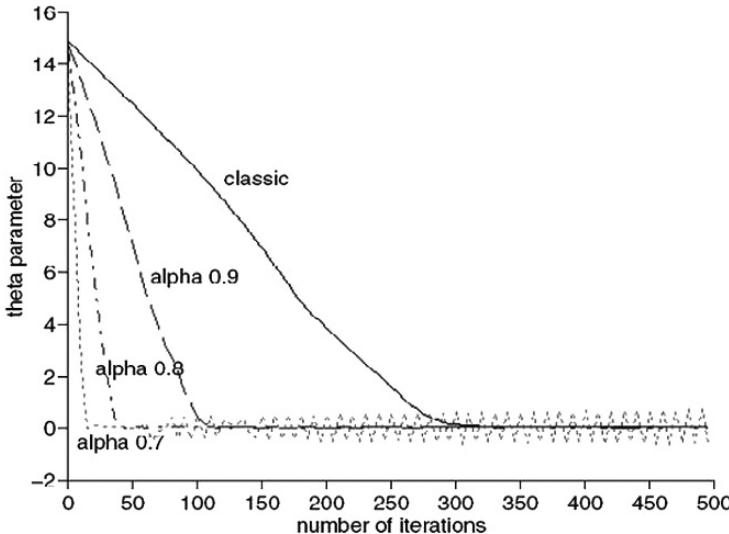
**Fig. 7.83** Image fusion metric based on  $q$ -generalized mutual information. The best correlation with the subjective quality of fused images is obtained for  $q \simeq 1.85$ . *Top panel:* The goal is to better distinguish the human profile. *Bottom panel:* The goal is to better distinguish the background. Further details in [765].

### iii. Medical applications

Signal processing of the EEG for direct medical use has been proposed for brain injury following severe situations such as cardiac arrest or asphyxia [776]. Typical results are indicated in Figs. 7.90 and 7.91. Further biomedical applications can be seen in [777–788].

## 7.6 Cellular Automata

A first connection between cellular automata (CA) and  $q$ -concepts has been attempted in [846], by introducing a long-memory in some typical Wolfram Class II CA. We have focused on Rules 61, 99, and 111. The weight of the memory decays towards the past as  $1/\tau^\alpha$  ( $\tau = 1, 2, 3, \dots; \alpha \geq 0$ ), so that  $\alpha \rightarrow \infty$  has no other



**Fig. 7.84** Magnetic Resonance and Computerized Tomography images. The goal is to make a fast and accurate image registration. It uses a  $q$ -generalized mutual information. The algorithm achieves up to *seven* times faster convergence and *four* times more precise registration for  $q \equiv \alpha < 1$  when compared to the classic case ( $q = 1$ ). Further details in [756].

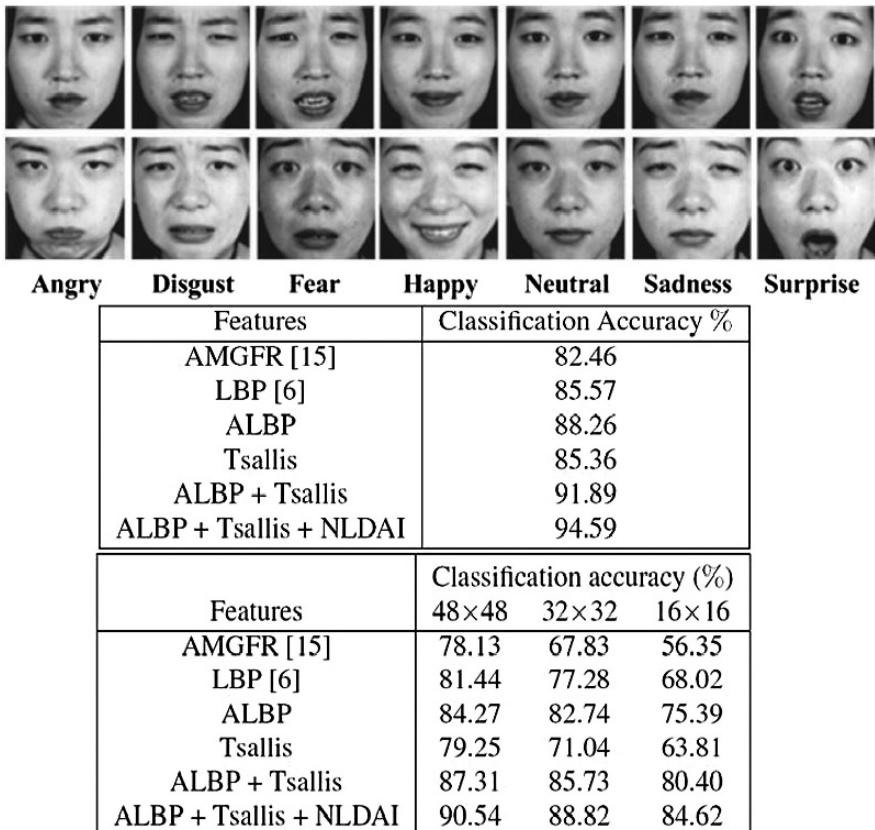
memory than that of the previous step, i.e., the model recovers the simple Wolfram CA. If  $\alpha = 0$  instead, we have infinitely long memory. Since the memory function is summable for  $\alpha > \alpha_c$  and nonsummable for  $0 < \alpha \leq \alpha_c$  with  $\alpha_c \simeq 1$ , we expect important changes to occur while crossing  $\alpha \simeq 1$ . This is indeed observed in the time behavior of the *Hamming distance*. Since this quantity plays a role totally analogous to the sensitivity to the initial conditions, it is natural to expect  $H(t) \propto e^{\lambda_q t} \propto t^{1/(1-q_{sen})}$ . The results can be seen in Figs. 7.92, 7.93, and 7.94.

## 7.7 Self-Organized Criticality

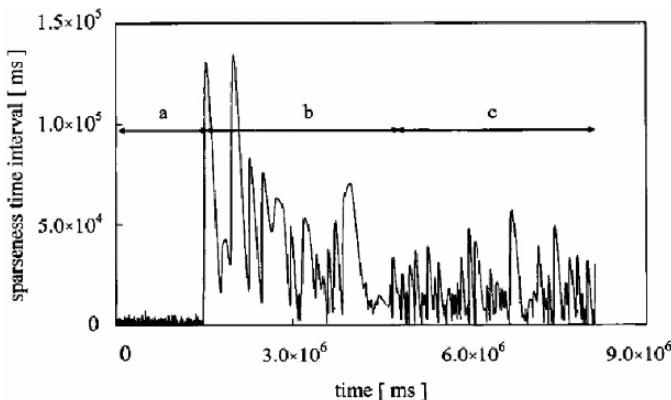
Several studies have been done in connection with self-organized criticality (SOC), in connection with biological evolution [847, 849, 851–853], imitation games [848], atmospheric cascades [850], earthquakes [855, 856], and others [854].

## 7.8 Scale-Free Networks

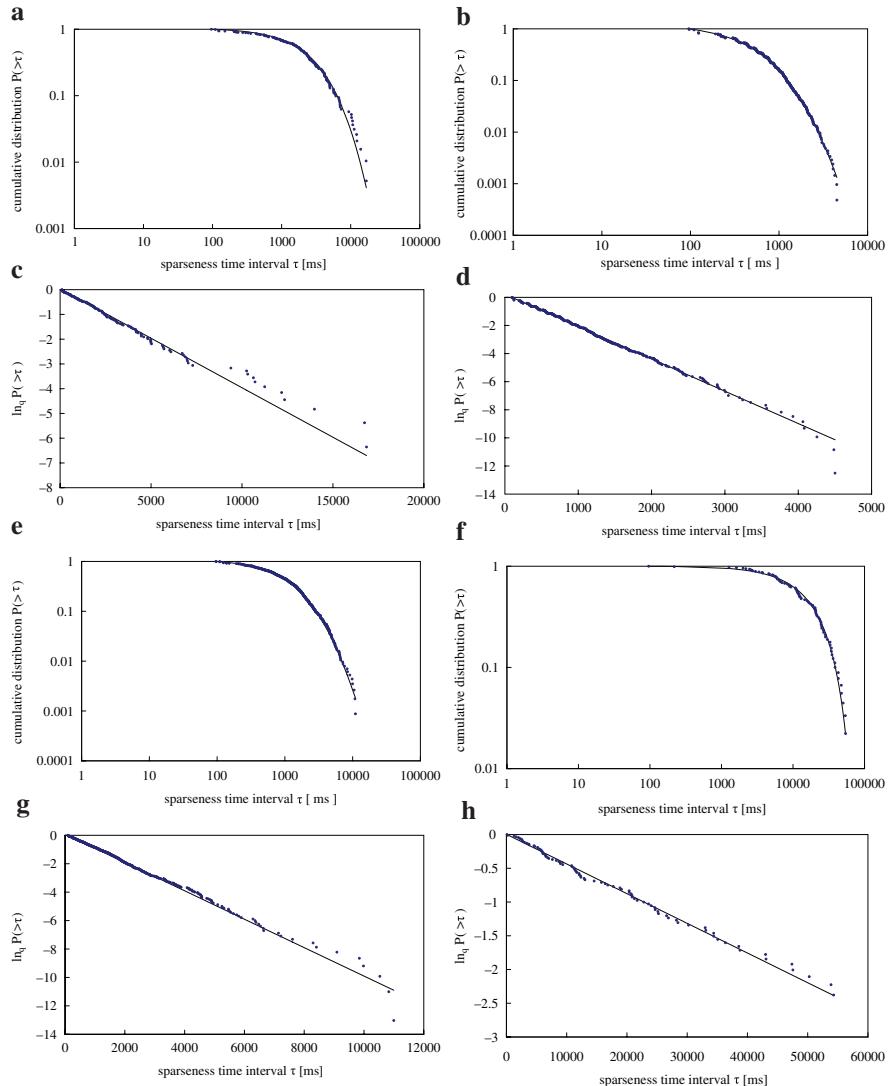
Networks exist of various types [858–862]. They are typically characterized by sets of *nodes* (*sites*) and sets of directed or nondirected *links* (*bonds*) joining the nodes. These are the most studied, although it is clear that it is easy to generalize the concept by also including plaquettes and other many-node, many-link, and



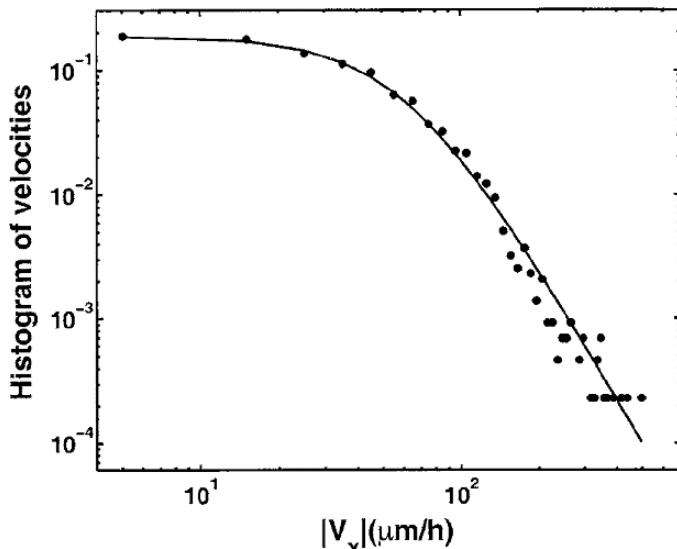
**Fig. 7.85** Facial expression recognition using Advanced Local Binary Patterns (ALBP), entropy  $S_q$ , and global appearance features. Sample images from the JAFFE database. At all resolution levels ( $64 \times 64$ ,  $48 \times 48$ ,  $32 \times 32$ , and  $16 \times 16$ ), the combination “ALBP + Tsallis + NLDAI” yields the highest accuracy. Further details in [763].



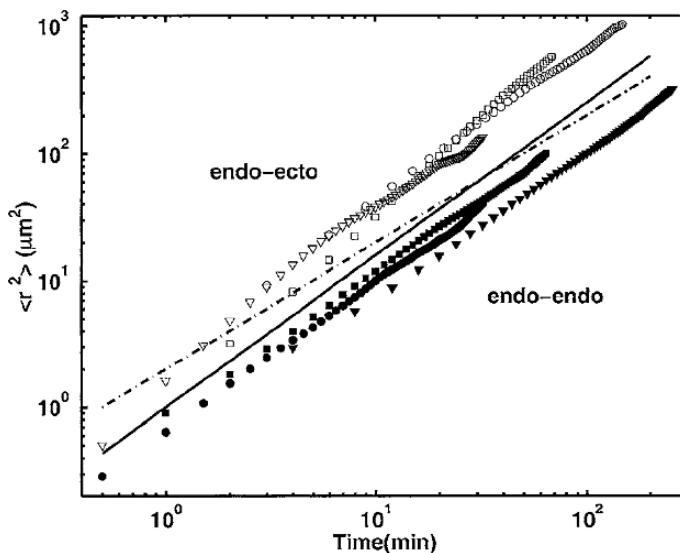
**Fig. 7.86** Time series data of the sparseness time interval. Approximately, three different nonequilibrium stationary states (denoted a, b and c) may be recognized (from [773]).



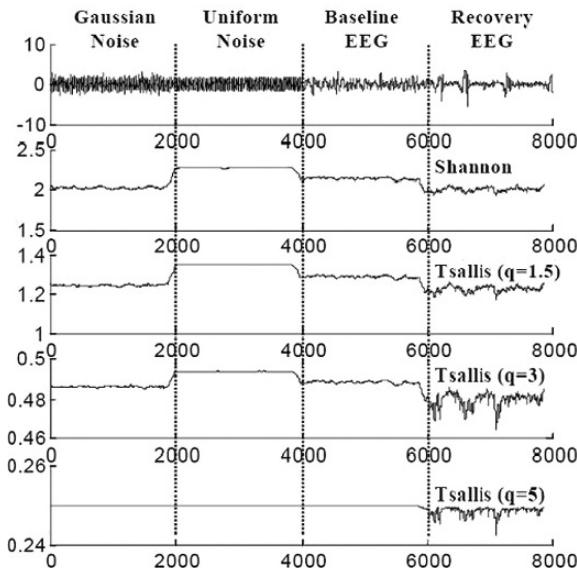
**Fig. 7.87** Cumulative probability of the measured sparseness time interval corresponding to four different nonequilibrium stationary states (the first three are precisely the states a, b, and c of Fig. 7.86; the fourth is still a different one. All four *upper panels* are in log–log representation; all four *lower panels* are the same data, in  $q$ -log vs. linear representation. The continuous curves are  $q$ -exponentials with  $q = 1.7$  (a and c),  $q = 1.12$  (b and d),  $q = 1.16$  (e and g), and  $q = 0.73$  (f and h), respectively. Notice that values of  $q$  both above and below unity occur (from [773]).



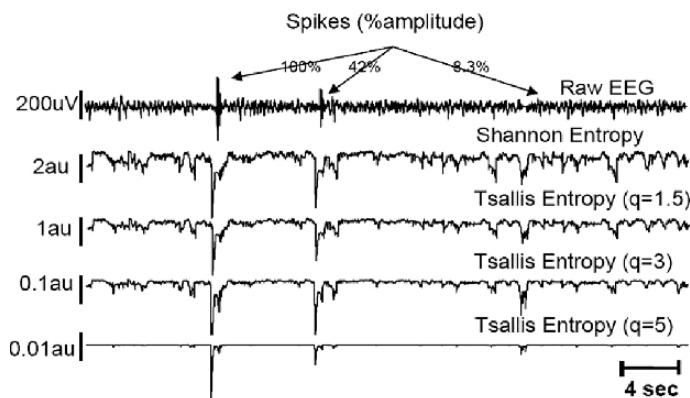
**Fig. 7.88** Probability distribution for the horizontal component of velocity for endodermal cells in an ectodermal aggregate. The *solid line* is a fit with a  $q$ -Gaussian using  $q = 1.5$ . See details in [774].



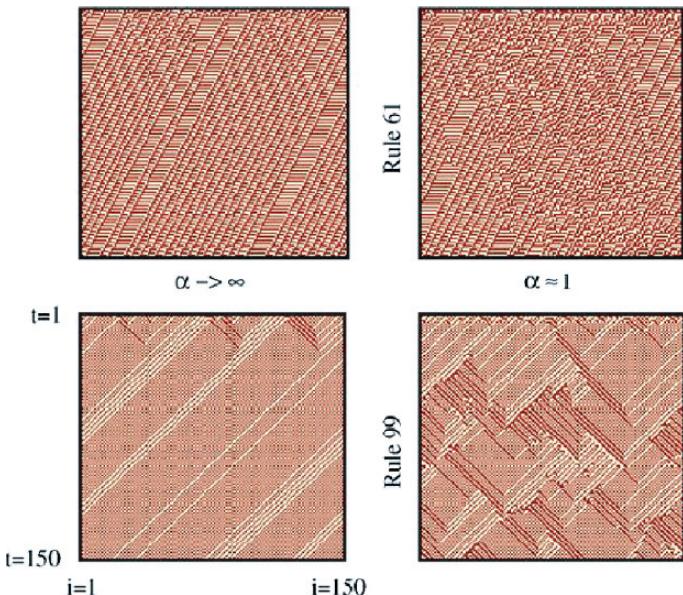
**Fig. 7.89**  $\langle r^2 \rangle$  vs.  $t$  plot for endodermal cells in an endodermal aggregate (*filled symbols*), and endodermal cells in an ectodermal aggregate (*open symbols*). The *solid line* has a slope of 1.23, while the *dashed line* has a slope of 1.0 (which would correspond to normal diffusion). See details in [774].



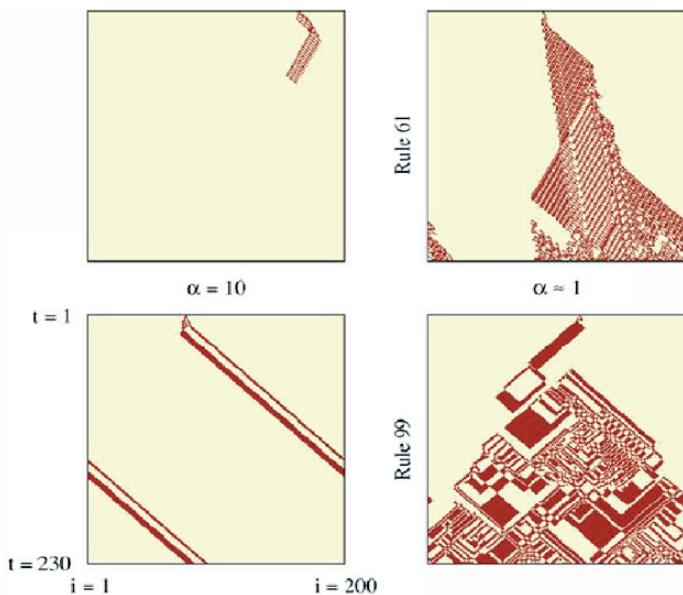
**Fig. 7.90** The goal is to distinguish between signals with different probability distributions, and between EEG from different physiological conditions. The optimal is achieved for  $q \simeq 3$ . See details in [776].



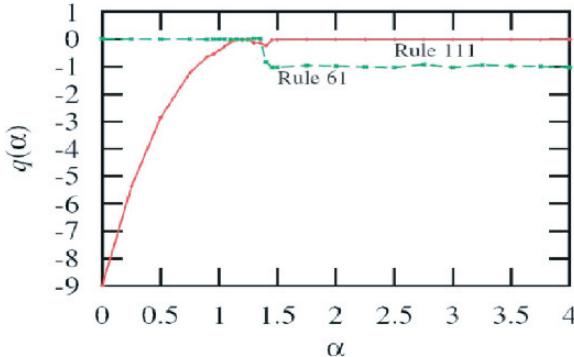
**Fig. 7.91** The goal is to detect the existence of three (artificially introduced) spikes which corrupt the raw EEG. Even the low amplitude spike becomes detectable after (entropic) processing with  $q \geq 3$ . See details in [776].



**Fig. 7.92** Space-time plots starting from random initial configurations. States  $\sigma_i = 0$  ( $\sigma_i = 1$ ) are shown yellow (red). See details in [846].



**Fig. 7.93** Difference patterns for CA with initial configurations differing in only one randomly chosen bit. Cells with different in both configurations at time  $t$  are shown in red. See details in [846].



**Fig. 7.94** The  $\alpha$ -dependence of  $q \equiv q_{sen}$ . See details in [846].

mixed connections. Networks can be *topological* in nature, in the sense that we are allowed to arbitrarily deform them as long as we do not modify the connections between nodes and links. But they can also be *metrical*, in the sense that they may have a “geography” with a concept of *distance*, which can sensibly influence a variety of properties. *Bravais lattices* can be thought as networks which are invariant through discrete *translations*. Through the concept of unitary crystalline cell, we can attribute to them a nonzero Lebesgue measure. *Hierarchical networks* typically are scale-invariant, and can be characterized through a *Hausdorff* or *fractal dimension*. More complex networks can exhibit a multifractal structure, and can thus be characterized by a  $f(\alpha)$  function [212]. In what follows we focus on the so-called *scale-free networks*. Indeed, they play an interesting role as systems that can be (at least for some of their properties) addressed by the entropy  $S_q$  and nonextensive statistical mechanics.

These networks are of the hierarchical kind, made of hubs, sub-hubs, sub-sub-hubs, and their links, the whole constituting a connected structure which exhibits (strict or statistical) invariance under *dilation*. Their basic characterization is done through the *degree distribution*  $p(k)$ , defined as the probability of a node having  $k$  links ( $k = 1, 2, \dots$ ). It happens that many of them exhibit a power-law dependence in  $k$  for large values of  $k$ . And many among those, precisely have the form

$$p(k) = p(0) e^{-k/\kappa} \quad (\kappa > 0), \quad (7.31)$$

where  $p(0)$  is a normalizing factor. This form is known to extremize  $S_q$  with simple constraints (see Section (3.5)). It appears frequently in the literature as

$$p(k) \propto \frac{1}{(k_0 + k)^\mu}, \quad (7.32)$$

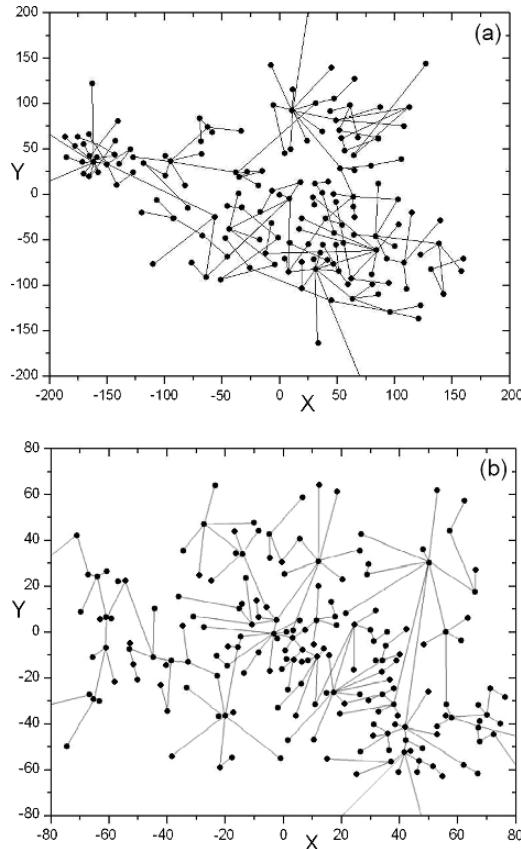
which is identical to Eq. (7.31) through the transformation

$$\mu \equiv \frac{1}{q-1}, \quad k_0 \equiv \frac{\kappa}{q-1}. \quad (7.33)$$

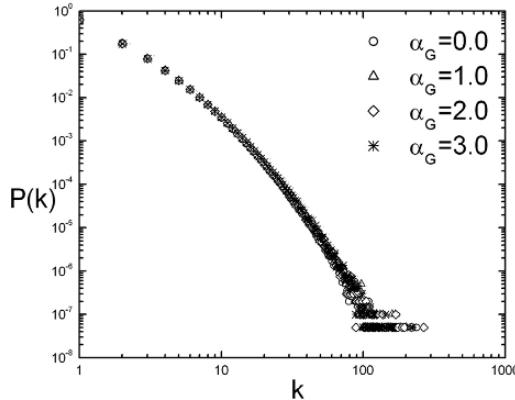
Let us exhibit now a few systems whose degree distribution is precisely of this type, in order to show later what the connection is between this type of networks and nonextensive statistical concepts [789].

### 7.8.1 The Natal Model

For convenience – and also as an homage – we shall refer to this growth model [790] as the *Natal* one because all four co-authors have deep connections with that sea-shore town of the North-East of Brazil. See Figs. 7.95, 7.96, 7.97, 7.98, and 7.99.



**Fig. 7.95** Typical  $N = 250$  network for (a)  $(\alpha_G, \alpha_A) = (1, 0)$  and (b)  $(\alpha_G, \alpha_A) = (1, 4)$ . The starting site at  $(X, Y) = (0, 0)$  is indicated with a *larger circle*. Notice the spontaneous emergence of hubs (from [790]).



**Fig. 7.96** Connectivity distribution for  $\alpha_A = 1$  and typical values of  $\alpha_G$ ; 2000 realizations of  $N = 10,000$  networks (from [790]).

### 7.8.2 Albert-Barabasi Model

Another growth model, also including *preferential attachment*, has been introduced and analytically solved in 2000 by Albert and Barabasi [864] as a prototype of emergence of the ubiquitous scale-free networks. At each time step,  $m$  new links are added with probability  $p$ , or  $m$  existing links are rewired with probability  $r$ , or a new node with  $m$  links is added with probability  $1 - p - r$ ; all linkings are done with probability  $\Pi(k_i) = (k_i + 1)/\sum_j(k_j + 1)$ , where  $k_i$  is the number of links of the  $i$ th node. The exact stationary state distribution of the number  $k$  of links at each site is given [864] by Eq. (7.32) with

$$k_0 = 1 + (p - r) \left[ 1 + \frac{2m(1 - r)}{1 - p - r} \right] > 0. \quad (7.34)$$

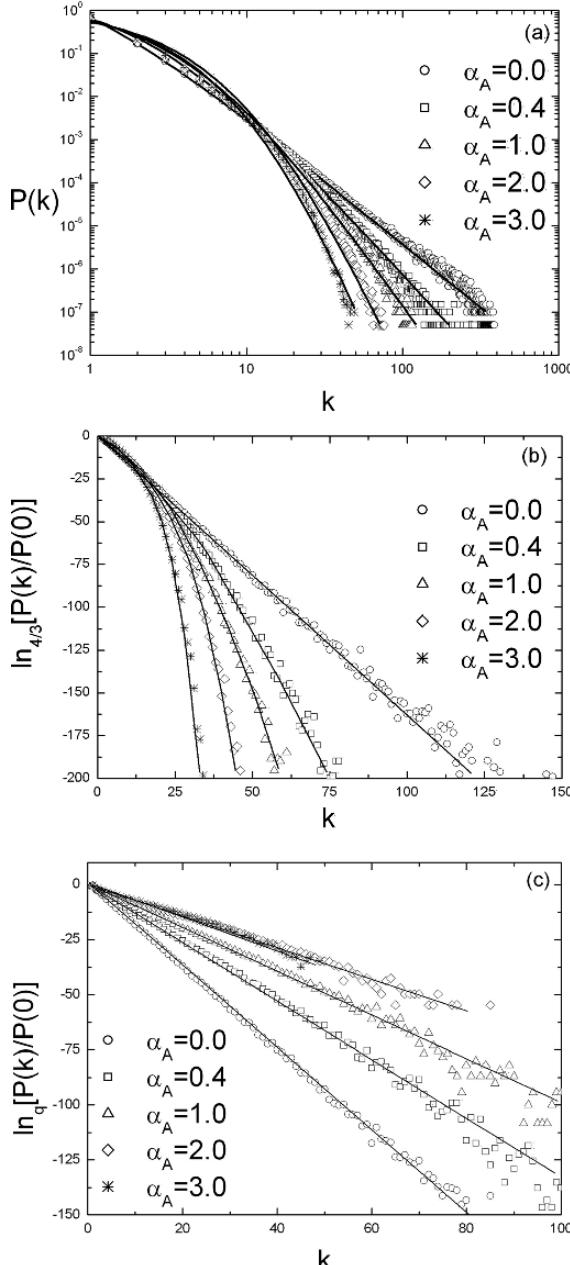
and

$$\mu = \frac{m(3 - 2r) + 1 - p - r}{m} > 0. \quad (7.35)$$

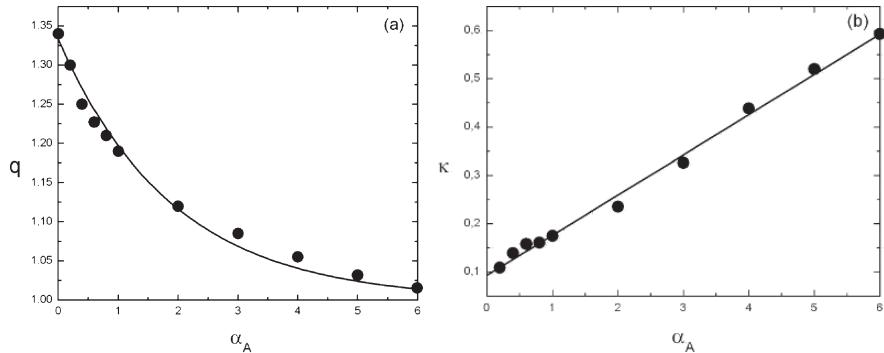
With the notation change (7.33), this degree distribution can be rewritten in the form of Eq. (7.31) with

$$q = \frac{2m(2 - r) + 1 - p - r}{m(3 - 2r) + 1 - p - r} \geq 1, \quad (7.36)$$

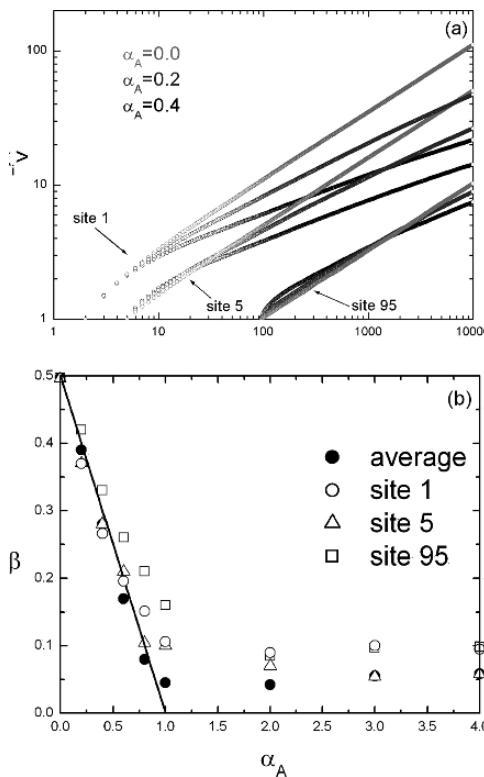
with  $\kappa > 0$  given by Eqs. (7.34) and (7.35) replaced into  $\kappa = k_0(q - 1)$ .



**Fig. 7.97** Connectivity distribution for typical values of  $\alpha_A$  (we have used  $\alpha_G = 2$  but we recall that this value is irrelevant). Points are our computer simulation results; continuous lines are the best fits with  $q$ -exponentials. (a)  $\log$ - $\log$  representation; (b)  $\ln_{4/3}$ -linear representation, with  $\ln_q x \equiv \frac{x^{1-q}-1}{1-q}$ ; (c)  $\ln_q$ -linear representation, where, for each value of  $\alpha_A$ , we have used its corresponding value of  $q$ . We have used three different representations to improve comprehension (from [790]).



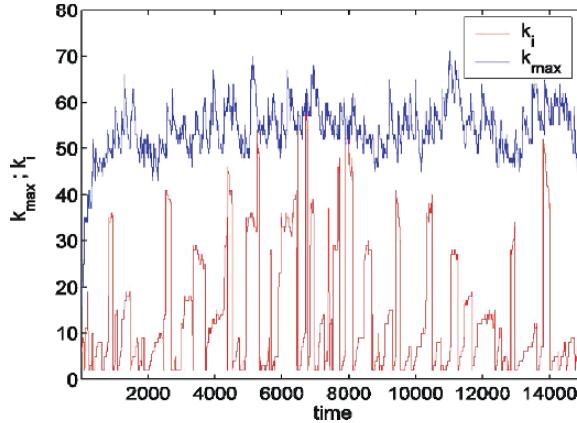
**Fig. 7.98** Values of  $q$  and  $\kappa$  used in the best fits indicated in Fig. 7.97. The (heuristic) solid curves are: (a)  $q = 1 + (1/3)e^{-0.526\alpha_A} (\forall \alpha_G)$ ; (b)  $\kappa \simeq 0.083 + 0.092\alpha_A (\forall \alpha_G)$  (from [790]).



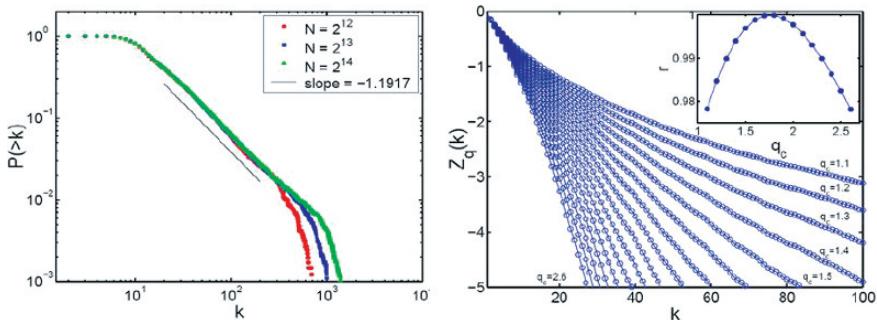
**Fig. 7.99** (a) Time dependence ( $t = N$ ) of the average number (over 2000 realizations) of links for typical values of  $\alpha_A$  for sites  $i = 1$ ,  $i = 5$ , and  $i = 95$  (compare with Fig. 2(c) of [863]). We have used  $\alpha_G = 2$ ; (b)  $\alpha_A$ -dependence of  $\beta$  (the straight line  $\beta = \frac{1}{2}(1 - \alpha_A)$  could be the exact answer) (from [790]).

### 7.8.3 Non-Growing Model

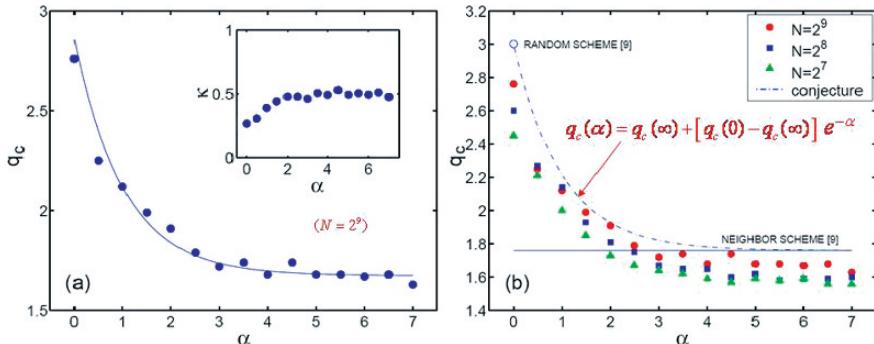
Scale-free networks without growth are known since long [865]. We focus here on a recent one [49], on which a  $q$ -exponential degree distribution has been numerically exhibited. See Figs. 7.100, 7.101, and 7.102.



**Fig. 7.100** A node collapsing (gas-like) model with a merging probability  $\propto 1/d_{ij}^\alpha$  ( $\alpha \geq 0$ ), where  $d_{ij}$  is the shortest topological distance between sites  $i$  and  $j$  on the network. We illustrate here the time evolution of the number of links of both the most important hub (blue) and of a typical node (red) of a network with  $N = 2^7 = 128$  nodes and  $\alpha = 0$ . In the present model the most linked hub maintains its “leadership” for ever (Figure following [49].).



**Fig. 7.101** Cumulative degree distribution of the same model as in Fig. 3 but for  $\alpha \rightarrow \infty$  and typical values of  $N$ , where the finite-size effects are visible. *Left:* log–log scale. *Right:* The same data in ( $q$ -log) – (linear) scale, for various values of  $q$ , the optimal value being  $q = 1.84$  [Inset: The  $q$ -dependance of the linear correlation  $r$ , which achieves its maximal value ( $r > 0.9999$ ) for  $q = 1.84$ ] (Figure following [49].).



**Fig. 7.102** Same model as in Figs. 3 and 4. *Left:*  $\alpha$ -dependance of the values of  $q$  and  $\kappa$  for the best  $q$ -exponential fitting of the numerical results for the  $N = 2^9$  network. *Right:* The same for the values of  $q$  for increasingly large networks. In the limits  $\alpha = 0$  and  $\alpha \rightarrow \infty$ , we recover the *random* and *neighbor* schemes of [51], respectively. The *dashed curve* corresponds to a possible heuristic analytical behavior (Figure following [49].).

#### 7.8.4 Lennard–Jones Cluster

Lennard–Jones small clusters (with  $N$  up to 14) have been numerically studied [866, 867]. The distributions of the number of local minima of the potential energy with  $k$  neighboring saddle-points in the configurational phase-space can be quite well fitted with  $q$ -exponentials with  $q = 2$ . No explanation is still available for this suggestive fact. Qualitatively speaking, however, the fact that we are talking of very *small* clusters makes that, despite the fact that the Lennard–Jones interaction is not a long-range one thermodynamically speaking (since  $\alpha/d = 6/3 > 1$ ), all the atoms sensibly “see” each other, therefore fulfilling roughly a nonextensive scenario. See Fig. 7.103. Most probably, a crossover to an extensive scenario might occur for increasingly large  $N$ .

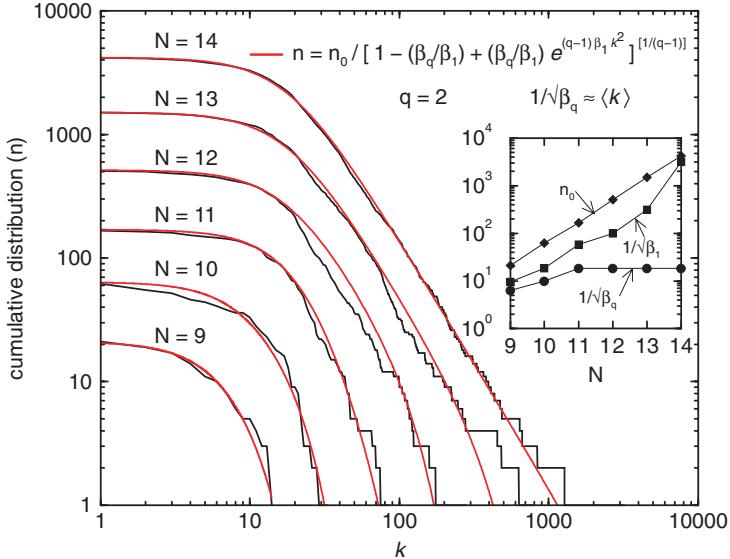
### 7.9 Linguistics

We briefly present here Zipf’s law and its generalizations. Some of the connections which exist with  $q$ -statistics are illustrated in Figs. 7.104, 7.105, and 7.106 from [791].

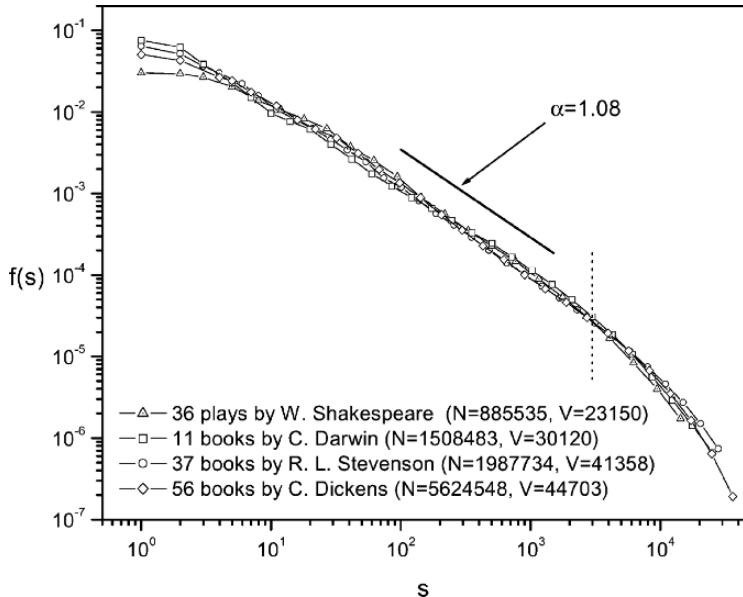
## 7.10 Other Sciences

### i. Citations

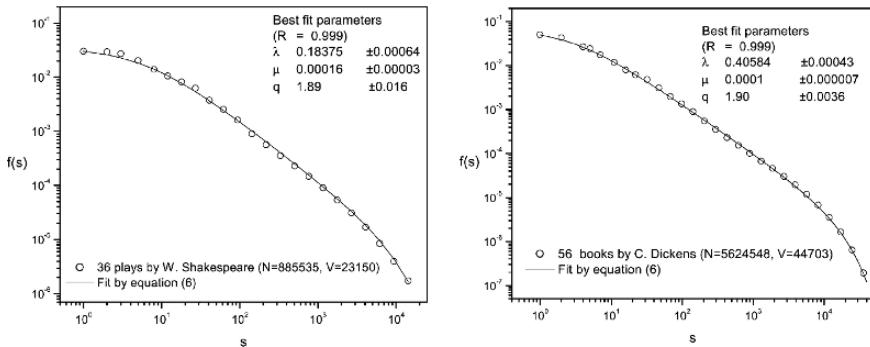
The statistical analysis of the citations of scientific papers has become possible thanks to internet research tools such as those implemented by ISI-Web of Science and Scopus/Elsevier. Some of these analyses [276, 278, 280, 796, 799]



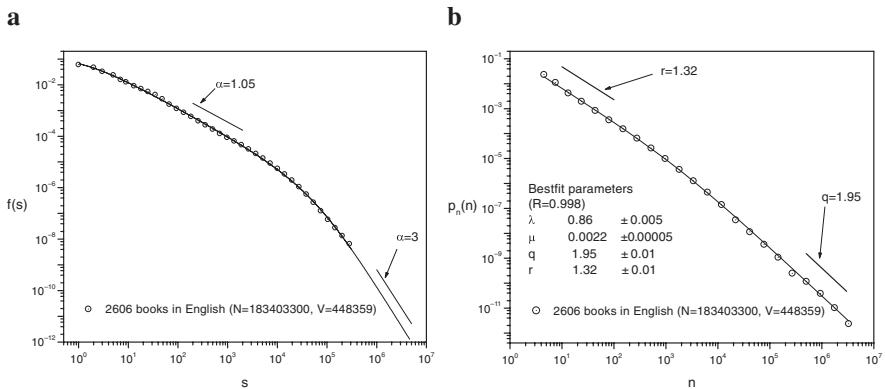
**Fig. 7.103** Degree distribution for Lennard-Jones clusters of  $N$  atoms. Black curves from [866, 867]. Red curves: fittings with the function indicated on the figure. Inset:  $N$ -dependence of the parameters of the fitting function.



**Fig. 7.104** Frequency-rank distribution of words for four large text samples. In order to reveal individual variations these corpora are built with literary works of four different authors, respectively (from [791]).



**Fig. 7.105** Frequency-rank distributions for corpus of Shakespeare and Dickens. The *solid lines* are fittings using Eq. (6.2) (from [791]).



**Fig. 7.106** Data from a corpus of 2606 books in English: frequency-rank distribution (*left*), and probability density function (*right*). The *solid lines* are fittings using crossover statistics: see details in [791].

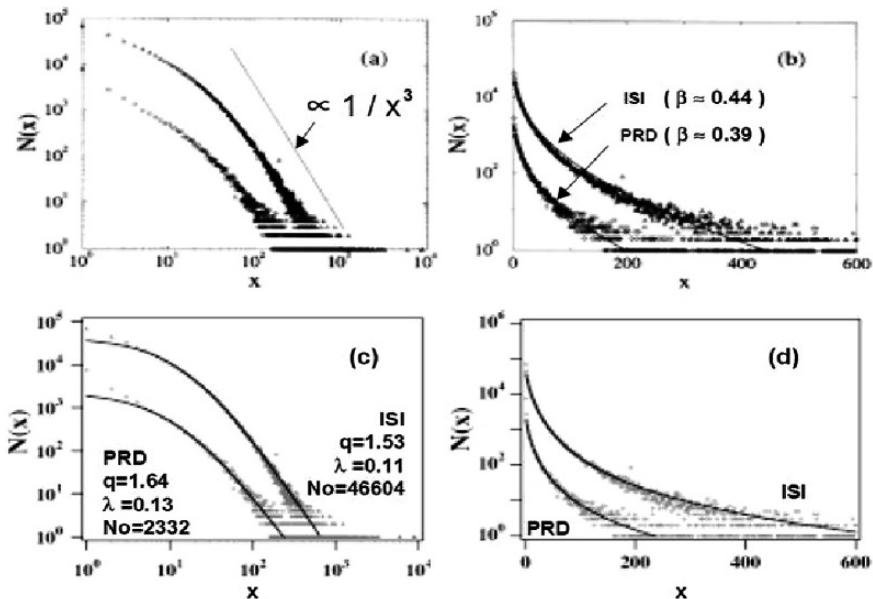
exhibit connections with nonextensive statistics. Illustrative results are shown in Figs. 7.107, 7.108, 7.109, and 7.110.

### ii. *Transportation*

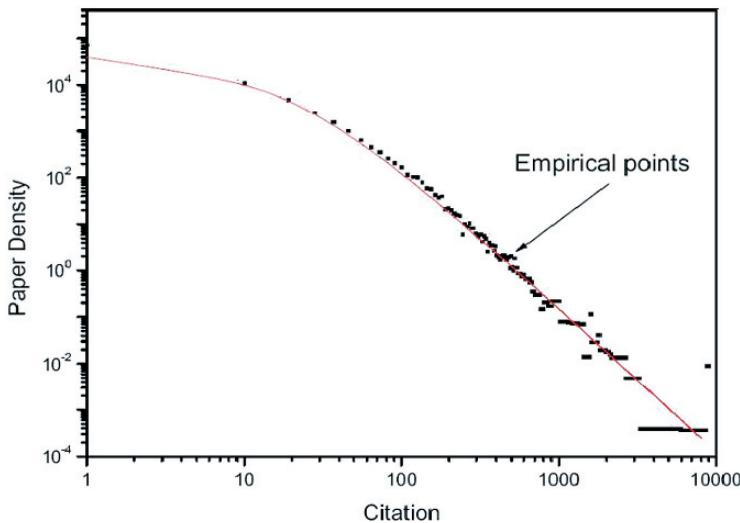
The train delays of the British railway network have been relatively well fitted by  $q$ -exponential forms [279]: see Fig. 7.111.

### iii. *Social sciences*

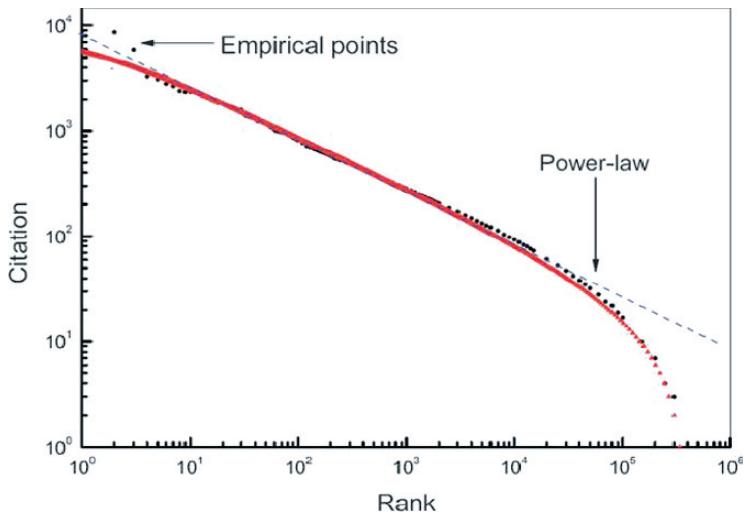
Many social phenomena have been addressed on grounds related to  $q$ -statistics, such as urban agglomerations [797], circulation of magazines and newspapers [798], football dynamics [800], among others. Some typical results are shown in Figs. 7.112 and 7.113. In the context of other sciences as well, such as musicology [281] and cognitive sciences [792–795], nonextensive concepts have been evoked.



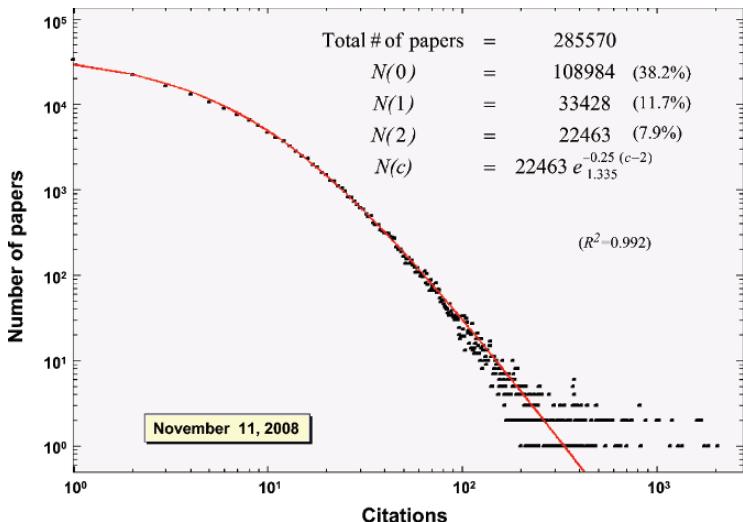
**Fig. 7.107** The same ISI and Physical Review D data (dots) are represented in the four panels. The two upper panels have been fitted with stretched exponentials [277], whereas the two lower ones have been fitted (with improved success) with  $q$ -exponentials (from [276]).



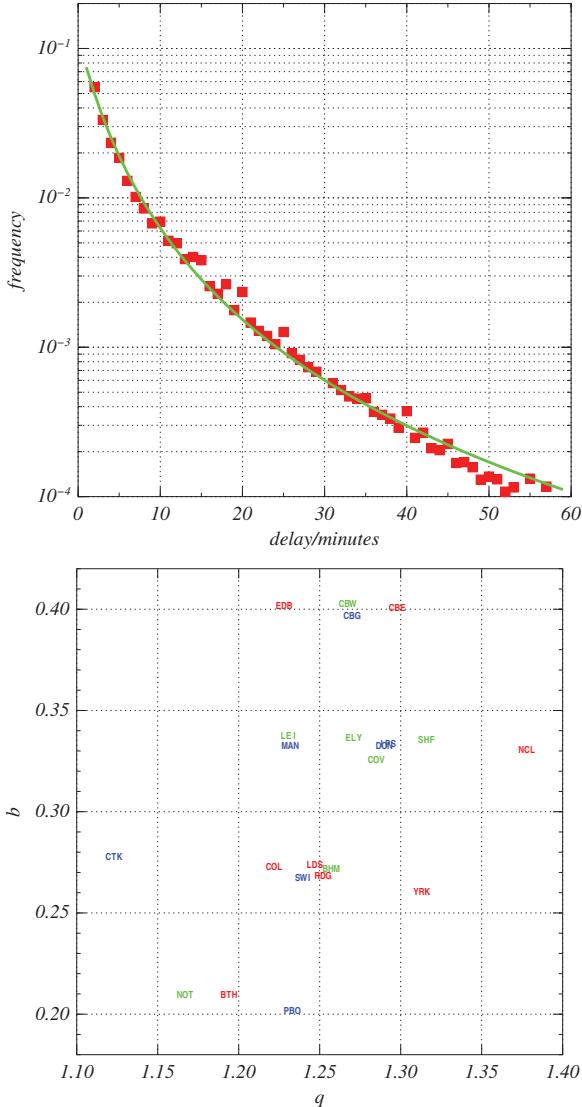
**Fig. 7.108** Publication density (publications per citation) vs. citation using 783,339 papers from the ISI data base. The *continuous line* is a fitting based on nonextensive-statistical-mechanical analytical expressions. See details in [278].



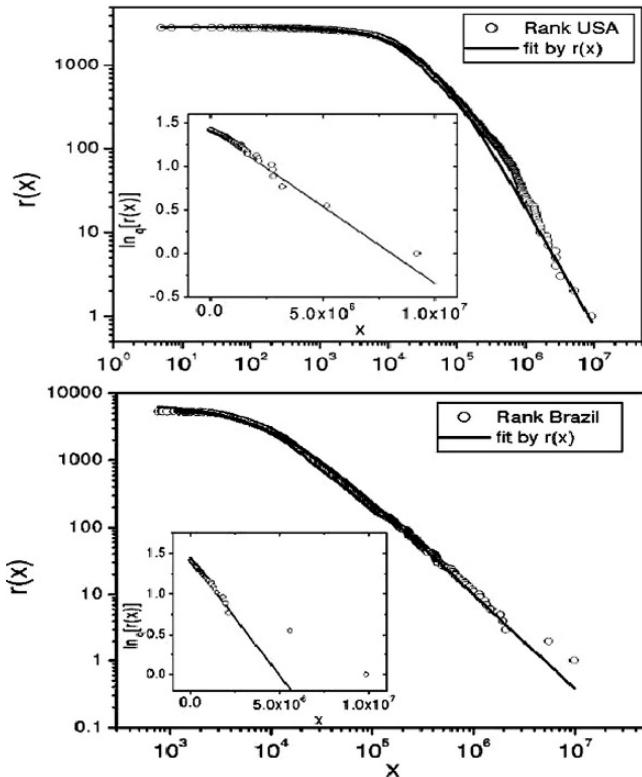
**Fig. 7.109** Zipf plot (number of citations of the  $n$ -th ranked paper) using the ISI data base. The continuous line is a fitting based on nonextensive-statistical-mechanical analytical expressions. The dashed line represents a power-law. See details in [278].



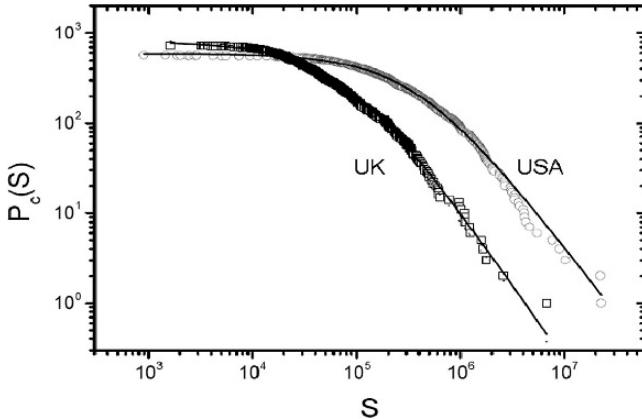
**Fig. 7.110** ISI citations of all papers ( $N(c)$ ) is the number of papers that have been cited  $c$  times involving at least one Brazilian institution (more precisely, having the word “Brazil” in the field “Address”), from 1945 on (from [796]).



**Fig. 7.111** *Top:* All train data and best-fit  $q$ -exponential  $frequency = c e_q^{-b t}$ , with  $q = 1.355 \pm 8.8 \times 10^{-5}$  and  $b = 0.524 \pm 2.5 \times 10^{-8}$  ( $c$  is a normalization factor). *Bottom:* The estimated pairs  $(q, b)$  for 23 stations (from [279]). Notice that we have here a *cloud* of points (and *not* a curve), kind of similarly to what was obtained in [773] for the *internet-quakes*.



**Fig. 7.112** Cumulative distributions for all cities in USA (top) and Brazil (bottom);  $x$  denotes the number of inhabitants. The *solid lines* are  $q$ -exponential fittings. Curiously enough, for both countries it has been found the same value for  $q$ , namely  $q = 1.7$ . Further details in [797].



**Fig. 7.113** Cumulative distributions for 570 USA magazines and 727 UK magazines in 2004,  $S$  denotes the circulation of the magazine. The *solid lines* are  $q$ -exponential fittings with  $q = 1.66$  for USA and  $q = 1.60$  for UK. Further details in [798].

**Part IV**  
**Last (But Not Least)**

# Chapter 8

## Final Comments and Perspectives

*I think it is safe to say that no one understands Quantum Mechanics*

Richard Feynman

### 8.1 Falsifiable Predictions and Conjectures, and Their Verifications

According to the deep epistemological observations of Karl Raimund Popper, a scientific theory cannot be considered as such if it is not capable of providing *falsifiable predictions*. This is to say predictions that *can* in principle be checked to be true or false. And a successful theory is of course that one which accumulates predictions that have been *verified to be correct*, and whose basic hypothesis has *not been proved to be violated* within the restricted domain of conditions for which the theory is thought to be applicable.

It is needless to say that nonextensive statistical mechanics cannot and must not escape to the necessity of satisfying such requirements. Although several such illustrations have already been presented in the body of this book, let us briefly and systematically list here some of the falsifiable predictions or conjectures of the theory, as well as their verification in recent years. This list is not exhaustive: for simplicity, I restrict here to those examples in which I have been, in one way or another, personally involved.

(a) *The scaling relation*  $\gamma = \frac{2}{3-q}$ .

Within the context of the nonlinear Fokker–Planck equation in the absence of external forces, and its exact  $q$ -Gaussian solution for all space-time  $(x, t)$ , it was analytically proved in 1996 [349] that  $x^2$  scales like  $t^\gamma$  with (Eq. (4.16))  $\gamma = \frac{2}{3-q}$  (hence, for instance, if  $\langle x^2 \rangle$  is finite, it must be  $\langle x^2 \rangle \propto t^{\frac{2}{3-q}}$ ). Through the perception of the crucial role that this equation plays in many complex systems addressed by nonextensive statistical mechanics, the rather generic applicability of this scaling relation was conjectured, and also illustrated, in 2004 [881]. Five verifications are available at the present date, namely in

- the experiments with *Hydra viridissima* reported in 2001 [774] (the measured value  $q = 1.5 \pm 0.05$  implies, through Eq. (4.16),  $\gamma = 1.33 \pm 0.05$ , which is consistent with the measured value  $\gamma = 1.24 \pm 0.1$ ; see Figs. 7.88 and 7.89);
- the experiments in defect turbulence reported in 2004 [427] (the measured value  $q \simeq 1.5$  implies, through Eq. (4.16),  $\gamma \simeq 1.33$ , which is consistent with the measured value  $\gamma = 1.16 - 1.50$ ; see Figs. 7.7, 7.8 and 7.9);
- the molecular dynamical simulations for the long-range classical inertial  $\alpha$ -*XY* ferromagnet reported in 2005 [41] ( $\gamma(3 - q)/2 = 1.0 \pm 0.1$ ; see also [820, 841], and Figs. 5.60 and 5.61);
- the computational simulations for silo drainage reported in 2007 [451, 452] ( $q \simeq 3/2$  and  $\gamma \simeq 4/3$ ; see Figs. 7.16 and 7.17);
- and the experiments with dusty plasma reported in 2008 [462] ( $\bar{\gamma}(3 - q)/2 = 1.00 \pm 0.016$ , where  $\bar{\gamma}$  is an averaged value; see Figs. 7.23, 7.24, 7.25 and 7.26).

In all but the molecular dynamics approach, the value for  $q$  was determined from the index of the  $q$ -Gaussian distribution of velocities. In the molecular dynamics case,  $q$  was determined from the time-relaxation of the velocity auto-correlation function. The precise relation (or even, perhaps, identity under some circumstances) of this  $q$  with that of the velocity distribution remains to be clarified.

(b)  *$q$ -Gaussian distributions of velocities of cold atoms in dissipative optical lattices*

Lutz predicted in 2003 [460] that the distribution of velocities of cold atoms in dissipative optical lattices should be  $q$ -Gaussian with  $q = 1 + \frac{44E_R}{U_0}$  (Eq. (7.1)). The prediction was checked in 2006 [461] through quantum Monte Carlo calculations, as well as through experiments with  $Cs$  atoms: see Fig. 7.1. The Monte Carlo calculations neatly confirmed both the  $q$ -Gaussian shape of the distribution (with a correlation factor  $R^2 = 0.995$ , and Lutz formula (Eq. (7.1)) within the range  $50 \leq U_0/E_R \leq 240$ . The laboratory experiments provided a laser-frequency dependence of  $q$  qualitatively the same as Lutz formula; the quantitative check would have demanded the direct measure of  $E_R$  and of  $U_0$ , which was out of the scope of the experiment. In what concerns the form of the distribution, the experiments verified the predicted  $q$ -Gaussian shape with  $R^2 = 0.9985$ , and obtained (in the illustration that is presented in [461])  $q = 1.38 \pm 0.12$  from the body of the distribution, and the consistent value  $q = 1.396 \pm 0.005$  from the tail of the distribution.

(c) *Generalized central limit theorem leading to stable  $q$ -Gaussian distributions*

The possible generalization of the standard and the Levy–Gnedenko Central Limit Theorems (CLT) was suggested in 2000 [826], and was then formally conjectured in 2004 [191]. Its proof started in 2006 [246], and was finally published in 2008 [247] (see also [252, 253]).

(d) *Existence of  $q$ ,  $\lambda_q$  and  $K_q$ , and the identity  $K_q = \lambda_q$*

It was argued in 1997 [127] that, whenever the Lyapunov exponent  $\lambda_1$  vanishes, (the upper bound of the) the sensitivity is given by  $\xi = e^{\lambda_{q_{sen}} t}$ , which determines a special value of  $q$ , noted  $q_{sen}$ . It was further argued that, at the edge of chaos,

$S_q(t)$  would increase *linearly* with  $t$  only for  $q = q_{sen}$ , and that the *slope* (entropy production per unit time) would satisfy  $K_{q_{sen}} = \lambda_{q_{sen}}$ , thus  $q$ -generalizing the  $q = 1$  Pesin-like identity  $K_1 = \lambda_1$ . This scenario was verified in various systems since 1997, and analytically proved since 2002: see [128–133, 139–142, 146, 147, 150, 153, 172, 358], among others.

(e) *Scaling with  $N^*$  for long-range-interacting systems*

An important class of two-body potentials  $V(r)$  in  $d$  dimensions consists in being smooth or integrable at short distances, and satisfying  $V(r) \sim -\frac{A}{r^\alpha}$  ( $A > 0; \alpha \geq 0$ ) at long distances. If the system is classical, such potentials are said *short-range-interacting* if  $\alpha/d > 1$ , and *long-range-interacting* if  $0 \leq \alpha/d \leq 1$  (see, for instance, Eq. (3.69)). The usual thermodynamical recipes address the short-range cases. Special scaling must be used in the long-range cases.

Since the successful verification done in 1995 [869] for ferro-fluids, it became natural to conjecture that, in order to have *finite* equations of states in the  $N \rightarrow \infty$  limit, it was necessary to divide by  $N^*$  (defined in Eq. (3.69)) quantities such as temperature, pressure, external magnetic field, chemical potential, etc., by  $N$  quantities such as volume, magnetization, entropy, number of particles, etc., and by  $NN^*$  quantities such as the internal energy and all the thermodynamical potentials. These prescriptions were verified since 1996 in many kinds of systems, such as Lennard–Jones-like fluids [870, 874], magnets [174, 175, 177, 871, 872, 875, 877], anomalous diffusion [873], and percolation [878, 879].

(f) *Vanishing Lyapunov spectrum for classical long-range-interacting many-body Hamiltonian systems*

It was first realized in 1977 [127] that the  $q$ -exponential functions emerge when the maximal Lyapunov exponent vanishes (see point (d) here above). It then became natural to conjecture that, in *any* anomalous stationary (or quasi-stationary) state, the Lyapunov spectrum should exhibit a generic tendency to approach zero at the  $N \rightarrow \infty$  limit for classical long-range-interacting Hamiltonian systems (whereas it is of course expected to be positive for short-range-interacting Hamiltonians). This was indeed verified, first in 1998 [177] for the  $\alpha$ - $XY$  ferromagnet (see Figs. 5.47 and 5.48), and since then in many other systems [178, 376–378] (see Figs. 5.49, 5.50, 5.51, and 5.52). In all these cases it was numerically verified that, in the  $N \gg 1$  limit, the Lyapunov spectrum vanishes for  $0 \leq \alpha/d \leq 1$ , and is nonzero for  $\alpha/d > 1$ .

(g) *Nonuniform convergence for long-range Hamiltonians associated with a divergent  $\lim_{N \rightarrow \infty} t_{\text{crossover}}(N)$*

It was conjectured in 1999 (see Fig. 4 in [63]) that classical long-range-interacting many-body systems could evolve, before attaining thermal equilibrium, through one (or more) nonequilibrium long-standing states. The departure from the longstanding states towards equilibration would occur (slowly, as indicated in Fig. 4, along something such as a logarithmic scale for time) at  $t_{\text{crossover}}(N)$ . Furthermore, it was conjectured that  $\lim_{N \rightarrow \infty} t_{\text{crossover}}(N) = \infty$ . Since 1999, the entire scenario was verified many times: see [45, 46, 373, 376–379, 820, 838–842], among others.

(h) *Existence of a  $q$ -triplet with  $q_{sen} < 1$ ,  $q_{rel} > 1$ , and  $q_{stat} > 1$*

It was conjectured in 2004 [880] that complex systems (of the nonextensive type) would exist exhibiting  $q$ -exponential behavior for the time dependence of the sensitivity to the initial conditions (with index  $q_{sen} < 1$ ), for the time dependence of the relaxation of relevant physical quantities towards the final stationary state (with index  $q_{rel} > 1$ ), and for the energy distribution at the stationary state (with index  $q_{stat} > 1$ ). In the Boltzmannian, thermal equilibrium, limit (corresponding to full mixing, and ergodicity) one would expect the collapse of this  $q$ -*triplet* (or  $q$ -*triangle*, as sometimes called) into  $q_{sen} = q_{rel} = q_{stat} = 1$ . This conjecture was indeed verified by Burlaga and Vinas in 2005 [361], through processing data sent to NASA by the Voyager 1, in the solar wind at the distant heliosphere, and also, more recently, in the heliosheath [362–364] (see also [365–368]). The Voyager 1 spacecraft was launched in 1977, over 30 years ago. It is therefore unreasonable to expect high precision results. This said, the values advanced by Burlaga and Vinas in 2005 [361] were  $(q_{sen}, q_{rel}, q_{stat}) = (-0.6 \pm 0.2, 3.8 \pm 0.3, 1.75 \pm 0.06)$ . Since only one of them is expected to be independent, one expects a priori two relations to exist between these three indices. Such relations were heuristically advanced in [199]. The outcome that was found is  $(q_{sen}, q_{rel}, q_{stat}) = (-1/2, 4, 7/4)$ , which, within the error bars, is consistent with the NASA results.

More recently, another  $q$ -triplet was completed, namely at the edge of chaos of the logistic map:  $(q_{sen}, q_{rel}, q_{stat}) = (0.24448..., 2.24978..., 1.65 \pm 0.05)$  (see [370, 371] and references therein). Although far from transparent, we have assumed here that the value of  $q$  corresponding to the  $q$ -Gaussian attractor (summing successive iterates) is to be identified with  $q_{stat}$ .

These and the NASA results together seem to indicate that perhaps the general scheme for the  $q$ -triplet is  $q_{sen} \leq 1 \leq q_{stat} \leq q_{rel}$ . A proof or clarifications would be welcome.

(i) *Degree distributions of the  $q$ -exponential type for scale-free networks*

The so-called scale-free networks (which are in fact only asymptotically scale-free) exhibit very frequently a degree distribution of the form  $k^\delta e_q^{-k/k_0}$  ( $q > 1; k_0 > 0$ ), with an exponent  $\delta$  than can be either zero or positive, or negative. This was first noticed in 2004 [803] with  $\delta = 0$ . The scale-invariance being a basic ingredient of nonextensive statistics (in particular in relation to the  $q$ -CLT), it was a kind of natural to expect that this  $q$ -exponential degree distribution would be something ubiquitous. Indeed, it has been so verified since 2005 in many models [49, 50, 52–54, 790]. However, it is yet elusive what motivates  $\delta$  to be zero or nonzero. Even its sign is presently an open question.

## 8.2 Frequently Asked Questions

As the history of sciences profusely shows to us, every possible substantial progress in the foundations of any science is accompanied by doubts and controversies. This

is a common and convenient mechanism for new ideas to be checked and better understood by the scientific community. Clearly, objections and critiques have frequently helped the progress of science. There is absolutely no reason to expect that statistical mechanics, and more specifically nonextensive statistical mechanics, would be out of such a process. Quite on the contrary – remember the words of Nicolis and Daems [2] that were cited in the Preface! – given the undeniable fact that entropy is one among the most subtle and rich concepts in physics. Some frequently asked points are addressed here. Indeed, we believe that some space dedicated here to such issues might well be useful at this stage (see also [803]).

This section only includes frequently asked questions, or critiques, the (basic) answer of which is believed to be known. Questions, frequent or not, whose answer is still a matter of research have been considered instead as “open questions,” and as such have been included in Section 8.3.

(a) *Finally, the entropy  $S_q$  is extensive or nonextensive?*

This question is incompletely posed. What can be simply answered is whether  $S_q$  is additive or not:  $S_1$  is *additive*, and  $S_q$  for  $q \neq 1$  is *nonadditive*. Extensivity is a more complex question. Indeed, the answer depends not only on the entropic functional but *also* on the system (more precisely, on the nature of the correlations between the elements of the system). If the elements have no correlation at all, or only local correlations, then typically  $S_1$  is *extensive* and  $S_q$  for  $q \neq 1$  is *not*. But if the correlations are nonlocal, then it can happen (e.g., the quantum magnetic chain analytically discussed in [201]) that  $S_q$  is *nonextensive* for all values of  $q$  (including  $q = 1$ ), *excepting a special value of  $q \neq 1$  for which  $S_q$  is extensive*.

(b) *If the entropic index  $q$  is chosen such that the entropy  $S_q$  is extensive, why this theory is named “nonextensive statistical mechanics?”*

This kind of mismatch has its historical roots on the fact that, during over one century of BG statistical mechanics, the entropy  $S_{BG}$ , known to be *additive*, was also *extensive* for all those systems (known today as *extensive systems*) for which the BG theory is plainly valid. This led imperceptibly to the abusive use of the words *additive* and *extensive* as practically synonyms. Later on, starting with the 1988 paper [39], the distinctive *nonadditivity property* (Eq. (3.21)) was wrongly, but frequently, referred to as the *nonextensivity property*. The expression *nonextensive statistical mechanics* was coined from there. When, many years later (see, for instance, the end of the Introduction of chapter I in [69]), this matter became gradually clear, the idea of course emerged to rather call this theory *nonadditive statistical mechanics*. But, on the other hand, the expression *nonextensive statistical mechanics* was already used in over one thousand papers. Furthermore, statistical mechanics has to do not only with *entropy* but also with *energy*. And the typical systems for which the present theory was devised are those involving long-range two-body interactions, for which the total energy is definitively *nonextensive*. The expression *nonextensive statistical mechanics* was therefore maintained. Nowadays, many authors call *nonextensive systems* those whose nonequilibrium stationary-state distribution (or similar properties, such as relaxation functions, and sensitivity to the

initial conditions) is of the  $q$ -exponential form, in contrast with *extensive systems*, which are therefore those whose stationary-state (thermal equilibrium) distribution (or similar properties) is of the usual BG exponential form. So, in extensive (BG) statistical mechanics, both the total energy and the total entropy are additive and extensive, whereas, in nonextensive statistical mechanics, the total energy is nonextensive but the total entropy is nonadditive and extensive! Regretfully it remains true that there was an inadvertence when the book [69] was named “Nonextensive Entropy” instead of “Nonadditive Entropy”!

(c) *How come ordinary differential equations play an important role in nonextensive statistical mechanics?*

Some remarks related to ordinary differential equations might surprise some readers, hence deserve a clarification. Indeed, in virtually all the textbooks of statistical mechanics, functions such as the energy distribution at thermal equilibrium are discussed *using a variational principle*, namely referring to the entropy functional, and *not using ordinary differential equations* and their solutions. In our opinion, it is so *not* because of some basic (and unknown) principle of exclusivity, but rather because the first-principle dynamical origin of the *BG* factor still remains, mathematically speaking, at the status of a *dogma* [34]. Indeed, as already mentioned, to the best of our knowledge, no theorem yet exists which establishes the necessary and sufficient *first-principles* conditions for being valid the use of the celebrated *BG* factor. Moreover, one must not forget that it was precisely through a differential equation that Planck heuristically found, as described in his famous October 1900 paper [312, 831],<sup>1</sup> the black-body radiation law. It was only in his equally famous December 1900 paper that he made the junction with the – at the time, quite controversial – Boltzmann factor by assuming the – at the time, totally bizarre – hypothesis of discretized energies.

A further point which deserves clarification is *why* have we *also* interpreted the linear ordinary differential equation in Section 5.5 as providing the typical time evolution of both the sensitivity to the initial conditions and the relaxation of relevant quantities. Although the bridging was initiated by Krylov [832], the situation still is far from completely clear on mathematical grounds. However, intuitively speaking, it seems quite natural to think that the sensitivity to the initial conditions is precisely what makes the system to relax to equilibrium, and therefore opens the door for the

<sup>1</sup> The celebrated equation in Planck’s 19 October 1900 paper is  $-(\frac{\partial^2 S}{\partial U^2})^{-1} = \alpha U + \beta U^2$  (where  $\alpha$  and  $\beta$  are constants), the heuristic interpolation between a term proportional to  $U$  and one proportional to  $U^2$ . By replacing in this equation the thermodynamic relation  $\frac{\partial S}{\partial U} = T^{-1}$ , one obtains  $\frac{\partial U}{\partial(1/T)} = -\alpha U - \beta U^2$ , which is precisely the  $q = 2$  particular case of the differential equation (6.1)! From the solution of this equation (see Eq. (6.2)), Planck readily arrived to his famous black-body radiation law  $u(v, T) = (av^3/c^3)/(e^{hv/T} - 1)$ . Two months later, in his 14 December 1900 paper, by incorporating a discretized energy within Boltzmann’s thermostatistical theory, he obtained the form which is used nowadays, namely  $u(v, T) = (8\pi v^2/c^3)hv/(e^{hv/kT} - 1)$  (where  $b$  was replaced by  $h/k$ ). The constant  $k$  (introduced and named *Boltzmann constant* by Planck) was the ratio between the gas constant  $R$  and the Avogadro number  $N$ ; the constant  $h$  was obtained by fitting the black-body experimental data available at the time.

$BG$  factor to be valid. In any case, although some of the statements in Section 5.4.4 are (yet) not proved, this by no means implies that they are generically false. Furthermore, they provide what we believe to be a powerful metaphor for generalizing the whole scheme into the nonlinear ordinary differential equations discussed in Section 3.1 (see also [804, 805]). Interestingly enough, the  $q$ -exponential functions thus obtained have indeed proved to be the correct answers for a sensible variety of specific situations reviewed in the present book, and this for *all three* interpretations – the  $q$ -triplet – as energy distribution for the stationary state, time evolution of the sensitivity to the initial conditions, and time evolution of basic relaxation functions.

(d) *Is it not possible to handle many-body long-range-interacting Hamiltonians just with BG statistical mechanics?*

Vollmayr-Lee and Luijten (VLL) presented in 2001 [806] a critique to nonextensive statistical mechanics. They consider a Kac-potential approach of nonintegrable interactions. They consider a  $d$ -dimensional classical fluid with two-body interactions exhibiting a hard core as well as an attractive potential proportional to  $r^{-\alpha}$  with  $0 \leq \alpha/d < 1$  (logarithmic dependence for  $\alpha/d = 1$ ; VLL use the notation  $\tau \equiv \alpha$ ). In their approach, they also include a Kac-like long-distance cutoff  $R$  such that no interactions exist for  $r > R$ , and then discuss the  $R \rightarrow \infty$  limit. They show that the exact solution within Boltzmann–Gibbs statistical mechanics is possible and that – no surprise (see VLL Ref. [12] and references therein) – it exhibits a mean field criticality. Moreover, the authors argue that very similar considerations hold for lattice gases,  $O(n)$  and Potts models.

VLL state “*Our findings imply that, contrary to some claims, Boltzmann–Gibbs statistics is sufficient for a standard description of this class of nonintegrable interactions.*”, and also that “*we show that nonintegrable interactions do not require the application of generalized  $q$ -statistics.*” In our opinion, these statements severely misguide the reader. The critique was rebutted in [803, 843], whose main points are summarized here. Indeed, the VLL discussion, along traditional lines, of their specific Kac-like model only exhibits that Boltzmann–Gibbs statistical mechanics is – as more than one century of brilliant successes guarantees! – *necessary* for calculating, *without doing time averages*, a variety of *thermal equilibrium* properties; by no means it proves that it is *sufficient*, as we shall soon clarify. Neither it proves that wider approaches such as, for instance, nonextensive statistical mechanics (VLL Refs. [6, 31] and present [39, 59, 60]), or any other similar formalism that might emerge, are not required or convenient. The crucial point concerns *time*, a word that nowhere appears in the VLL paper. The key role of  $t$  has been emphasized in several occasions, for instance in Fig. 4 of VLL Ref. [31]. For integrable or short-range interactions (i.e., for  $\alpha/d > 1$ ), we expect that the  $t \rightarrow \infty$  and  $N \rightarrow \infty$  limits are commutable in what concerns the equilibrium distribution  $p(E)$ ,  $E$  being the total energy level associated with the macroscopic system. More precisely, we expect naturally that (excepting for the possible presence in all these expressions of the density of states, which we are, for simplicity, skipping here)

$$p(E) \equiv \lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty} p(E; N; t) = \lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} p(E; N; t)$$

$$\propto \exp[-E/kT] \quad (\tau/d > 1) \quad (8.1)$$

if the system is in thermal equilibrium with a thermostat at temperature  $T$ . In contrast, the system is expected to behave in a more complex manner for nonintegrable (or long-range) interactions, i.e., for  $0 \leq \alpha/d \leq 1$ . In this case, no generic reason seems to exist for the  $t \rightarrow \infty$  and  $N \rightarrow \infty$  limits to be commutable, and consistently we expect the results to be not necessarily the same. The simplest of these results (which is in fact the one to be associated with the VLL paper, although therein these two relevant limits and their ordering are not mentioned) is, as we shall soon further comment,

$$\lim_{N \rightarrow \infty} \lim_{t \rightarrow \infty} p(E; N; t) \propto \exp[-(E/\tilde{N})/(kT/\tilde{N})]. \quad (8.2)$$

$\tilde{N} \equiv [N^{1-\alpha/d} - \alpha/d]/[1 - \alpha/d]$  has been introduced in order to stress that *generically* (see also [807])

- (i)  $E$  is *not* extensive, i.e., is *not* proportional to  $N$  but it is instead  $E(N) \propto N\tilde{N}$  [more precisely,  $E$  is extensive if  $\alpha/d > 1$  (see [97–99] and VLL Refs. [4, 5]), and it is nonextensive if  $0 \leq \alpha/d \leq 1$ ]; and
- (ii)  $T$  needs, in such calculation, to be rescaled (a feature which is frequently absorbed in the literature by artificially size-rescaling the coupling constants of the Hamiltonian), in order to guarantee nontrivial *finite* equations of states. Of course, for  $\alpha = 0$ , we have  $\tilde{N} = N$ , which recovers the traditional Mean Field scaling.

But, *depending on the initial conditions*, which determine the time evolution of the system if it is assumed isolated, quite *different* results can be obtained for the ordering  $\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty} p(E; N; t)$ . This fact has been profusely detected and stressed in the related literature (see, for instance, VLL Ref. [31], present Refs. [373, 376, 379, 820, 833, 837–842] and references therein). Unfortunately, this important fact has been missed in the VLL critique. Such metastable states can *by no means* be described within BG statistical mechanics. For example, the distribution of velocities is *not* Gaussian (even less the specific Gaussian which we commonly refer to as *Maxwellian*). Even more, as shown earlier in this book, there are nowadays increasing indications that they might be intimately related to nonextensive statistical mechanics. In any case, it is plain that, for such long-range Hamiltonians, BG statistics is necessary but not sufficient, in contrast with the VLL statements. In particular, since the time-average distribution of velocities along the QSS appears to be [45, 46] a  $q$ -Gaussian with  $q > 1$ , the BG distribution is highly inadequate (except of course if we are disposed to handle, through a series such as that of Eq. (A.19), an infinite number of BG-like terms!).

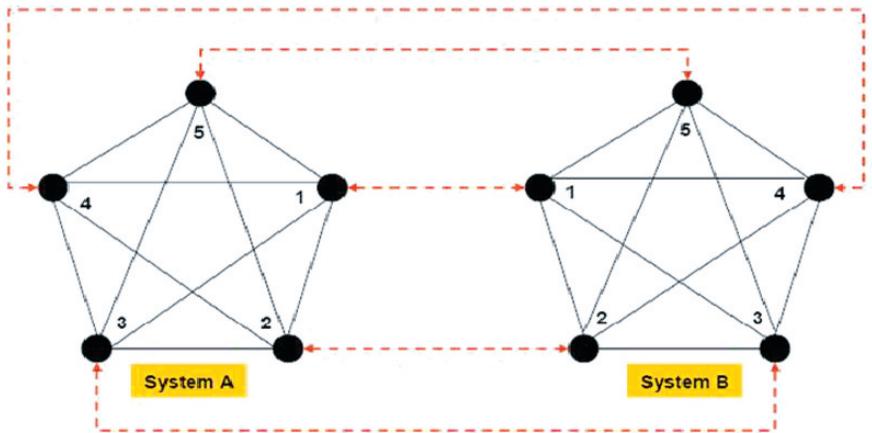
(e) *Is the zeroth principle of thermodynamics valid at the quasi-stationary states of long-range-interacting Hamiltonian systems, and in nonextensive statistical mechanics?*

This important question was raised up to me for the first time by Oscar Nassif de Mesquita [808]. The question concerns whether the zeroth principle of thermodynamics and thermometry are consistent with nonextensive statistical mechanics. Such questioning has already been addressed in a couple of dozens of papers that are available in the literature. It has been recently raised once again, this time by Nauenberg [809]. He concludes, among many other critiques, that it is not possible to have thermalization between systems with different values of  $q$ . It appears to be exactly the opposite which is *factually* shown in [810], where his critique is rebutted. One of the crucial points that is unfortunately missed in [809], concerns discussion of “weak coupling” in Hamiltonian systems. Indeed, if we call  $c$  the coupling constant associated with long range interactions (i.e.,  $0 \leq \alpha/d \leq 1$ ), we have that  $\lim_{N \rightarrow \infty} \lim_{c \rightarrow 0} c\tilde{N} = 0$ , whereas  $\lim_{c \rightarrow 0} \lim_{N \rightarrow \infty} c\tilde{N}$  diverges. No such anomaly exists for short-range interactions (i.e.,  $\alpha/d > 1$ ). Indeed, in this simpler case, we have that  $\lim_{N \rightarrow \infty} \lim_{c \rightarrow 0} c\tilde{N} = \lim_{c \rightarrow 0} \lim_{N \rightarrow \infty} c\tilde{N} = 0$ . The nonuniform convergence that, for long-range interactions, exists at this level possibly is related to the concomitant nonuniform convergence associated with the  $t \rightarrow \infty$  and  $N \rightarrow \infty$  limits discussed previously in this paper. These subtleties probably play an important role in the present question.

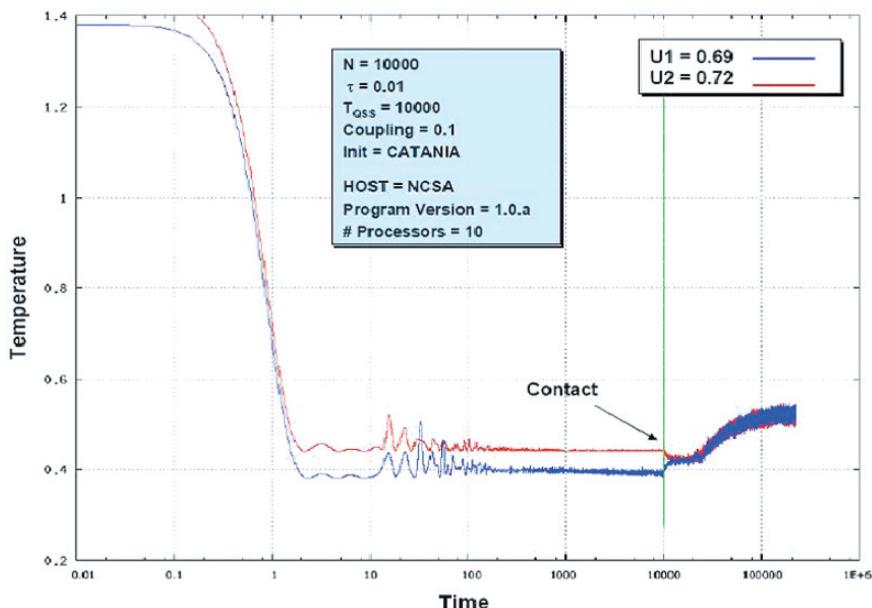
The strict verification of the zeroth principle of thermodynamics demands checking the transitivity of the concept of temperature through successive thermal contacts between three, initially disconnected systems,  $A$ ,  $B$ , and  $C$ . Such a study is in progress [811] for the paradigmatic HMF model (which corresponds to infinitely-long-range interactions). As a first step, two (equal) systems,  $A$  and  $B$ , are put into thermal contact. The Hamiltonian is given by (see Fig. 8.1)

$$\begin{aligned} \mathcal{H} = & \sum_{i=1}^N \frac{(L_i^A)^2}{2} + \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N [1 - \cos(\theta_i^A - \theta_j^A)] \\ & + \sum_{i=1}^N \frac{(L_i^B)^2}{2} + \frac{1}{N} \sum_{i=1}^N \sum_{j=1}^N [1 - \cos(\theta_i^B - \theta_j^B)] \\ & + l \sum_{k=1}^N [1 - \cos(\theta_k^A - \theta_k^B)]. \end{aligned} \quad (8.3)$$

As we see, there are long-range interactions within system  $A$  and within system  $B$ , but only short-range interactions connecting systems  $A$  and  $B$  through the coupling constant  $l$ . See in Fig. 8.2 the time evolution of the temperatures of  $A$  and  $B$ . We verify that, after the thermal contact being established, the two temperatures merge into an intermediate one, as they would do if they were at thermal equilibrium... *but they are not!* Indeed, those are quasi-stationary states. Only later, the two systems go together towards thermal equilibrium. A discussion such as the present



**Fig. 8.1** Systems *A* and *B* that will be put in thermal contact at a certain moment by allowing the coupling constant  $l$  to become different from zero (see Eq. (8.4)). Here  $N = 5$  (from [811]).



**Fig. 8.2** Time evolution of the temperatures of *A* and *B*. The initial conditions are water bag for both *A* and *B*, at slightly different initial internal energies, hence slightly different initial temperatures. Here  $N = 10,000$ , and  $l$  is taken zero until the moment indicated with a green vertical line, and  $l = 0.1$  after that moment (from [811]).

one, but involving three instead of two systems, is expected to be able to illustrate the possible validity of the zeroth principle for anomalous systems such as the HMF one.

(f) *Does the quasi-stationary state in long-range-interacting Hamiltonians really exist?*

A re-analysis was done by Zanette and Montemurro [819] of the molecular dynamics approach and results presented in [373] for the infinitely-long-range interacting planar rotators already discussed here. They especially focus on the time dependence of the temperature  $T(t)$  defined as the mean kinetic energy per particle. For total energy slightly below the second-order critical point and a non-zero-measure class of initial conditions, a long-standing nonequilibrium state emerges before the system achieves the terminal BG thermal equilibrium. When  $T$  vs.s  $\log t$  is plotted, an inflection point exists. If we call  $t_{\text{crossover}}$  the value of  $t$  at which the inflection point is located, it has been repeatedly verified numerically by various authors, including Zanette and Montemurro [819], that  $\lim_{N \rightarrow \infty} t_{\text{crossover}}(N)$  diverges. Therefore, if the system is very large (in the limit  $N \rightarrow \infty$ , mathematically speaking) it remains virtually for ever in the anomalous state, currently called *quasi-stationary state* or *metastable state*. Zanette and Montemurro point out (correctly) that, if a linear scale is used for  $t$ , the inflection point disappears.<sup>2</sup> For increasingly large  $N$ ,  $T(t)$  remains constant, and *different from the BG value*, within a quite small error bar. This effect appears in an even more pronounced way because of a slight minimum that  $T(t)$  presents just before going up to the BG value. This intriguing minimum had already been observed in [373], and has been detected with higher precision in [819]. Further details are presented in [820]. It remains nevertheless a fact that the nature of this quasi-stationary state is quite unusual (with aging and other indications of glassy-like dynamics [821–824]), and surely deserves further studies.

(g) *Are the  $q$ -exponential distributions compatible with the central limit theorems which only allow, in the thermodynamic limit, for Gaussian and Lévy distributions?*

This interesting issue has been raised in several occasions by several people. For example, soon after their previous critique, Zanette and Montemurro advanced a second one [825] objecting the validity of nonextensive statistical mechanics for thermodynamical systems. This line of critique addresses the possibility of the ubiquity of the  $q$ -exponential form as a stable law in nature. The argument essentially goes that only Gaussians and Lévy distributions would be admissible, because of the

<sup>2</sup> From this, these authors conclude that this well-known metastable state is but a kind of mathematical artifact, and no physically relevant quasi-stationarity exists. Such an argument is mathematically similar to stating that the high-to-low energies crossing occurring, at a given temperature, in Fermi–Dirac statistics would have no physical meaning! Indeed, if instead of using the linear scale for the energies we were to use a faster scale (e.g., an exponential scale), the well-known inflection point would disappear. Nevertheless, there is no point to conclude from this that the textbook crossing in Fermi–Dirac statistics is but a mathematical artifact. In fact, *any* inflection point on *any* curve will disappear by sufficiently “accelerating” the abscissa. The crossover will obviously remain.

respective central limit theorems. Such question has been preliminarily addressed long ago in [826], and once again in [585] as a rebuttal to [825]. The answer basically reminds that the stability observed in the usual central limit theorems is intimately related to the hypothesis of independence (or quasi-independence) of the random variables that are being composed. If important global correlations are present even in the  $N \rightarrow \infty$  limit, different central limit theorems are applicable, as proved in [247–249, 251–253]. Under these circumstances, stable distributions differing from Gaussians and Levy ones are to be expected in nature.

(h) *Is entropy  $S_q$  “physical”?*

Another question (or line of critique) that might emerge concerns the “physicality” of  $S_q$  (see [812]). Or whether it could exist a “physical” entropy different from  $S_{BG}$ . Since such issues appear to be of a rather discursive/philosophical nature, we prefer to put these critiques on slightly different, more objective, grounds. We prefer to ask, for instance, (i) whether  $S_q$  is useful in theoretical physics in a sense similar to that in which  $S_{BG}$  undoubtedly is useful; (ii) whether  $q$  necessarily is a fitting parameter, or whether it can be determined a priori, as it should if we wish the present theory to be a complete one; (iii) whether there is no other way of addressing the thermal physics of the anomalous systems addressed here, very specifically whether one could not do so by just using  $S_{BG}$ ; (iv) whether  $S_q$  is special in some physical sense, or whether it is to be put on the same grounds as the thirty or forty entropic functionals popular in cybernetics, control theory, and information theory—generally speaking.

Such questions have received answers in [150, 813–818] and elsewhere. (i) The usefulness of this theory seems to be answered by the large amount of applications it has already received, and by the ubiquity of the  $q$ -exponential form in nature. (ii) The a priori calculation of  $q$  from microscopic dynamics has been specifically illustrated in Chapter 5 (see also point (m) here below). (iii) The optimization of  $S_q$ , as well as of almost any other entropic form, with a few constraints has been shown in [814] to be equivalent to the optimization of  $S_{BG}$  with an infinite number of appropriately chosen constraints. Therefore, we could in principle restrain to the exclusive use of  $S_{BG}$ . If we followed that line, we would be doing like a hypothetical classical astronomer who, instead of using the extremely convenient Keplerian elliptic form for the planetary orbits, would (equivalently) use an infinite number of Ptolemaic epicycles. Obviously, it is appreciably much simpler to characterize, whenever possible, a complex structure of constraints with a single index  $q \neq 1$  (in analogy with the fact that the ellipticity of a Keplerian orbit can be simply specified by a single parameter, namely the eccentricity of the ellipse). (iv) The entropy  $S_q$  shares with  $S_{BG}$  an impressive set of important properties (see also point (j) here below), which includes, among others, concavity, extensivity, Lesche-stability, and finiteness of the entropy production per unit time,  $\forall q > 0$ . The difficulty of simultaneously satisfying all these four properties can be illustrated by the fact that the (additive) Renyi entropy (usefully used in the geometric characterization of multifractals) satisfies, under the hypothesis of probabilistic independence or quasi-independence (and only then), extensivity  $\forall q$ , and *none* of the other three

properties for all  $q > 0$ . Such features point  $S_q$  as being very special, although probably not unique, for thermostatistical purposes.

(i) *By adjusting the constraints under which the entropy optimization is done, one can obtain virtually any desired distribution. Is that not a serious problem?*

Soon after their second critique, Zanette and Montemurro advanced a third one [827]. This time the objection addresses nonthermodynamical systems, in contrast to the previous critiques which mainly addressed thermodynamical ones. It is argued by these authors that nonthermodynamical applications of nonextensive statistics are ill-defined, essentially because of the fact that *any* probability distribution can be obtained from the nonadditive entropy  $S_q$  by conveniently adjusting the constraint used in the optimization. We argue here that, since it is well known to be so for *any* entropic form and, in particular, for the (additive) Boltzmann–Gibbs entropy  $S_{BG}$  (see [828]), the critique brings absolutely no novelty to the area. In other words, it has *nothing* special to do with the entropy  $S_q$ . In defense of the usual simple constraints, typically averages of the random variable  $x_i$  or of  $x_i^2$  (where  $x_i$  is to be identified according to the nature of the system), we argue, *and this for all entropic forms*, that they can hardly be considered as arbitrary, as Zanette and Montemurro seem to consider. Indeed, once the natural variables of the system have been identified (e.g., constants of motion of the system), the variable itself and, in some occasions, its square obviously are the most basic quantities to be constrained. Such constraints are used in hundreds (perhaps thousands) of useful applications outside (and also inside) thermodynamical systems, along the information theory lines of Jaynes and Shannon, and more recently of A. Plastino and others. And this is so for  $S_{BG}$ ,  $S_q$ , and any other entropic form. If, however, other quantities are constrained (e.g., an average of  $x^\sigma$  or of  $|x|^\sigma$ ) for specific applications, it is clear that, at the present state-of-the-art of information theory, *and for all entropic forms*, this must be discussed case by case. Rebuttals of this critique can be found in [803, 829].

As a final comment let us mention that statistical mechanics is much more than just a stationary-state (e.g., thermal equilibrium) distribution. Indeed, under exactly the same constraints, the optimization of  $S_{BG}$  and  $(S_{BG})^3$  yield precisely the same distribution. This is obviously not a sufficient reason for using  $(S_{BG})^3$ , instead of  $S_{BG}$ , in a thermostatistical theory which must also satisfy thermodynamical requirements.

(j) *What properties are common to  $S_{BG}$  and  $S_q$ ?*

The additive entropy  $S_{BG}$  and the nonadditive entropy  $S_q$  share a huge amount of mathematical properties. These include nonnegativity, expansibility ( $\forall q > 0$ ), optimality for equal probabilities, concavity ( $\forall q > 0$ ), extensivity, Lesche-stability (or experimental robustness) ( $\forall q > 0$ ), finiteness of the entropy production per unit time, existence of partition function depending only on temperature, composability, the Topsøe factorizability property [830] ( $\forall q > 0$ ), the mathematical relationship of the Helmholtz free energy with the partition function is the same as the microscopic energies with their probabilities, the function (namely  $\ln_q x$ ) which (through a stan-

dard probabilistic mean value) defines the entropy is precisely the inverse of the function (namely  $e_q^x$ ) which provides the energy distribution at the stationary state. We are unaware of the existence of *any* other entropic functional form having all these properties in common with  $S_{BG}$ .

Let us stress, at this point, that a property that  $S_{BG}$  and  $S_q$  do *not* share is additivity. This difference is extremely welcome. It is precisely this fact which makes possible for *both* entropies to be *thermodynamically extensive* for a special value of  $q$ , more specifically  $q = 1$  for extensive systems (i.e., those whose correlations are generically short-ranged), and  $q < 1$  for nonextensive ones (i.e., a large class among those whose correlations are generically long-ranged).

(k) *Is nonextensive statistical mechanics necessary or just convenient?*

Let us first address a somewhat simpler question, namely: *Is Boltzmann–Gibbs statistical mechanics necessary or just convenient?* The most *microscopic* level at which collective properties of a system can be answered is that of *mechanics* (classical, quantum, or any other that might be appropriate for the case). Let us illustrate this with classical Hamiltonian systems. Let us consider a system constituted of  $N$  well-defined interacting particles. Its time evolution is fully determined by the initial conditions. So, for every admissible set of initial conditions we have a point evolving along a unique trajectory in the *full phase-space*  $\Gamma$ . We can in principle calculate all its mechanical properties, its time averages, its ensemble averages (over well-defined sets of initial conditions). For example, its time-dependent “temperature” can be defined as being proportional to the average total kinetic energy of  $N$  particles divided by  $N$ . If we wish to approach a more thermodynamical definition of temperature, we might wish to consider the average of this quantity over an ensemble of initial conditions. This ensemble can be uniformly distributed over the entire  $\Gamma$  space, or be as special or particular as we wish. Of course, in practice, this road is almost always analytically untractable; moreover, it quickly becomes computationally untractable as well when  $N$  increases above some number... well below the Avogadro number!

Another approach, which is not so powerful but surely is more tractable (both analytically and computationally), consists in considering the projection of the  $\Gamma$  into the *single-particle phase-space*  $\mu$ , where the coordinates and momenta of only one particle are taken into account. In other words, we might be interested in discussing only those properties that are well defined in terms of the single-particle marginal probabilities. Such is the case of the *Vlasov equation* (see, for instance, [299]), and analogous approaches such as the *Boltzmann transport equation* itself. These procedures are expected to be very useful whenever mixing and ergodic hypothesis are (strictly or nearly) verified in  $\Gamma$  space. This surely is the case of almost all Hamiltonian systems whose many elements interact through a potential which is nowhere singular, and which decays quickly enough at long distances. In other cases, the situation might be more complex. For example, such an approach is not expected to be very reliable if the microscopic dynamics are such that structures (e.g., hierarchical ones) emerge in  $\Gamma$  space, which might or might not reflect into

nontrivial structures in the  $\mu$  space itself.<sup>3</sup> This could be the case if the interactions decay very slowly with distance, at least for various classes of initial conditions.

A third possible approach is that of *stochastic equations*. The paradigm of such a level of description is the *Langevin equation*. One particle is selected (and followed) from the entire system, and part of the action of all the others is seen as a noise, typically a white Gaussian-like one. Such a description has the advantage of being relatively simple. It has however the considerable disadvantage of being partially phenomenological, in the sense that one has to introduce quite ad hoc types of noises. If we are not interested in following the possible trajectories of a single particle, but rather in the time evolution of probability distributions associated with such particles, we enter into the level of description of the *Fokker–Planck equation*, and the alike. At this *mesoscopic level*, exact analytical calculations, or relatively easy numerical ones, are relatively frequent.

A fourth possible approach is that of *statistical mechanics*. It directly connects – and this is where its beauty and power come from – the relevant microscopic information contained, for instance, in the Hamiltonian (with appropriate boundary conditions), to useful macroscopic quantities such as equations of states, specific heats, susceptibilities, and even various important correlation functions. In some epistemological sense, it superseeds all the previous types of approaches, excepting the fully microscopic one *with which it should always be consistent*. This last point is kind of trivial since statistical mechanics is nothing but a “shortcuted path” from the microscopic world to the macroscopic one. Let us precisely qualify the sense in which statistical mechanics “superseeds” other approaches such as those of Vlasov, Langevin, and Fokker–Planck. We mean that, whenever the collective states (usually at thermal equilibrium) and the quantities that are being calculated are *exactly the same*, no admissible mesoscopic description could be inconsistent with the statistical mechanical one.

A fifth possible approach is that of *thermodynamics*. It directly connects many types of *macroscopic* quantities with sensible simplicity. However, it is incapable of calculating from first principles quantities such as specific heats, susceptibilities, among many others. One expects, of course, that the results and connections obtained at the thermodynamical level will be consistent with those obtained at any of the previous levels, whenever comparison is justified and possible.

After this brief overview, it becomes kind of trivial to answer *part* of our initial question. Indeed, statistical mechanics is *not necessary*, but it can be extremely *convenient*; also, it provides an *unifying description* of a great variety of useful questions. A point which remains to be answered is the following one. Given the fact that we *do* have – since more than one century – *BG* statistical mechanics, *do we need, or is it convenient, a more general one?* We can say that it is *not necessary* in the very same sense that, as we saw above, *BG* statistical mechanics is *not necessary* either. Is it convenient? We may say that, whenever possible,

<sup>3</sup> Nontrivial structures in  $\mu$  space imply nontrivial ones in  $\Gamma$  space. The other way around is not true: structures could exist in  $\Gamma$  space which would not be seen in  $\mu$  space (the “shadow” of a fractal sponge on a wall can be a quite smooth surface).

it is so in the same sense that the *BG* theory is convenient. The next point that has to be addressed in order to satisfactorily handle our initial question follows. Assuming that – because of its convenience and unifying power – we indeed want to make, whenever possible, a statistical mechanical approach of a given problem, *do we need a generalization of the BG theory?* The answer is *yes*. For instance, quasi-stationary and other intermediate states are known to exist for long-range interacting classical Hamiltonian systems whose one-particle velocity distributions (both ensemble-averaged and time-averaged) are *not* Gaussians. This *excludes* the exponential form of the *BG* distribution law for the stationary state. Indeed, the marginal probability for the one-particle velocities derived from an exponential of the total Hamiltonian *necessarily is Gaussian*. Therefore, we definitively need something more general, if it can be formulated. Nonextensive statistical mechanics (as well as its variations such as the Beck–Cohen superstatistics, and others) appears to be at the present time a strong operational paradigm. And this is so because of a variety of reasons which include the following inter-related facts: (i) Many of the functions that emerge in long-range interacting systems are known to be precisely of the  $q$ -exponential form; (ii) The entropy  $S_q$  is consistent with nonergodic (and/or slowly mixing) occupancy of the  $\Gamma$  space; (iii) The entropy  $S_q$  is, in many nonlinear dynamical systems, appropriate when the system is weakly chaotic (vanishing maximal Lyapunov exponent); (iv) In the presence of long-range interactions, the elements of the system tend to evolve in a rather synchronized manner, which makes virtually impossible an exponential divergence of nearby trajectories in  $\Gamma$  space: this prevents the system from quick mixing, and, in some cases, violates ergodicity, one of the pillars of the *BG* theory; (v) The central limit theorem, on which the *BG* theory is based, has been generalized in the presence of a (apparently large) class of global correlations, and the  $N \rightarrow \infty$  basic attractors are  $q$ -Gaussians (see, for instance, [45, 46, 370, 371]); (vi) The block entropy  $S_q$  of paradigmatic Hamiltonian systems in quantum entangled collective states is extensive only for a special value of  $q$  which differs from unity (see [201, 202]).

(I) *Why do we need to use escort distributions and  $q$ -expectation values instead of the ordinary ones?*

The essential mathematical reason for this can be seen in the set of Eq. (4.81) and the following ones, and is based on connections that have been shown recently [258]. When we are dealing with distributions that decay quickly at infinity (e.g., an exponential decay), then their characterization can be done with standard averages (e.g., first and second moments). This is the typical case within BG statistical mechanics, and such moments precisely are the constraints that are normally imposed for the extremization of the entropy  $S_{BG}$ . But if we are dealing with distributions that decay slowly at infinity (e.g., power-law decay), the usual characterization becomes inadmissible since all the moments above a given one (which depends on the asymptotic behavior of the distribution) diverge. The characterization can, however, be done with mathematically well-defined quantities by using  $q$ -expectation values (i.e., with escort distributions). This is the typical case within nonextensive statistical mechanics.

Let us illustrate with the  $q = 2$   $q$ -Gaussian (i.e., the Cauchy–Lorentz distribution)  $p_2(x) \propto 1/(1 + \beta x^2)$ . Its width is characterized by  $1/\sqrt{\beta}$ . However, its second moment diverges. At variance, its  $q = 2$   $q$ -expectation value is finite and given by  $\langle x^2 \rangle_q \propto 1/\beta$ . This is therefore a natural constraint to be used for extremizing the entropy  $S_q$ .

Further arguments yielding consistently the escort distributions as the appropriate ones for expressing the constraints under which the entropy  $S_q$  is to be extremized can be found in [259, 803], and in Appendix B.

(m) *Is it  $q$  just a fitting parameter? Does it characterize universality classes?*

From a first-principle standpoint, the basic universal constants of contemporary physics, namely  $c$ ,  $h$ ,  $G$ , and  $k_B$ , are fitting parameters, but  $q$  is not. The indices  $q$  are in principle determined a priori from the microscopic or mesoscopic dynamics of the system. Very many examples illustrate this fact. However, when the micro- or meso-scopic dynamics are unknown (which is virtually always the case in real, empirical systems), or when, even if known, the problem turns out to be mathematically untractable (also this case is quite frequent), then and only then  $q$  is to be handled, *faute de mieux*, as a fitting parameter.

To make this point clear cut, let us remind here a nonexhaustive list of examples in which  $q$  is analytically known in terms of microscopic or mesoscopic quantities, or similar indices:

Standard critical phenomena at finite critical temperature:  $q = \frac{1+\delta}{2}$  (see Eq. (5.58));

Zero temperature critical phenomena of quantum entangled systems:  $q = \frac{\sqrt{9+c^2}-3}{c}$  (see Eq. (3.145));

Lattice Lotka–Volterra models:  $q = 1 - \frac{1}{D}$  (see Eq. (7.22));

Boltzmann lattice models:  $q = 1 - \frac{2}{D}$  (see Eq. (7.4));

Probabilistic correlated models with cutoff:  $q = 1 - \frac{1}{d}$  (see Eq. (3.137));

Probabilistic correlated models without cutoff:  $q = \frac{v-2}{v-1}$  (see Eq. (4.67));

Unimodal maps:  $\frac{1}{1-q} = \frac{1}{\alpha_{min}} - \frac{1}{\alpha_{max}}$  (see Eq. (5.9));

The particular case of the  $z$ -logistic family of maps:  $\frac{1}{1-q(z)} = (z-1)\frac{\ln \alpha_F(z)}{\ln b}$  (see Eq. (5.11));

The  $z = 2$  particular case of the  $z$ -logistic maps:  $q = 0.244487701341282066198$  .... (see Eq. (5.13));

Scale-free networks:  $q = \frac{2m(2-r)+1-p-r}{m(3-2r)+1-p-r}$  (see Eq. (7.36));

Nonlinear Fokker–Planck equation:  $q = 2 - \nu$  (see Eq. (4.10)), and  $q = 3 - \frac{2}{\mu}$  (see Eq. (4.16));

Langevin equation including multiplicative noise:  $q = \frac{\tau+3M}{\tau+M}$  (see Eq. (4.107));

Langevin equation including colored symmetric dichotomous noise:  $q = \frac{1-2\gamma/\lambda}{1-\gamma/\lambda}$  (see Eq. (4.109));

Ginzburg–Landau discussion of point kinetics for  $n = d$  ferromagnets:  $q = \frac{d+4}{d+2}$  (see Eq. (4.111));

The  $q$ -generalized central limit theorems:  $q_{\alpha,n} = \frac{(2+\alpha)q_{\alpha,n+2}-2}{2q_{\alpha,n+2}+\alpha-2}$  (see Eq. (4.91)).

Further analytical expressions for  $q$  in a variety of other physical systems are presented in [232]. See also [A.B. Adib, A.A. Moreira, J.S. Andrade Jr. and M.P. Almeida, *Tsallis thermostatistics for finite systems: A Hamiltonian approach*, Physica A 322, 276 (2003)] for connections between  $q$  and finite-sized systems.

As we readily verify, in some cases  $q$  characterizes universality classes (of nonadditivity), in total analogy with those of standard critical phenomena. Relations (5.58), (3.145), and (5.11) constitute such examples. In other cases, analogously to the two-dimensional short-range-interacting isotropic XY ferromagnetic model and to the Baxter line of the square-lattice Ashkin–Teller ferromagnet [233] (whose critical exponents depend on the temperature and on the details of the Hamiltonian),  $q$  depends on model details. Relations (7.36), (4.107), and (4.109) constitute such examples. A case which is believed to be of the universality class type is that of classical long-range Hamiltonian systems. The index  $q$  is expected to depend only on  $\alpha$  (which characterizes the range of the forces) and on  $d$  (spatial dimension of the system), possibly even only on  $\alpha/d$ . However, this remains an open problem at the time when this book is being written.

(n) *Why are there so many different values of  $q$  for the same system?*

The basic function ubiquitously emerging in the BG theory is a very universal one, namely the exponential one. It is present in the sensitivity to the initial conditions, in the relaxation of many physical quantities, in the distribution of energy states at thermal equilibrium (in particular, in the distribution of velocities), in the solution of the linear Fokker–Planck equation in the absence of external forces (and even for linear external forces), in the attractor in the sense of the Central Limit Theorem (CLT). In all these cases, the only quantity which is not universal is the *scale* of the independent variable. Of course, functions different from the exponential also appear in BG statistical mechanics, but at the crucial and generic points we find it again and again.

For many complex systems (the realm of nonextensive statistical mechanics), this function is generalized into a less universal one, namely the  $q$ -exponential function (a power-law, in the asymptotic region). It is this one which ubiquitously emerges now at the same crucial and generic points. The  $q$ -exponential function depends not only on the *scale*, but also on the *exponent* (i.e., on the value of  $q$ ) of the power-law. Therefore, for a given system, different physical quantities are associated with different values of  $q$ . The indices  $q$  are expected to appear in the theory in infinite number. However, only a few of them should be necessary to characterize the most important features of the system. And several of these few are expected to be interrelated in such a way that only very few would be independent. A paradigmatic case has been analytically shown to occur in the context of the  $q$ -generalization of the CLT: see Eq. (4.91) and Fig. 4.20. Once the values of  $\alpha$  and  $q \equiv q_{\alpha,0}$  are fixed, the entire family of infinite countable indices  $q$  is uniquely determined. Analogously, it is expected that, for classical  $d$ -dimensional long-range-interacting many-body Hamiltonians, all relevant values of  $q$  would be fixed once the exponent  $\alpha$  (which fixes how quickly the force decays with distance, independently from the intensity of the force as long as it is nonzero) is fixed.

(o) *Do we need to microscopically discuss every single new dynamical system in order to know the numerical values associated with say its  $q$ -triplet?*

The examples for which analytical and/or numerical results are available today (e.g., Eqs. (3.145) and (5.58), and Fig. 5.52) suggest that the generic answer is *no*. What we need is to know the relevant values of  $q$  for the universality classes of nonextensivity. This step of the problem being solved, we just use the values associated with the universality class to which our specific system belongs.

(p) *Are  $q$ -Gaussians ubiquitous?*

In the same sense that Gaussians are ubiquitous (meaning by this that they appear very frequently, and in very diverse occasions), the answer is *yes*. The  $q$ -Gaussians are well-defined distributions which extremize the entropy  $S_q$  under quite generic constraints, and which are normalizable for  $q < 3$ , with finite (diverging) variance for  $q < 5/3$  ( $q \geq 5/3$ ), and with compact (infinite) support for  $q < 1$  ( $q \geq 1$ ). They are *analytical extensions* of the Student's  $t$ -distributions ( $r$ -distributions) for  $q \geq 1$  (for  $q \leq 1$ ). The cause of their ubiquity presumably is the fact that, within the  $q$ -generalization of the central limit theorem,  $q$ -Gaussians are *attractors* in probability space [234] (see also [235–237, 254]). Through a related viewpoint,  $q$ -Gaussians are *stable* distributions (i.e., independent from the initial conditions) of an ubiquitous nonlinear Fokker–Planck equation. Moreover, these distributions are deeply related to scale-invariance (see, for instance, [244]), an ubiquitous property of many natural, artificial and social systems. Finally, they have already been detected under a large variety of experimental and computational circumstances (see [45, 46, 361, 363, 370, 371, 427, 451, 452, 461, 462, 583, 584, 774] among others).

An interesting analysis involving  $q$ -Gaussian distributions for  $q \leq 1$  deserves to be mentioned here. Two (physically and mathematically interesting) probabilistic models were introduced and numerically analyzed in 2005–2006, namely the MTG [239] and the TMNT [240], which were thought to yield  $q$ -Gaussian distributions (with  $q \leq 1$ ) in the  $N \rightarrow \infty$  limit. However, the *exact* limiting distributions were analytically found in 2007 [241], and, although amazingly close numerically to  $q$ -Gaussians, they are *not*  $q$ -Gaussians.<sup>4</sup> Further news were to come along this fruitful line. Indeed, three more probabilistic models were introduced in 2008 [244] (see details in Section 4.6.4). Let us refer to them as RST1, RST2, and RST3. The models RST1<sup>5</sup> and RST2 exactly yield  $q$ -Gaussian limiting distributions (RST1 for  $q \leq 1$  and RST2 for arbitrary values of  $q$ , both above and below unity), the first one on a probabilistic first-principle basis, the second one by construction. The model RST3, such as the MTG and TMNT ones, approach limiting distributions which are not  $q$ -Gaussians. So, as we see, all types of situations can occur, and the whole picture surely deserves further clarification, especially since all five models

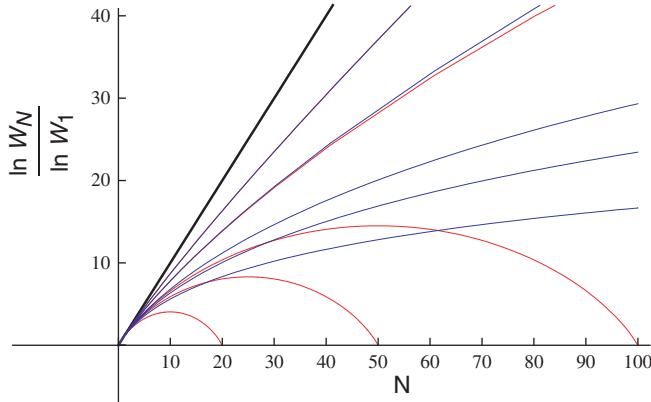
<sup>4</sup> This was immediately commented in [242] in a quite misleading manner, which generated a vague impression that there was something wrong with the  $q$ -Gaussian distributions themselves. This critique was soon replied [243], the confusing point being hopefully clarified.

<sup>5</sup> The model RST1 has been very recently extended to the entire range of  $q$ , both below and above unity [R. Hanel, S. Thurner and C. Tsallis, *Scale-invariant correlated probabilistic model yields q Gaussians in the thermodynamic limit*, (2008), preprint].

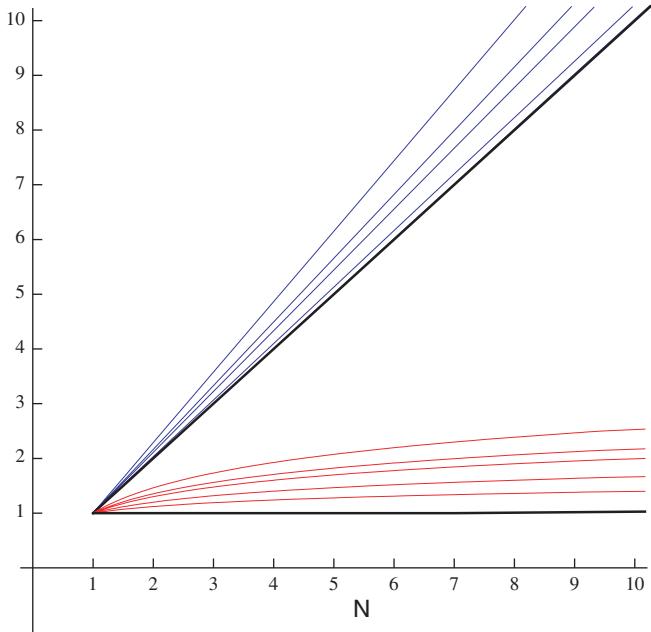
are scale-invariant (the MTG, TMNT, RST1, and RST3 models strictly, and the RST2 model only asymptotically).

(q) *Can we have some intuition on what is the physical origin of the nonadditive entropy  $S_q$ , hence of  $q$ -statistics?*

Yes, we can. Although rarely looked at this way, a very analogous phenomenon occurs at the emergence, for an ideal gas, of Fermi–Dirac and Bose–Einstein quantum statistics. Indeed, their remarkably different mathematical expressions compared to Maxwell–Boltzmann statistics come from a drastic reduction of the admissible physical states. Indeed, let us note  $\mathcal{E}_H^{(N)}$  the Hilbert space associated with  $N$  particles; the  $N$ -particle wavefunctions are of the form  $|m_1, m_2, \dots, m_N\rangle = \prod_{i=1}^N \phi_{m_i}(\mathbf{r}_i)$ , where  $\phi_{m_i}(\mathbf{r}_i)$  represents the wavefunction of the  $i$ th particle being in the quantum state characterized by the quantum number (or set of quantum numbers)  $m_i$ . If for any reason (e.g., localization of the particles) we are allowed to consider the  $N$  particles as *distinguishable*, then Boltzmann–Gibbs equal-probability hypothesis for an isolated system at equilibrium is to be applied to the entire Hilbert space  $\mathcal{E}_H^{(N)}$ . At thermal equilibrium with a thermostat, we consistently obtain, for the occupancy of the quantum state characterized by the wave-vector  $\mathbf{k}$  and energy  $E_{\mathbf{k}}$ ,  $f_{\mathbf{k}}^{MB} = e^{-\beta(E_{\mathbf{k}}-\mu)} = Ne^{-\beta E_{\mathbf{k}}}$ , where  $\mu$  is the chemical potential, and  $MB$  stands for *Maxwell–Boltzmann*. If however, the particles are to be considered as *indistinguishable*, then only *symmetrized (anti-symmetrized)*  $N$ -particle wavefunctions are physically admissible for bosons (fermions). For example, for  $N = 2$ , we have  $|m_1, m_2\rangle = \frac{1}{\sqrt{2}}[\phi_{m_1}(\mathbf{r}_1)\phi_{m_2}(\mathbf{r}_2) + \phi_{m_1}(\mathbf{r}_2)\phi_{m_2}(\mathbf{r}_1)]$  for bosons, and  $|m_1, m_2\rangle = \frac{1}{\sqrt{2}}[\phi_{m_1}(\mathbf{r}_1)\phi_{m_2}(\mathbf{r}_2) - \phi_{m_1}(\mathbf{r}_2)\phi_{m_2}(\mathbf{r}_1)]$  for fermions. For the general case of  $N$  particles, let us note, respectively,  $\mathcal{E}_H^{(N)}(S)$  and  $\mathcal{E}_H^{(N)}(A)$  the Hilbert spaces associated with symmetrized and anti-symmetrized wavefunctions. We have that  $\mathcal{E}_H^{(N)}(S) \oplus \mathcal{E}_H^{(N)}(A) \subseteq \mathcal{E}_H^{(N)}$ , the equality holding only for  $N = 2$ . For increasing  $N$ , the reduction of both  $\mathcal{E}_H^{(N)}(S)$  and  $\mathcal{E}_H^{(N)}(A)$  becomes more and more relevant. It is precisely for this reason that statistics is profoundly changed. Indeed, the occupancy is now given by  $f_{\mathbf{k}}^{BE} = 1/[e^{\beta(E_{\mathbf{k}}-\mu)} - 1]$  for bosons ( $BE$  standing for *Bose–Einstein*), and by  $f_{\mathbf{k}}^{FD} = 1/[e^{\beta(E_{\mathbf{k}}-\mu)} + 1]$  for fermions ( $FD$  standing for *Fermi–Dirac*). The corresponding entropies are consistently changed from  $S^{MB}/k_B = -\sum_{\mathbf{k}} f_{\mathbf{k}} \ln f_{\mathbf{k}}$  to  $S^{BE}/k_B = \sum_{\mathbf{k}} [-f_{\mathbf{k}} \ln f_{\mathbf{k}} + (1 + f_{\mathbf{k}}) \ln(1 + f_{\mathbf{k}})]$  for bosons, and  $S^{FD}/k_B = -\sum_{\mathbf{k}} [f_{\mathbf{k}} \ln f_{\mathbf{k}} + (1 - f_{\mathbf{k}}) \ln(1 - f_{\mathbf{k}})]$  for fermions. The need, in nonextensive statistical mechanics, for an entropy more general than the BG one, comes from essentially the same reason, i.e., a restriction of the space of the physically admissible states. Indeed, for the classical case for instance, vanishing Lyapunov exponents possibly generate, in regions of  $\Gamma$ -space, orbits which are (multi)fractal-like. Since such orbits are generically expected to have zero Lebesgue-measure, an important restriction emerges for the physically admissible space (see also [21]). The basic ideas are illustrated for the microcanonical entropy in Fig. 8.3 for ideal Maxwell–Boltzmann, Fermi–Dirac and Bose–Einstein  $N$ -particle systems ( $W_1$  being the number of states, assumed non-degenerate, of the one-particle system), and in Fig. 8.4 for a highly correlated  $N$ -body system.



**Fig. 8.3** All one-particle  $W_1$  states ( $W_1 = 1, 2, 3, \dots$ ) are assumed nondegenerate. We consider the  $N$ -particle case assuming no interaction energy between the particles.  $W_N^{(MB)} = W_1^N, N > 0$  (black curve);  $W_N^{(FD)} = \frac{W_1!}{N!(W_1-N)!}, 0 < N \leq W_1$  (red curves);  $W_N^{(BE)} = \frac{(N+W_1-1)!}{N!(W_1-1)!}, N > 0$  (blue curves).  $N = 20, 50, 100, 1000, 100,000$ . In the present scale, the FD and BE curves for  $N = 100,000$  appear superimposed. In the limit  $N \rightarrow \infty$  and  $W_1 \rightarrow \infty$  with  $N/W_1 \rightarrow 0$ ,  $W_N^{(FD)}$  and  $W_N^{(BE)}$  collapse onto the  $W_N^{(MB)}$  result; they both satisfy  $W_N \propto (W_1/N)^N$ .



**Fig. 8.4**  $N$ -dependence of  $\frac{\ln_q W_N}{\ln_q W_1}$ , where  $W_N = W_1 N^\rho$  ( $\rho > 0$ ) with  $q = 1 - \frac{1}{\rho}$  ( $\rho = 2$  hence  $q = 1/2$ ;  $W_1 > 1, N \geq 1$ ).  $\lim_{N \rightarrow \infty} \frac{\ln_{1-1/\rho} W_N}{\ln_{1-1/\rho} W_1} = \frac{W_1^{1/\rho}}{W_1^{1/\rho}-1} N$ , which asymptotically approaches  $N$  in the limit  $W_1 \rightarrow \infty$ . Under the same conditions  $\lim_{N \rightarrow \infty} \frac{\ln W_N}{\ln W_1}$  approaches unity,  $\forall N$ . Blue (red) set of curves for  $q = 1/2$  (for  $q = 1$ ), with  $W_1 = 20, 50, 100, 1000, 100,000$  from top to bottom. Black curves:  $\frac{\ln_q W_N}{\ln_q W_1} = N$  for  $q = 1 - 1/\rho$ , and  $\frac{\ln_q W_N}{\ln_q W_1} = 1$  for  $q = 1$ .

We verify in Fig. 8.3 that, in the limit of large systems ( $N \rightarrow \infty$  and  $W_1 \rightarrow \infty$ ), the MB, FD, and BE systems yield a BG entropy which is extensive, i.e., thermodynamically admissible. This is not the case for the highly correlated  $N$ -body system. Indeed, the BG entropy asymptotically becomes independent from  $N$ , whereas the nonadditive entropy  $S_q$  exhibits extensivity for a special value of  $q$ , and is therefore thermodynamically admissible. In other words, when the reduction of the (physically) admissible number of states is nonexistent (MB model), or moderate (FD and BE models), the BG entropy is extensive. But if this reduction is very severe (present highly correlated model), then we are obliged to introduce a different entropy in order to satisfy thermodynamics. Obviously this point is most important, since it basically makes legitimate the use of virtually all general formulas of textbooks of thermodynamics.

### 8.3 Open Questions

As in any physical theory in intensive development, a large amount of open questions still exist within nonextensive statistical mechanics. Since we do not intend here to make a lengthy description, we will simply mention some of those few points that we find particularly intriguing and fruitful.

- (a) *What are the  $q$ -indices relevant to the stationary-state associated with a  $d$ -dimensional classical many-body Hamiltonian including (say attractive) interactions that are not singular (or are, at least, integrable) at the origin and decay with distance  $r$  like  $1/r^\alpha$  ( $\alpha \geq 0$ )?*

We know that, for  $\alpha/d > 1$  (i.e., short-range interactions),  $q = 1$  (hence  $q_{sen} = q_{rel} = q_{stat} = 1$ ). What happens for  $0 \leq \alpha/d \leq 1$  (i.e., long-range interactions)? What would be the possible  $(\alpha, d)$ -dependences (perhaps  $(\alpha/d)$ -dependences) of indices such as  $(q_{sen}, q_{rel}, q_{stat})$ ?

- (b) *Compatibility between the (presumably) scale-invariant correlations leading to an extensive  $S_q$  and the  $q$ -exponential form for the stationary-state distribution of energy for many-body Hamiltonian systems*

More precisely, what must be satisfied by the interaction Hamiltonian  $\mathcal{H}_{AB}$  within the form  $\mathcal{H}_{A+B} = \mathcal{H}_A + \mathcal{H}_B + \mathcal{H}_{AB}$  when  $A$  and  $B$  are two large systems? Let us be more concrete and discuss the  $q = 1$  case. Assume that we are dealing with short-range interactions, and that  $A$  and  $B$  are two equally sized  $d$ -dimensional systems. Let  $L$  be the linear size of each of them. Then the energy corresponding to  $\mathcal{H}_A$  increases like  $L^d$ , and the same happens with system  $B$ . Let us also assume that  $A$  and  $B$  are in contact only through a common  $(d - 1)$ -dimensional surface. Then the energy corresponding to  $\mathcal{H}_{AB}$  increases like  $L^{d-1}$ . In the limit  $L \rightarrow \infty$ , we can neglect the interaction energy, i.e., consider  $\mathcal{H}_{AB} = 0$ . Then  $\mathcal{H}_{A+B} = \mathcal{H}_A + \mathcal{H}_B$  is clearly compatible with  $p_i^A = e^{-\beta E_i^A}/Z_A$ ,  $p_i^B = e^{-\beta E_i^B}/Z_B$  and  $p_{ij}^{A+B} = p_i^A p_j^B$ . The question we would like to answer is what exactly happens for  $q \neq 1$ ?

- (c) *What is the geometrical-dynamical interpretation of the escort distribution?*

This is a frequently asked question whose full answer is still unclear. We have presented in a previous section a variety of mathematical reasons pointing the relevance of the escort distributions within the present theory. However, a clear-cut physical interpretation in terms of the dynamics and occupancy geometry within the full phase-space  $\Gamma$  is still lacking. Some important hints can be found in [55–57].

(d) *What is the logical connection between the class of systems whose extensivity requires the adoption of the entropy  $S_q$  with  $q \neq 1$ , and the class of systems whose probabilities distributions of occupancy of phase-space leads, in the limit  $N \rightarrow \infty$ , to anomalous central limit theorems?*

The present scenario is that asymptotic scale-invariance is necessary but not sufficient. Hints can be found in [245], in Section 4.6.4, and in the nonlinear Fokker–Planck equation.

(e) *Under what generic conditions nonlinear dynamics such as those emerging at the edge of chaos as well as in long-range-interacting many-body classical Hamiltonians at their quasi-stationary state tend to create, in the full phase-space, structures geometrically similar to scale-free networks?*

The scenario is that probabilistic correlations of the  $q$ -independent class tend to create a (multi)fractal occupation of phase-space. The clarification of this point would most probably also provide an answer to the above point (c).

(f) *What are the precise physical quantities associated with the infinite set of inter-related values of  $q$  emerging in relations such as Eq. (4.90)? What is their precise connection to sets such as the  $q$ -triplet?*

This is a most important open question. The scenario is that somehow the  $q$ -triplet essentially corresponds to central elements (such as  $n = 0, \pm 1, \pm 2$ , etc) of the relation (4.90).

The solution, or at least crucial hints pointing along that direction, of these and other similar questions would be more than welcome!

# Appendix A

## Useful Mathematical Formulae

$$\ln_q x \equiv \frac{x^{1-q} - 1}{1 - q} \quad (x > 0, q \in \mathcal{R}) \quad (\text{A.1})$$

$$\ln_q x = x^{1-q} \ln_{2-q} x \quad (x > 0; \forall q) \quad (\text{A.2})$$

$$\ln_q(1/x) + \ln_{2-q} x = 0 \quad (x > 0; \forall q) \quad (\text{A.3})$$

$$q \ln_q x + \ln_{(1/q)}(1/x^q) = 0 \quad (x > 0; \forall q) \quad (\text{A.4})$$

$$e_q^x \equiv [1 + (1 - q)x]_+^{\frac{1}{1-q}} \equiv \begin{cases} 0 & \text{if } q < 1 \text{ and } x < -1/(1 - q), \\ [1 + (1 - q)x]^{\frac{1}{1-q}} & \text{if } q < 1 \text{ and } x \geq -1/(1 - q), \\ e^x & \text{if } q = 1 \quad (\forall x), \\ [1 + (1 - q)x]^{\frac{1}{1-q}} & \text{if } q > 1 \text{ and } x < 1/(q - 1). \end{cases} \quad (\text{A.5})$$

$$e_q^x e_{2-q}^{-x} = 1 \quad (\forall q) \quad (\text{A.6})$$

$$(e_q^x)^q e_{(1/q)}^{-qx} = 1 \quad (\forall q) \quad (\text{A.7})$$

$$e_q^{x+y+(1-q)xy} = e_q^x e_q^y \quad (\forall q) \quad (\text{A.8})$$

$$x \oplus_q y \equiv x + y + (1 - q)x y \quad (\text{A.9})$$

For  $x \geq 0$  and  $y \geq 0$ :

$$x \otimes_q y \equiv [x^{1-q} + y^{1-q} - 1]_+^{\frac{1}{1-q}} \equiv \begin{cases} 0 & \text{if } q < 1 \text{ and } x^{1-q} + y^{1-q} < 1, \\ [x^{1-q} + y^{1-q} - 1]^{\frac{1}{1-q}} & \text{if } q < 1 \text{ and } x^{1-q} + y^{1-q} \geq 1, \\ xy & \text{if } q = 1 \quad \forall(x, y), \\ [x^{1-q} + y^{1-q} - 1]^{\frac{1}{1-q}} & \text{if } q > 1 \text{ and } x^{1-q} + y^{1-q} > 1. \end{cases} \quad (\text{A.10})$$

$$x \otimes_q y = [1 + (1 - q)(\ln_q x + \ln_q y)]^{\frac{1}{1-q}} \quad (\text{A.11})$$

$$e_q^{x \oplus_q y} = e_q^x e_q^y \quad (\forall q) \quad (\text{A.12})$$

$$e_q^{x+y} = e_q^x \otimes_q e_q^y \quad (\forall q) \quad (\text{A.13})$$

$$\frac{d \ln_q x}{dx} = \frac{1}{x^q} \quad (x > 0; \forall q) \quad (\text{A.14})$$

$$\frac{d e_q^x}{dx} = (e_q^x)^q \quad (\forall q) \quad (\text{A.15})$$

$$(e_q^x)^q = e_{2-(1/q)}^{qx} \quad (\forall q) \quad (\text{A.16})$$

$$(e_q^x)^a = e_{1-(1-q)/a}^{ax} \quad (\forall q) \quad (\text{A.17})$$

$$x^a e_q^{-\frac{x}{b}} = \left[ \frac{b}{q-1} \right]^{1/(q-1)} x^{a-\frac{1}{q-1}} e_q^{-\frac{b(q-1)^2}{x}} \quad (b > 0; q > 1) \quad (\text{A.18})$$

$$\begin{aligned} e_q^x = & e^x [1 - \frac{1}{2}(1-q)x^2 + \frac{1}{3}(1-q)^2x^3(1 + \frac{3}{8}x) - \frac{1}{4}(1-q)^3x^4(1 + \frac{2}{3}x + \frac{1}{12}x^2) \\ & + \frac{1}{5}(1-q)^4x^5(1 + \frac{65}{72}x + \frac{5}{24}x^2 + \frac{5}{384}x^3) \\ & - \frac{1}{6}(1-q)^5x^6(1 + \frac{11}{10}x + \frac{17}{48}x^2 + \frac{1}{24}x^3 + \frac{1}{640}x^4) + \dots] \quad (q \rightarrow 1; \forall x) \end{aligned} \quad (\text{A.19})$$

$$\begin{aligned} \ln_q x = & \ln x [1 + \frac{1}{2}(1-q)\ln x + \frac{1}{6}(1-q)^2\ln^2 x + \frac{1}{24}(1-q)^3\ln^3 x \\ & + \frac{1}{120}(1-q)^4\ln^4 x + \frac{1}{720}(1-q)^5\ln^5 x + \dots] \quad (q \rightarrow 1; x > 0) \end{aligned} \quad (\text{A.20})$$

$$\begin{aligned} x \otimes_q y = & xy \left[ 1 - (1-q)(\ln x)(\ln y) \right. \\ & + \frac{1}{2}(1-q)^2 [(\ln^2 x)(\ln y) + (\ln x)(\ln^2 y) + (\ln^2 x)(\ln^2 y)] \\ & - \frac{1}{12}(1-q)^3 [2(\ln^3 x)(\ln y) + 9(\ln^2 x)(\ln^2 y) + 2(\ln x)(\ln^3 y) \\ & + 6(\ln^3 x)(\ln^2 y) + 6(\ln^2 x)(\ln^3 y) + 2(\ln^3 x)(\ln^3 y)] \\ & + \frac{1}{24}(1-q)^4 [(\ln^4 x)(\ln y) + 14(\ln^3 x)(\ln^2 y) \\ & + 14(\ln^2 x)(\ln^3 y) + (\ln x)(\ln^4 y) \\ & + 7(\ln^4 x)(\ln^2 y) + 24(\ln^3 x)(\ln^3 y) + 7(\ln^2 x)(\ln^4 y) \\ & \left. + 6(\ln^4 x)(\ln^3 y) + 6(\ln^3 x)(\ln^4 y) + (\ln^4 x)(\ln^4 y) \right] + \dots \end{aligned} \quad (\text{A.21})$$

$$\begin{aligned} e_q^x = & 1 + x + \frac{1}{2}x^2q + \frac{1}{6}x^3q(2q-1) + \frac{1}{24}x^4q(2q-1)(3q-2) \\ & + \frac{1}{120}x^5q(2q-1)(3q-2)(4q-3) + \dots \quad (x \rightarrow 0; \forall q) \end{aligned} \quad (\text{A.22})$$

$$\begin{aligned} \ln_q(1+x) = & x - \frac{1}{2}x^2q + \frac{1}{6}x^3q(1+q) - \frac{1}{24}x^4q(1+q)(2+q) \\ & + \frac{1}{120}x^5q(1+q)(2+q)(3+q) + \dots \quad (x \rightarrow 0; \forall q) \end{aligned} \quad (\text{A.23})$$

$$x^a e_q^{-\frac{x}{b}} = \left[ \frac{b}{q-1} \right]^{\frac{1}{q-1}} x^{a-\frac{1}{q-1}} e_q^{-\frac{b/(q-1)^2}{x}} \quad (q > 1; b > 0) \quad (\text{A.24})$$

$$\ln_{q,q'} x \equiv \ln_{q'} e^{\ln_q x} \quad (x > 0, (q, q') \in \mathcal{R}^2) \quad (\text{A.25})$$

$$\ln_{q,q'}(x \otimes_q y) = \ln_{q,q'} x \oplus_{q'} \ln_{q,q'} y \quad (x > 0, (q, q') \in \mathcal{R}^2) \quad (\text{A.26})$$

$$e_q^{-\beta z} = \frac{1}{\Gamma(\frac{1}{q-1})} \frac{1}{[\beta(q-1)]^{\frac{1}{q-1}}} \int_0^\infty d\alpha \alpha^{\frac{2-q}{q-1}} e^{-\frac{\alpha}{\beta(q-1)}} e^{-\alpha z} \quad (\alpha > 0; \beta > 0; 1 < q < 2) \quad (\text{A.27})$$

The following relations are useful for the Fourier transform of  $q$ -Gaussians (with  $\beta > 0$ ):

$$F_q(p) \equiv \int_{-\infty}^\infty dx \frac{e^{ipx}}{[1 + (q-1)\beta x^2]^{1/(q-1)}} \\ = 2 \int_0^\infty dx \frac{\cos(xp)}{[1 + (q-1)\beta x^2]^{1/(q-1)}} \\ = \begin{cases} \sqrt{\frac{\pi}{(1-q)\beta}} \Gamma(\frac{2-q}{1-q}) \left(\frac{2\sqrt{\beta(1-q)}}{p}\right)^{\frac{3-q}{2(1-q)}} J_{\frac{3-q}{1-q}}\left(\frac{p}{\sqrt{\beta(1-q)}}\right) & \text{if } q < 1, \\ \sqrt{\frac{\pi}{\beta}} e^{-\frac{p^2}{4\beta}} & \text{if } q = 1, \\ \frac{2}{\Gamma(\frac{1}{q-1})} \sqrt{\frac{\pi}{\beta(q-1)}} \left(\frac{|p|}{2\sqrt{\beta(q-1)}}\right)^{\frac{3-q}{2(q-1)}} K_{\frac{3-q}{2(q-1)}}\left(\frac{|p|}{\sqrt{\beta(q-1)}}\right) & \text{if } 1 < q < 3, \end{cases} \quad (\text{A.28})$$

where  $J_\nu(z)$  and  $K_\nu(z)$  are, respectively, the Bessel and the modified Bessel functions. For the three successive regions of  $q$  we have respectively used formulae 3.387-2 (page 346), 3.323-2 (page 333) and 8.432-5 (page 905) of [228] (see also [868]). For the  $q < 1$  result we have taken into account the fact that the  $q$ -Gaussian identically vanishes for  $|x| > \frac{1}{\sqrt{\beta(1-q)}}$ .

$$F_q[f](\xi) \equiv \int_{-\infty}^\infty dx e_q^{i\xi x} \otimes_q f(x) = \int_{-\infty}^\infty dx e_q^{i\xi x [f(x)]^{q-1}} f(x) \quad (q \geq 1) \quad (\text{A.29})$$

$$F_q[f](0) = \int_{-\infty}^\infty dx f(x) \quad (q \geq 1) \quad (\text{A.30})$$

$$\left. \frac{dF_q[f](\xi)}{d\xi} \right|_{\xi=0} = i \int_{-\infty}^\infty dx x [f(x)]^q \quad (q \geq 1) \quad (\text{A.31})$$

$$\left. \frac{d^2 F_q[f](\xi)}{d\xi^2} \right|_{\xi=0} = -q \int_{-\infty}^\infty dx x^2 [f(x)]^{2q-1} \quad (q \geq 1) \quad (\text{A.32})$$

$$\frac{d^3 F_q[f](\xi)}{d\xi^3} \Big|_{\xi=0} = -i q (2q-1) \int_{-\infty}^{\infty} dx x^3 [f(x)]^{3q-2} \quad (q \geq 1) \quad (\text{A.33})$$

$$\begin{aligned} \frac{d^{(n)} F_q[f](\xi)}{d\xi^n} \Big|_{\xi=0} &= (i)^n \left\{ \prod_{m=0}^{n-1} [1 + m(q-1)] \right\} \int_{-\infty}^{\infty} dx x^n [f(x)]^{1+n(q-1)} \\ &\quad (q \geq 1; n = 1, 2, 3, \dots) \end{aligned} \quad (\text{A.34})$$

$$F_q[af(ax)](\xi) = F_q[f](\xi/a^{2-q}) \quad (a > 0; 1 \leq q < 2). \quad (\text{A.35})$$

The *generating function*  $I(t)$  ( $t \in R$ ) of a given distribution  $P_N$  ( $N = 0, 1, 2, \dots$ ) is defined as follows:

$$I(t) \equiv \sum_{N=0}^{\infty} t^N P_N \quad \left( \sum_{N=0}^{\infty} P_N = 1 \right). \quad (\text{A.36})$$

The *negative binomial distribution* is defined as follows:

$$P_N(\bar{N}, k) \equiv \frac{(N+k-1)!}{N!(k-1)!} \left( \frac{\bar{N}/k}{1+\bar{N}/k} \right)^N \left( \frac{1}{1+\bar{N}/k} \right)^k \quad (\bar{N} > 0, k > 0), \quad (\text{A.37})$$

where

$$\bar{N} = \sum_{N=0}^{\infty} N P_N(\bar{N}, k), \quad (\text{A.38})$$

$$\frac{1}{k} = \frac{[\sum_{N=0}^{\infty} (N - \bar{N})^2 P_N] - \bar{N}}{\bar{N}^2}. \quad (\text{A.39})$$

Its generating function is given by

$$I(t) = e_q^{\bar{N}(t-1)}, \quad (\text{A.40})$$

with

$$q \equiv 1 + \frac{1}{k}. \quad (\text{A.41})$$

The particular case  $q = 1$  (i.e.,  $k \rightarrow \infty$ ) corresponds to the *Poisson distribution*

$$P_N(\bar{N}) = \frac{\bar{N}^N}{N!} e^{-\bar{N}}, \quad (\text{A.42})$$

which satisfies the property that the width equals the mean value, i.e.,

$$\sum_{N=0}^{\infty} (N - \bar{N})^2 P_N = \bar{N}. \quad (\text{A.43})$$

# Appendix B

## Escort Distributions and $q$ -Expectation Values

### B.1 First Example

In order to illustrate the practical utility and peculiar properties of escort distributions and their associated  $q$ -expectation values, we introduce and analyze here a pedagogical example [884].<sup>1</sup>

Let us assume that we have a set of empirical distributions  $\{f_n(x)\}$  ( $n = 1, 2, 3, \dots$ ) defined as follows:

$$f_n(x) = \frac{A_n}{(1 + \lambda x)^\alpha} \quad (\lambda > 0; \alpha \geq 0), \quad (\text{B.1})$$

if  $0 \leq x \leq n$ , and zero otherwise. Normalization of  $f_n(x)$  immediately yields

$$A_n = \frac{\lambda(\alpha - 1)}{1 - (1 + \lambda n)^{1-\alpha}}. \quad (\text{B.2})$$

In order to have finite values for  $A_n$ ,  $\forall n$ , including  $n \rightarrow \infty$  (i.e.,  $0 < A_\infty < \infty$ ),  $\alpha > 1$  is needed. Consequently

$$A_\infty = \lambda(\alpha - 1). \quad (\text{B.3})$$

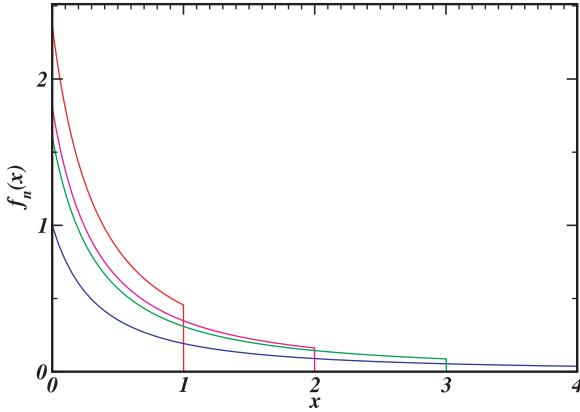
By identifying

$$\alpha = \frac{1}{q - 1}, \quad (\text{B.4})$$

$$\lambda = \beta(q - 1), \quad (\text{B.5})$$

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<sup>1</sup> The present illustration has greatly benefited from lengthy discussions with S. Abe, who launched [885] interesting questions regarding  $q$ -expectation values, and with E.M.F. Curado.



**Fig. B.1** The distributions  $f_n(x)$  for  $n = 1, 2, 3, \infty$  (from top to bottom) for  $(\lambda, \alpha) = (2, 3/2)$  (from [884]).

Equation (B.1) can be rewritten as

$$f_n(x) = A_n e_q^{-\beta x} \quad (\beta > 0; q \geq 1). \quad (\text{B.6})$$

The variable  $x \geq 0$  could be a physical quantity, say earthquake intensity, measured along small intervals, say  $10^{-6}$ , so small that sums can be replaced by integrals within an excellent approximation. The empiric distribution  $f_n(x)$  could correspond to different seismic regions, say region 1 (for  $n = 1$ ), region 2 (for  $n = 2$ ), and so on. See Fig. B.1. Suppose we want to characterize the distribution  $f_n(x)$  through its mean value. A straightforward calculation yields

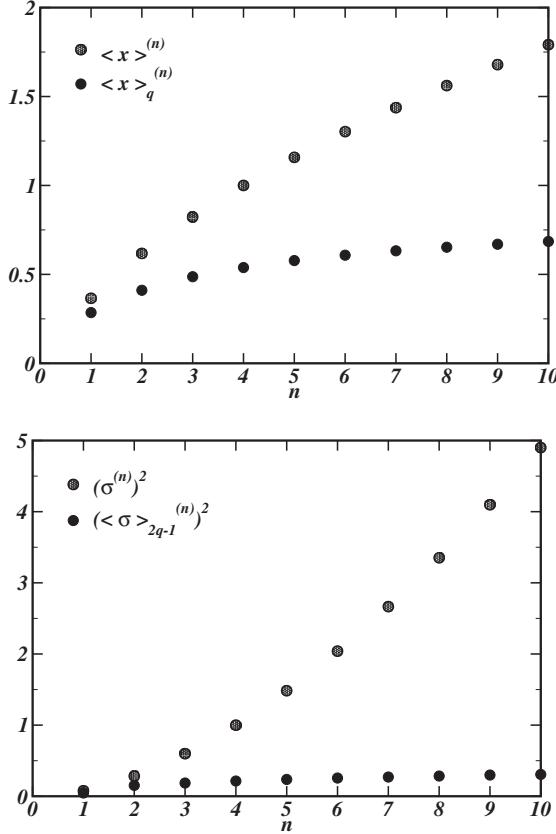
$$\langle x \rangle^{(n)} \equiv \int_0^n dx x f_n(x) = \frac{1 - (1 + \lambda n)^\alpha + \lambda n [\alpha + (\alpha - 1)\lambda n]}{(\alpha - 2)\lambda(1 + \lambda n)[1 - (1 + \lambda n)^{\alpha-1}]} . \quad (\text{B.7})$$

This quantity is *finite* for all  $n$  (including  $n \rightarrow \infty$ ) for  $\alpha > 2$ , but  $\langle x \rangle^{(\infty)}$  diverges for  $1 < \alpha \leq 2$ . In other words, we can use it to characterize  $f_n(x)$ ,  $\forall n$ , for  $\alpha > 2$ , but we *cannot* for  $1 < \alpha \leq 2$ . The problem is illustrated in Fig. B.2 for  $\alpha = 3/2$ . This difficulty disappears if we use instead the  $q$ -expectation value, defined as follows

$$\langle x \rangle_q^{(n)} \equiv \frac{\int_0^n dx x [f_n(x)]^q}{\int_0^n dx [f_n(x)]^q} = \frac{(1 + \lambda n)^\alpha - 1 - \lambda \alpha n}{\lambda(\alpha - 1)[(1 + \lambda n)^\alpha - 1]} , \quad (\text{B.8})$$

which equals of course the standard mean value but calculated with the *escort distribution* (first introduced in chaos theory [212])

$$F_n(x) \equiv \frac{[f_n(x)]^q}{\int_0^n dx [f_n(x)]^q} . \quad (\text{B.9})$$



**Fig. B.2** The  $n$ -dependences of relevant average quantities of the model  $(\lambda, \alpha) = (2, 3/2)$ ;  $q = 1 + \frac{1}{\alpha}$ . *Top:* Expectation value  $\langle x \rangle^{(n)} \equiv \int_0^n dx x f_n(x)$  ( $\lim_{n \rightarrow \infty} \langle x \rangle^{(n)} = \infty$ ), and  $q$ -expectation value  $\langle x \rangle_q^{(n)} \equiv \frac{\int_0^n dx x [f_n(x)]^q}{\int_0^n dx [f_n(x)]^q}$  ( $\lim_{n \rightarrow \infty} \langle x \rangle_q^{(n)} = \frac{1}{\lambda(\alpha-1)}$ ). *Bottom:* Variance  $[\sigma^{(n)}]^2 \equiv \langle x^2 \rangle^{(n)} - [\langle x \rangle^{(n)}]^2$  ( $\lim_{n \rightarrow \infty} [\sigma^{(n)}]^2 = \infty$ ), and  $(2q-1)$ -variance  $[\sigma_{2q-1}^{(n)}]^2 \equiv \langle x^2 \rangle_{2q-1}^{(n)} - [\langle x \rangle_{2q-1}^{(n)}]^2$  ( $\lim_{n \rightarrow \infty} [\sigma_{2q-1}^{(n)}]^2 = \frac{1+\alpha}{\lambda^2 \alpha^2 (\alpha-1)}$ ) (from [884]).

instead of with the original distribution  $f_n(x)$ . It follows immediately that

$$\langle x \rangle_q^{(\infty)} = \frac{1}{\lambda(\alpha-1)}, \quad (\text{B.10})$$

which is *finite* for *all* values  $\alpha > 1$ , i.e., as long as the norm itself is finite. The problem that we exhibited with the standard mean value reappears, and even worse, if we are interested in the second moment of  $f_n(x)$ . We have that

$$[\sigma^{(n)}]^2 \equiv \langle x^2 \rangle^{(n)} - [\langle x \rangle^{(n)}]^2 \quad (\text{B.11})$$

is *finite* for all values of  $n$  (including for  $n \rightarrow \infty$ ) only if  $\alpha > 3$ , but  $\sigma^{(\infty)}$  diverges for  $1 < \alpha \leq 3$ : see Fig. B.2. This divergence can be regularized by considering [258]<sup>2</sup>

$$[\sigma_{2q-1}^{(n)}]^2 \equiv \langle x^2 \rangle_{2q-1}^{(n)} - [\langle x \rangle_{2q-1}^{(n)}]^2 = \frac{\int_0^n dx x^2 [f_n(x)]^{2q-1}}{\int_0^n dx [f_n(x)]^{2q-1}} - \left[ \frac{\int_0^n dx x [f_n(x)]^{2q-1}}{\int_0^n dx [f_n(x)]^{2q-1}} \right]^2, \quad (\text{B.12})$$

whose  $n \rightarrow \infty$  limit is given by

$$[\sigma_{2q-1}^{(\infty)}]^2 = \frac{1 + \alpha}{(\alpha - 1)\alpha^2\lambda^2}. \quad (\text{B.13})$$

This quantity, such as the norm and  $\langle x \rangle_q^{(\infty)}$ , is finite for all  $\alpha > 1$ : see Fig. B.2. As a matter of fact, the moments of *all* orders are finite for  $\alpha > 1$  if, instead of the original distribution  $f_n(x)$ , we use the appropriate escort distributions [258]. Indeed, if we consider the  $m$ th order moment  $\langle x^m \rangle_{q_m}^{(n)}$  with  $q_m = mq - (m - 1)$  and  $m = 0, 1, 2, 3, \dots$ , *all* these moments are *finite* for any  $\alpha > 1$  and any  $n$ , and they *all diverge* for  $\alpha \leq 1$  and  $n \rightarrow \infty$  (see also Section 4.7).

Summarizing,

- (i) If we want to characterize, for *all* values of  $n$  (including  $n \rightarrow \infty$ ), the functional density form (B.1) for all  $\alpha > 1$ , we can perfectly well do so by using the appropriate escort distributions, whereas the standard mean value is admissible only for  $\alpha > 2$ , and the standard variance is admissible only for  $\alpha > 3$ ;
- (ii) If we only want to characterize, for all  $\alpha > 1$  and finite  $n$ , which seismic region (in our example with earthquakes) is more dangerous, we can do so either with the standard mean value or with the  $q$ -mean value; obviously, the larger  $n$  is, the more seismically dangerous the region is;
- (iii) If we only want to characterize, for all  $\alpha > 1$  and finite  $n$ , the size of the fluctuations, we can do so either with the standard variance or with the  $q$ -variance; obviously, the larger  $n$  is, the larger the fluctuations are.

As we have illustrated, the problem of the empirical verification of a specific *analytic form* for a distribution of probabilities theoretically argued is quite different from the problem on how *successive experimental data keep filling this functional form*. In particular, the problem of its largest empirical values constitutes an entire branch of mathematical statistics, usually referred to as *extreme value statistics* (or *extreme value theory*) (see, for instance, [883]), and remains out of the scope of the present book.

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<sup>2</sup> For the present purpose, we can also use  $\langle (x - \langle x \rangle_q)^2 \rangle_{2q-1}^{(n)} = \langle x^2 \rangle_{2q-1}^{(n)} - 2\langle x \rangle_q^{(n)}\langle x \rangle_{2q-1}^{(n)} + (\langle x \rangle_q^{(n)})^2$ . In contrast, we cannot use  $\langle x^2 \rangle_{2q-1}^{(n)} - (\langle x \rangle_q^{(n)})^2$ ; indeed, it becomes negative for  $n$  large enough.

## B.2 Second Example

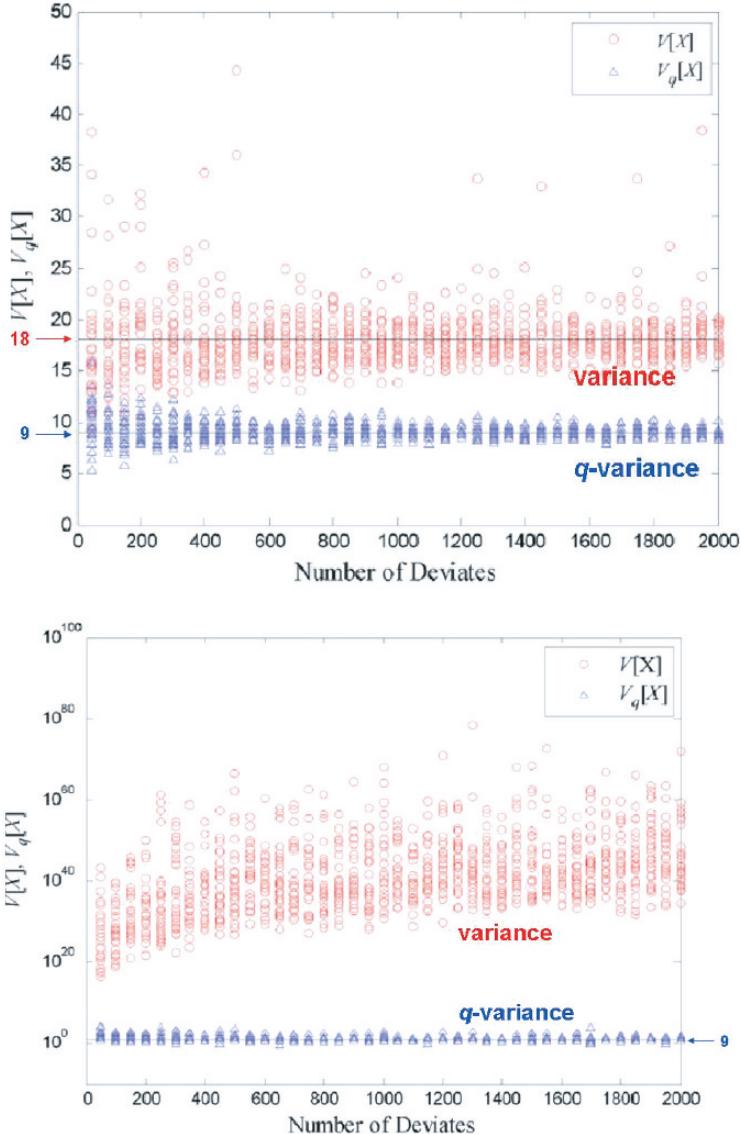
In the previous example, we have used academically constructed “empiric” distributions. However, exactly the same scenario is encountered if we use random models such as the one introduced in [627]. The variance of  $q$ -Gaussian distributions is finite for  $q < 5/3$ , and diverges for  $5/3 \leq q < 3$ ; their norm is finite for  $q < 3$ . Two typical cases are shown in Fig. B.3, one of them for  $q < 5/3$ , and the other one for  $q > 5/3$ . In both cases, the fluctuations of the variance  $V[X] \equiv \sigma^2$  are considerably larger than those of the  $q$ -variance  $V_q[X] \equiv \sigma_q^2$ . For  $q < 5/3$ , the variance converges very slowly to its exact asymptotic value; for  $q > 5/3$  does not converge at all. In all situations, the  $q$ -variance quickly converges to its asymptotic value, which is always finite, thus constituting a very satisfactory characterization. The reasons for precisely considering in this example the  $q$ -variance  $V_q[X]$ , and not any other, are the same that have been indicated in the previous example (see [258] and Section 4.7).

## B.3 Remarks

Let us end by some general remarks. Abe has shown [885] that the  $q$ -expectation value  $\langle Q \rangle_q \equiv \frac{\sum_{i=1}^W Q_i p_i^q}{\sum_{i=1}^W p_i^q}$ , where  $\{Q_i\}$  corresponds to any physical quantity, is unstable (in a uniform continuity sense, i.e., similar to the criterion introduced by Lesche for any entropic functional [79], *not* in the thermodynamic sense) for  $q \neq 1$ , whereas it is stable  $q = 1$ . If we consider the particular case  $Q_i = \delta_{i,j}$ , where we use Kroenecker’s delta function, we obtain as a corollary that the escort distribution itself is unstable for  $q \neq 1$ <sup>3</sup> This fact illustrates a simple property, namely that two quantities can be Lesche-stable, and nevertheless their ratio can be Lesche-unstable. In the present example, both  $p_i^q$  and  $\sum_{i=1}^W p_i^q$  are stable,  $\forall q > 0$ , but  $\frac{p_i^q}{\sum_{j=1}^W p_j^q}$  is unstable for  $q \neq 1$ . The possible epistemological implications of such subtle properties for the 1998 formulation [60] of nonextensive statistical mechanics deserve further analysis. The fact stands, however, that the characterization of the (asymptotic) *power-laws* which naturally emerge within this theory undoubtedly is very conveniently done through  $q$ -expectation values, whereas it is not so through standard expectation values (which *necessarily* diverge for *all* moments whose order exceeds some specific one, which depends on the exponent of the power-law). The situation is well illustrated for the constraints to be used for the canonical ensemble (the system being in contact with some thermostat). If, together with the norm constraint  $\sum_{i=1}^W p_i = 1$ , we impose the energy constraint as  $\langle \mathcal{H} \rangle_q \equiv \frac{\sum_{i=1}^W E_i p_i^q}{\sum_{i=1}^W p_i^q} = U_q$ , where  $\{E_i\}$  are the energy eigenvalues and  $U_q$  a fixed *finite* real number, we are dealing (unless we provide some additional qualification) with an unstable quantity.

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<sup>3</sup> This special property was also directly established by Curado [886].



**Fig. B.3** Behavior, as functions of the number of deviates, of the variance  $V[X] \equiv \sigma^2$  and the  $q$ -variance  $V_q[X] \equiv \sigma_q^2$  of typical, stochastically generated,  $q$ -Gaussians. *Top:* For  $q = 1.4 (< 5/3)$ ;  $\lim_{\# \text{of deviates} \rightarrow \infty} V[X] = 18$ , and  $\lim_{\# \text{of deviates} \rightarrow \infty} V_{1.4}[X] = 9$ . Notice that the level of fluctuations of  $V[X]$  for 2000 deviates is similar to that of  $V_{1.4}[X]$  for only 200 deviates. *Bottom:* For  $q = 2.75 (> 5/3)$ ;  $\lim_{\# \text{of deviates} \rightarrow \infty} V[X] = \infty$ , and  $\lim_{\# \text{of deviates} \rightarrow \infty} V_{2.75}[X] = 9$ . Notice how huge is the ordinate scale (from [627]).

However, it has been shown [887] that, for all the physically relevant cases, this quantity is *robust*. In other words, nothing indicates whatsoever difficulty at the practical level for the experimentally falsifiable predictions of nonextensive statistical mechanics.

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