GENERALIZAÇÃO DA MECÂNICA ESTATÍSTICA DE BOLTZMANN-GIBBS - TEORIA E APLICAÇÕES

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Escola CBPF – Rio de Janeiro, Julho 2017

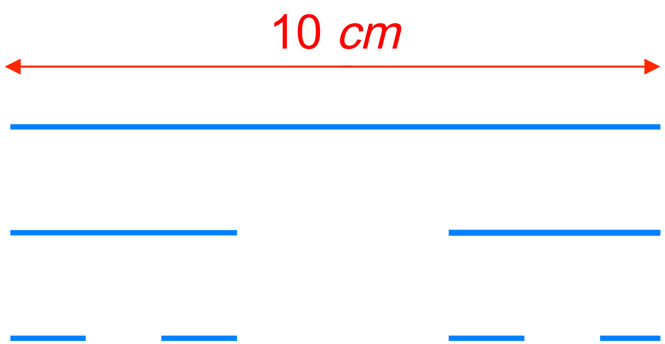
Para um melhor aproveitamento do conteúdo ministrado, recomendamos à audiência que mantenha os aparelhos eletrônicos (celulares, laptops) desligados durante as aulas.

Comissão Organizadora
XI Escola do CBPF

World champion
of complexity!

(Photo taken in London by Luciano Pietronero)

TRIADIC CANTOR SET:



$$d_F = \frac{\ln 2}{\ln 3} = 0.6309...$$

Hence the interesting measure is

$$(10\ cm)^{0.6309...} \cong 4.275\ cm^{0.6309}$$

It is the natural (or artificial or social) system itself which, through its geometrical-dynamical properties, mandates the specific informational tool --- entropy --- to be meaningfully used for the study of its thermostatistical and thermodynamical properties.

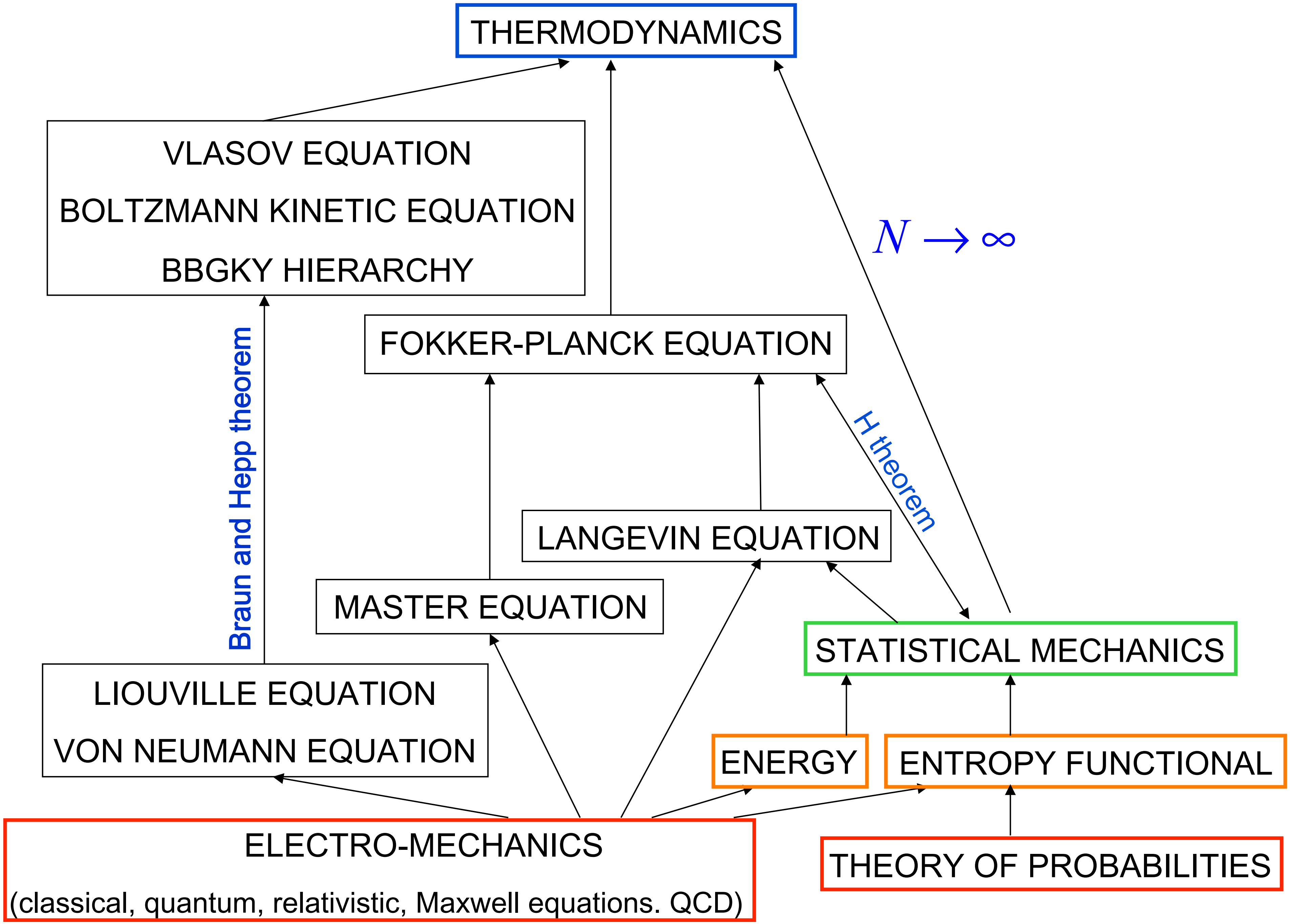
Enrico FERMI *Thermodynamics* (Dover, 1936)

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.

Ettore MAJORANA

The value of statistical laws in physics and social sciences.
Original manuscript in Italian published by G. Gentile Jr. in *Scientia* **36**, 58 (1942); translated into English by R. Mantegna (2005).

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 indefinitively, 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.


THERMODYNAMICS
VLASOV EQUATION
BOLTZMANN KINETIC EQUATION
BBGKY HIERARCHY
$N \to \infty$
FOKKER-PLANCK EQUATION
Braun and Hepp theorem
H theorem
LANGEVIN EQUATION
MASTER EQUATION
STATISTICAL MECHANICS
LIOUVILLE EQUATION
VON NEUMANN EQUATION
ENERGY
ENTROPY FUNCTIONAL
ELECTRO-MECHANICS
(classical, quantum, relativistic, Maxwell equations. QCD)
THEORY OF PROBABILITIES

ENTROPIC FUNCTIONALS

	$p_i = \frac{1}{W} \quad (\forall i)$ equiprobability	$\forall p_i \ (0 \le p_i \le 1)$ $\left(\sum_{i=1}^{W} p_i = 1 \right)$
BG entropy (*q* =*1*)	$k \ln W$	$-k \sum_{i=1}^{W} p_i \ln p_i$
Entropy *Sq* (*q real*)	$k \frac{W^{1-q} - 1}{1-q}$	$k \frac{1 - \sum_{i=1}^{W} p_i^q}{q-1}$

additive

Concave

Extensive

Lesche-stable

Finite entropy production per unit time

Pesin-like identity (with largest entropy production)

Composable (**unique** trace form; Enciso-Tempesta)

Topsoe-factorizable (unique)

Amari-Ohara-Matsuzoe conformally invariant geometry (unique)

Biro-Barnafoldi-Van thermostat universal independence (unique)

nonadditive (if $q \neq 1$)

Possible generalization of Boltzmann-Gibbs statistical mechanics

C.T., J. Stat. Phys. **52**, 479 (1988)

DEFINITIONS: *q-logarithm*: $\ln_q x \equiv \frac{x^{1-q}-1}{1-q}$ $(x>0;\ \ln_1 x = \ln x)$

q-exponential: $e_q^x \equiv [1+(1-q)\,x]^{\frac{1}{1-q}}$ $(e_1^x = e^x)$

Hence, the entropies can be rewritten:

	equal probabilities	generic probabilities
BG entropy $(q=1)$	$k\ \ln W$	$k \sum_{i=1}^{W} p_i \ln \frac{1}{p_i}$
entropy S_q $(q \in R)$	$k\ \ln_q W$	$k \sum_{i=1}^{W} p_i \ln_q \frac{1}{p_i}$

Full bibliography (regularly updated):

http://tsallis.cat.cbpf.br/biblio.htm

6224 articles by 12691 scientists (96 countries)

[14 July 2017]

CONTRIBUTORS (6224 MANUSCRIPTS)

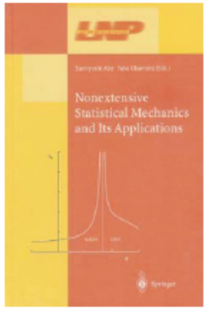
USA	2229	HUNGARY	89	SLOVENIA	19	VIETNAM	5
ITALY	1034	PORTUGAL	89	SAUDI ARABIA	17	BOLIVIA	4
GERMANY	959	AUSTRALIA	88	IRELAND	14	INDONESIA	4
BRAZIL	873	ROMANIA	80	VENEZUELA	14	NIGERIA	4
UNITED KINGDOM	778	NORWAY	75	LITHUANIA	12	SENEGAL	4
FRANCE	683	SWEDEN	69	CYPRUS	11	BELARUS	3
CHINA	670	TAIWAN	63	MOROCCO	11	MACEDONIA	3
SWITZERLAND	642	UKRAINE	57	ARMENIA	10	MOLDOVA	2
RUSSIA	536	EGYPT	48	BELARUS	10	NORTH CYPRUS	2
JAPAN	484	PAKISTAN	46	PUERTO RICO	10	PANAMA	2
INDIA	388	SLOVAKIA	45	SINGAPORE	10	PHILIPINES	2
SPAIN	360	DENMARK	43	NEW ZEALAND	9	UN. ARAB EMIRATES	2
POLAND	202	SERBIA	36	FRENCH GUIANA	8	BAHRAIN	1
GREECE	187	FINLAND	34	GEORGIA	8	BENIN	1
CANADA	177	SOUTH AFRICA	33	KHAZHAKSTAN	8	ECUADOR	1
NETHERLANDS	147	BELGIUM	32	ESTONIA	7	ETHIOPIA	1
CZECH REPUBLIC	140	CHILE	31	ALBANIA	6	IRAQ	1
ARGENTINA	132	BANGLADESH	30	AZERBAIJAN	6	LUXENBOURG	1
TURKEY	128	COLOMBIA	29	CAMEROON	6	OMAN	1
IRAN	126	ALGERIA	26	JORDAN	6	QATAR	1
SOUTH KOREA	111	CROATIA	25	ICELAND	5	SRI LANKA	1
ISRAEL	109	BULGARIA	20	PERU	5	TUNISIA	1
MEXICO	108	CUBA	19	THAILAND	5	UZBEKISTAN	1
AUSTRIA	93	MALAYSIA	19	URUGUAY	5	YEMEN	1

12691 SCIENTISTS **96 COUNTRIES**

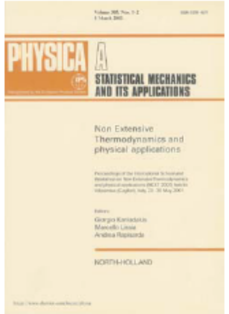
[Updated 14 July 2017]

BOOKS AND SPECIAL ISSUES ON NONEXTENSIVE STATISTICAL MECHANICS

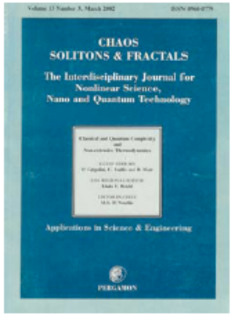
1999



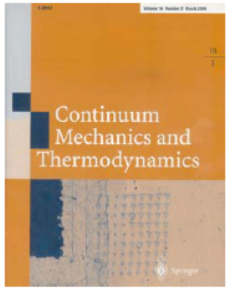
2001



2002

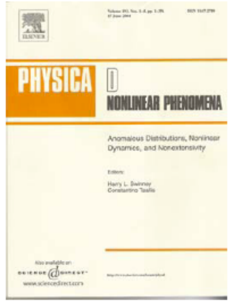


2002



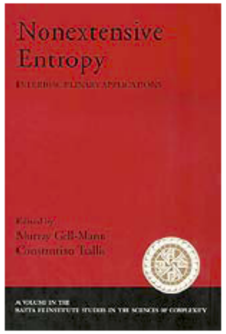
2004

2004

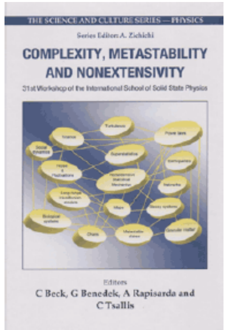


2004

2004



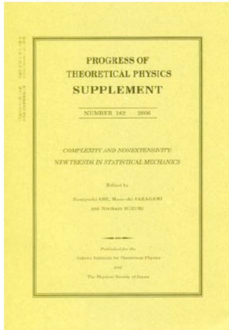
2004



2005

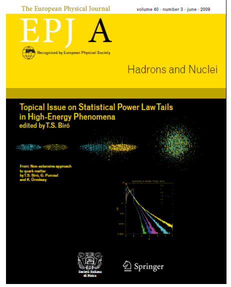
2005

2006



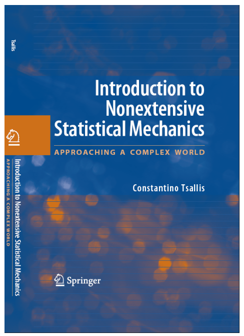
2006

2007

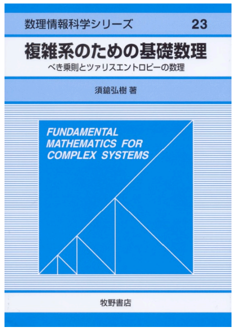


2009

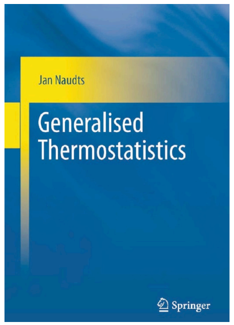
2009



2009



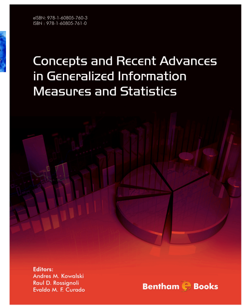
2010



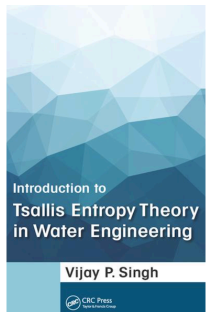
2011

2011

2012



2013

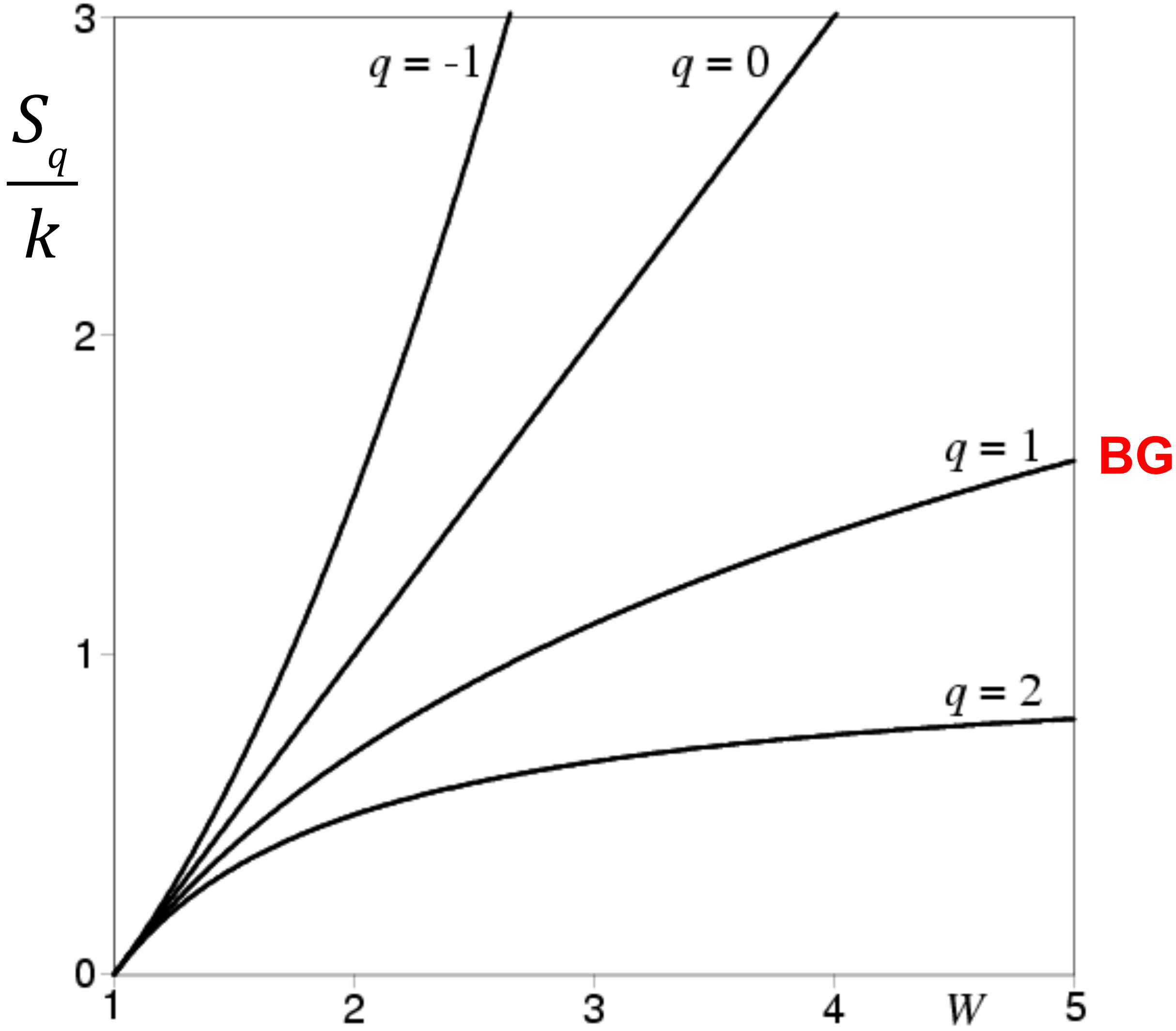


2016

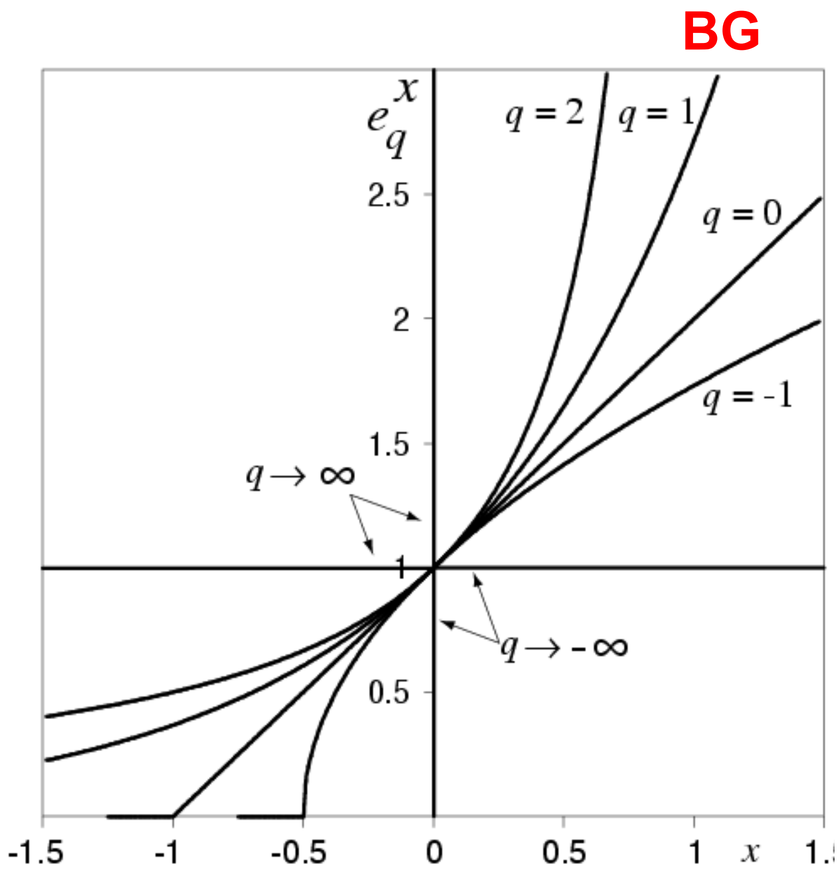
Generalized Entropies:
C.T., E.M.F. Curado and F.D. Nobre, Cambridge Univ. Press, in preparation

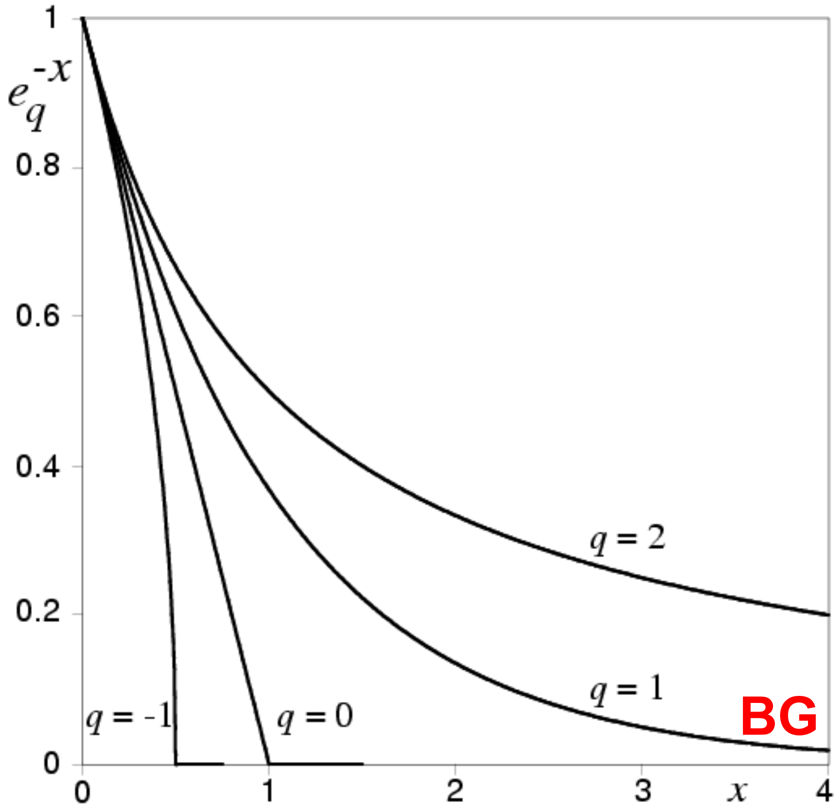
~2017

$$S_q = k \ln_q W \equiv k \frac{W^{1-q} - 1}{1-q}$$

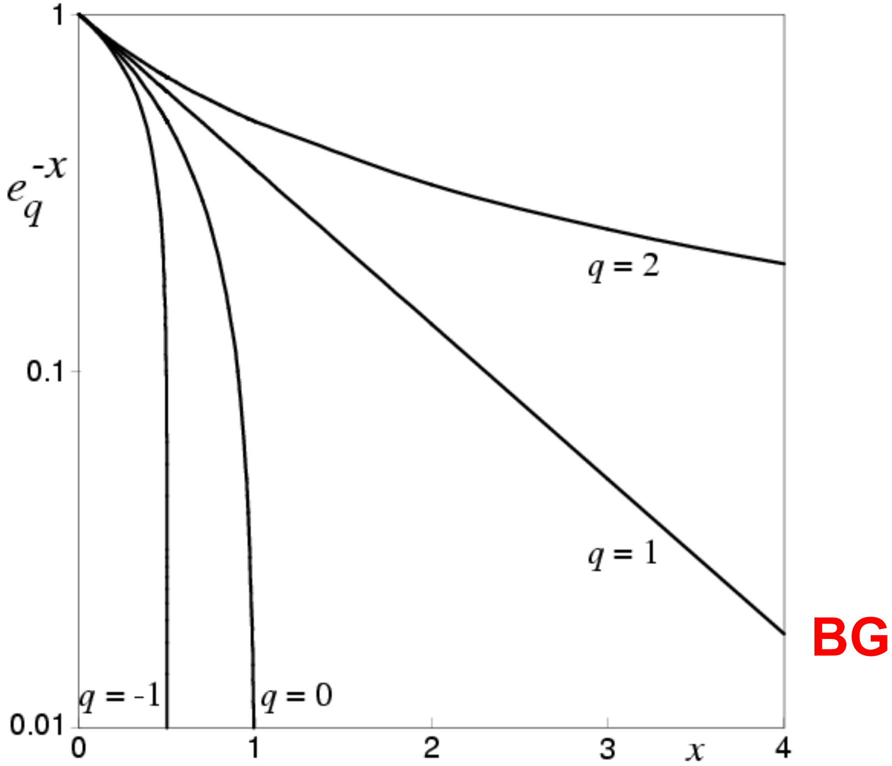


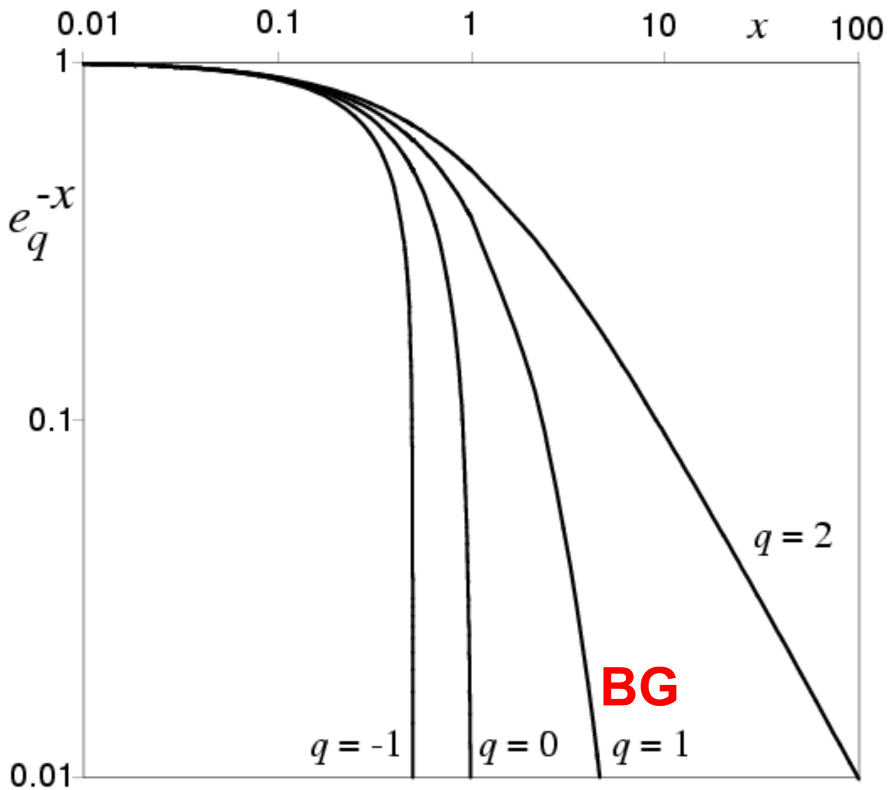
$$e_q^x = [1 + (1-q)x]^{\frac{1}{1-q}}$$





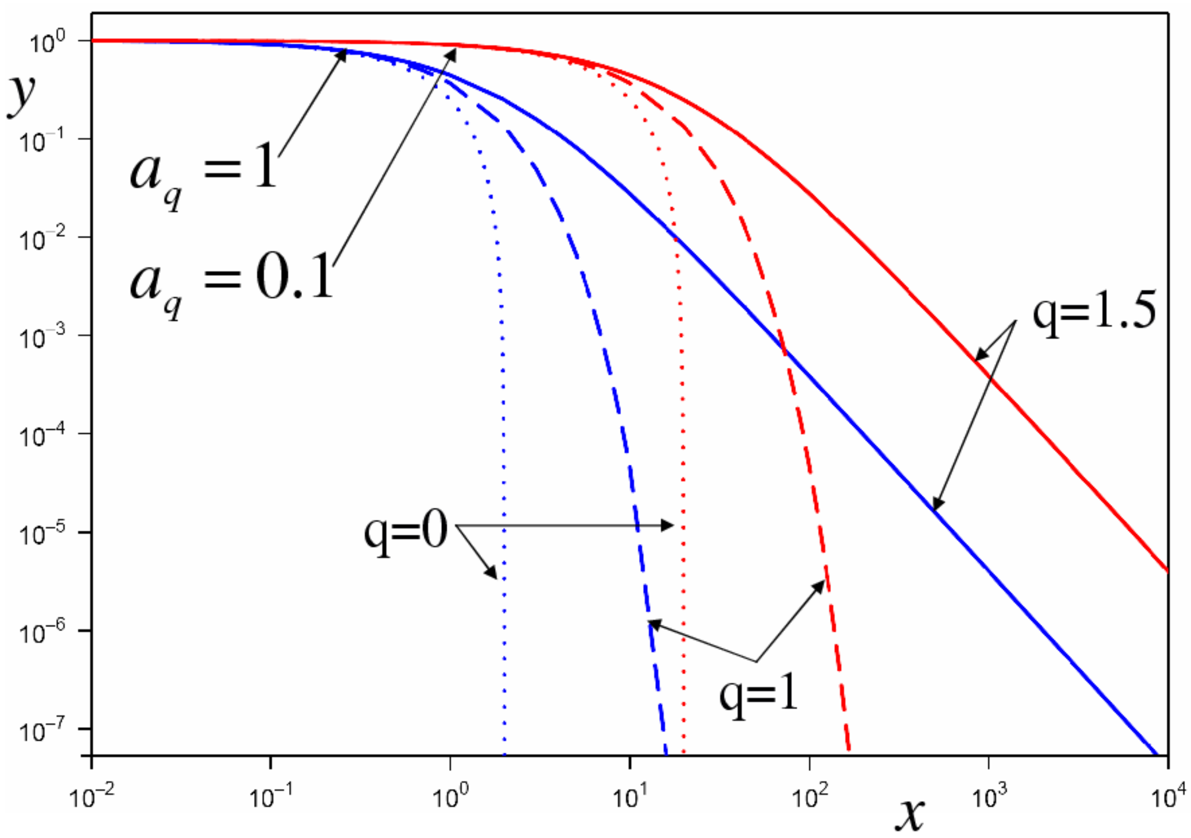
$$e_q^x = [1+(1-q)x]^{\frac{1}{1-q}}$$





$$\frac{dy}{dx} = -a_q y^q \quad \text{with } y(0) = 1$$

$$\Rightarrow y = e_q^{-a_q x} \equiv \frac{1}{\left[1 + (q-1)a_q x\right]^{\frac{1}{q-1}}}$$



TYPICAL SIMPLE SYSTEMS:

$$W(N) \propto \mu^N \;\; (\mu > 1)$$

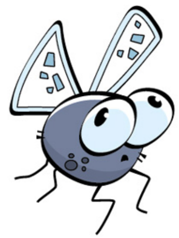
Short-range space-time correlations

Markovian processes (short memory), Additive noise

Strong chaos (positive maximal Lyapunov exponent), **Ergodic**, Riemannian geometry

Short-range many-body interactions, weakly quantum-entangled subsystems

Linear and homogeneous Fokker-Planck equations, Gausssians



→ **Boltzmann-Gibbs entropy (additive)**

→ **Exponential dependences (Boltzmann-Gibbs weight, ...)**

TYPICAL COMPLEX SYSTEMS:

$$\text{e.g.,} \;\; W(N) \propto N^\rho \;\; (\rho > 0)$$

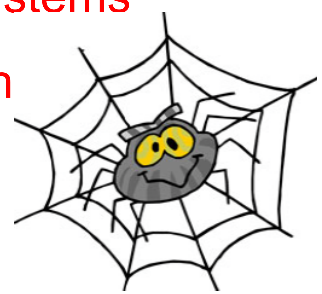
Long-range space-time correlations

Non-Markovian processes (long memory), Additive and multiplicative noises

Weak chaos (zero maximal Lyapunov exponent), **Nonergodic**, Multifractal geometry

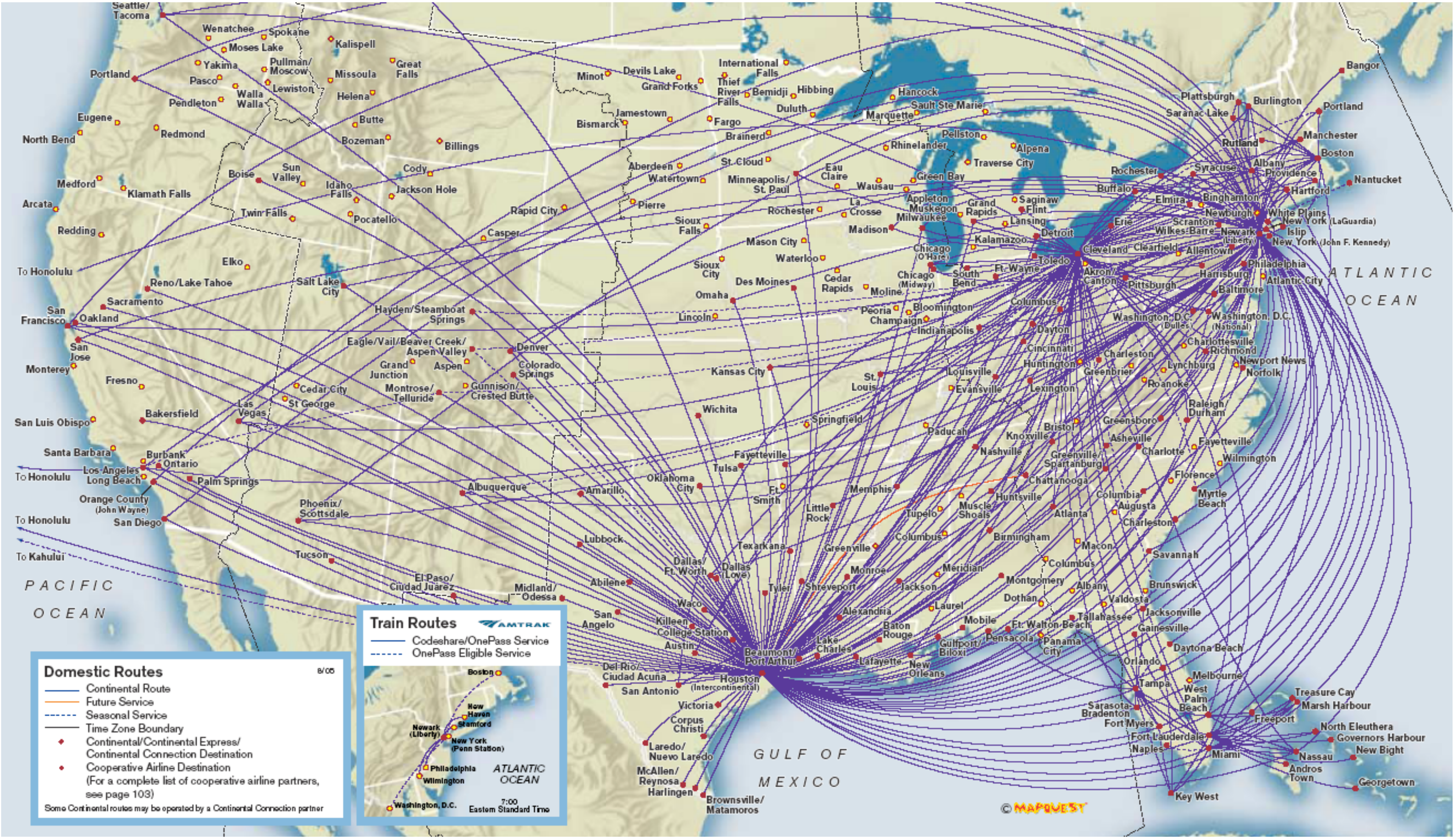
Long-range many-body interactions, strongly quantum-entangled sybsystems

Nonlinear and/or inhomogeneous Fokker-Planck equations, *q*-Gaussian



→ **Entropy S_q (nonadditive)**

→ ***q*-exponential dependences (asymptotic power-laws)**



Continental Airlines

ADDITIVITY: O. Penrose, *Foundations of Statistical Mechanics: A Deductive Treatment* (Pergamon, Oxford, 1970), page 167

An entropy is additive if, for any two probabilistically independent systems A and B,

$$S(A+B)=S(A)+S(B)$$

Therefore, since

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

S_{BG} and $S_q^{Renyi}\,(\forall q)$ are additive, and $S_q\ (\forall q\neq 1)$ is nonadditive .

EXTENSIVITY:

Consider a system $\Sigma\equiv A_1+A_2+\ldots+A_N$ made of N (not necessarily independent) identical elements or subsystems A_1 and A_2, ..., A_N.

An entropy is extensive if

$$0<\lim_{N\to\infty}\frac{S(N)}{N}<\infty\ ,\ i.e.,\ \ S(N)\propto N\ \ (N\to\infty)$$

EXTENSIVITY OF THE ENTROPY $(N \to \infty)$

$W \equiv$ total number of possibilities with nonzero probability,

assumed to be equally probable

If $W(N) \sim \mu^N \quad (\mu > 1)$

$$\Rightarrow S_{BG}(N) = k_B \ln W(N) \propto N \qquad \text{OK!}$$

If $W(N) \sim N^\rho \quad (\rho > 0)$

$$\Rightarrow S_q(N) = k_B \ln_q W(N) \propto [W(N)]^{1-q} \propto N^{\rho(1-q)}$$

$$\Rightarrow S_{q=1-1/\rho}(N) \propto N \qquad \text{OK!}$$

If $W(N) \sim \nu^{N^\gamma} \quad (\nu > 1;\ 0 < \gamma < 1)$

$$\Rightarrow S_\delta(N) = k_B \left[\ln W(N)\right]^\delta \propto N^{\gamma\,\delta}$$

$$\Rightarrow S_{\delta=1/\gamma}(N) \propto N \qquad \text{OK!}$$

IMPORTANT: $\boxed{\mu^N >> \nu^{N^\gamma} >> N^\rho \quad \text{if} \quad N >> 1}$

All happy families are alike; each unhappy family is unhappy in its own way.

Leo Tolstoy (*Anna Karenina*, 1875-1877)

SYSTEMS $W(N)$ (*equiprobable*)	ENTROPY S_{BG} (ADDITIVE)	ENTROPY S_q $(q \neq 1)$ (NONADDITIVE)	ENTROPY S_δ $(\delta \neq 1)$ (NONADDITIVE)
e.g., μ^N $(\mu > 1)$	EXTENSIVE	NONEXTENSIVE	NONEXTENSIVE
e.g., N^ρ $(\rho > 0)$	NONEXTENSIVE	EXTENSIVE $(q = 1 - 1/\rho)$	NONEXTENSIVE
e.g., ν^{N^γ} $(\nu > 1;$ $0 < \gamma < 1)$	NONEXTENSIVE	NONEXTENSIVE	EXTENSIVE $(\delta = 1/\gamma)$

King Thutmosis I
18^{th} Dynasty
circa 1500 BC

A theory is the more impressive the greater the simplicity of its premises is, the more different kinds of things it relates, and the more extended is its area of applicability. Therefore the deep impression that classical thermodynamics made upon me. It is the only physical theory of universal content concerning which I am convinced that, within the framework of applicability of its basic concepts, it will never be overthrown.

Albert Einstein (1949)

THERMODYNAMICS:

$$G(V,T,p,\mu,H,\ldots)=U(V,T,p,\mu,H,\ldots)-TS(V,T,p,\mu,H,\ldots)$$
$$+pV-\mu N(V,T,p,\mu,H,\ldots)-HM(V,T,p,\mu,H,\ldots)-\ldots$$

where $S,V,N,M,\ldots$ scale like $V\equiv L^d$ (extensivity)

$T,p,\mu,H,\ldots$ scale like L^θ

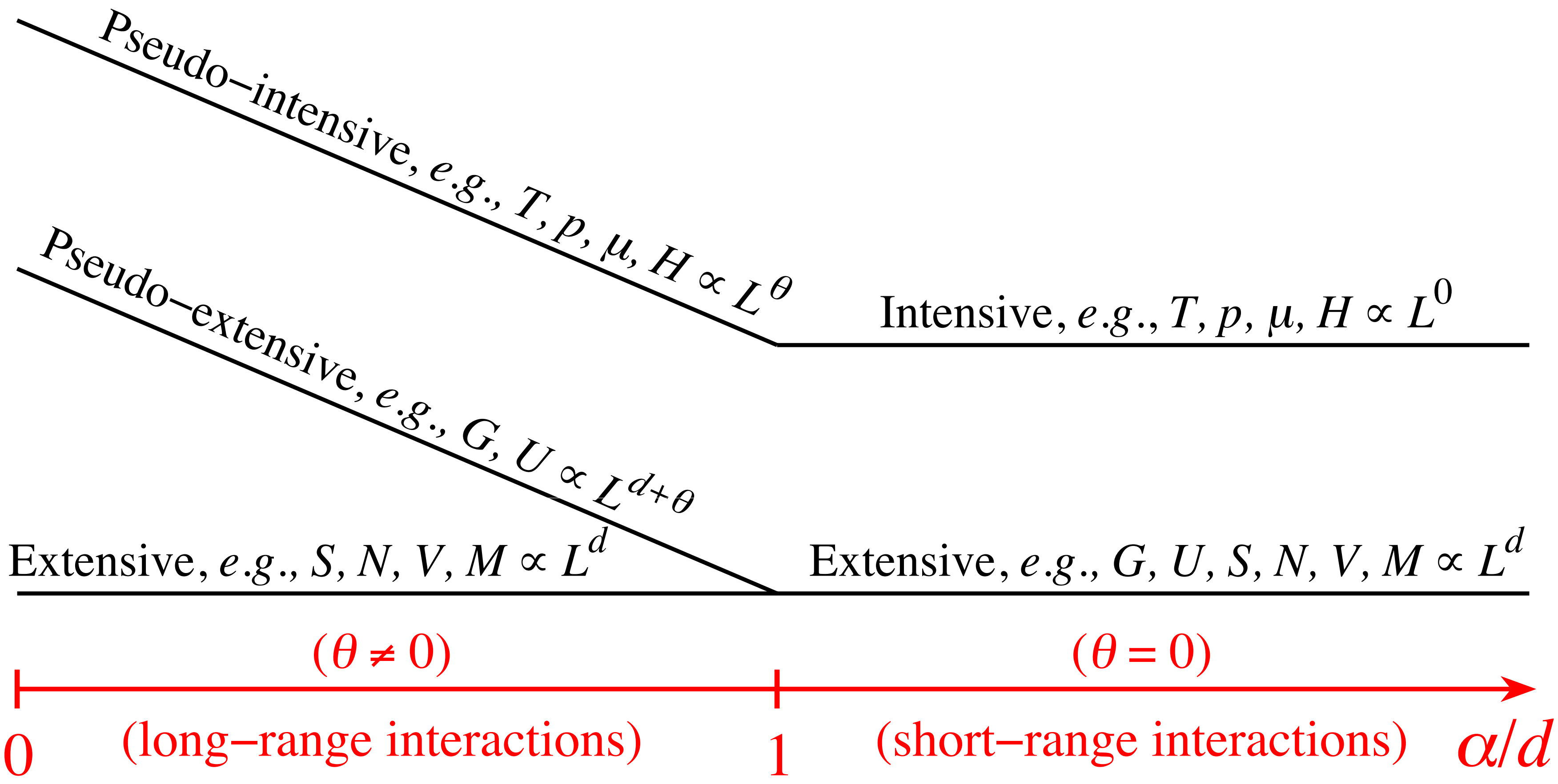
$G,U,\ldots$ scale like L^ε

hence $\varepsilon=\theta+\mathrm{d}$

Dividing by $L^{\theta+d}$ we obtain

$$g\left(\frac{T}{L^\theta},\frac{p}{L^\theta},\frac{\mu}{L^\theta},\frac{H}{L^\theta},\ldots\right)=u\left(\frac{T}{L^\theta},\frac{p}{L^\theta},\frac{\mu}{L^\theta},\frac{H}{L^\theta},\ldots\right)-\frac{T}{L^\theta}s\left(\frac{T}{L^\theta},\frac{p}{L^\theta},\frac{\mu}{L^\theta},\frac{H}{L^\theta},\ldots\right)$$
$$+\frac{p}{L^\theta}-\frac{\mu}{L^\theta}n\left(\frac{T}{L^\theta},\frac{p}{L^\theta},\frac{\mu}{L^\theta},\frac{H}{L^\theta},\ldots\right)-\frac{H}{L^\theta}m\left(\frac{T}{L^\theta},\frac{p}{L^\theta},\frac{\mu}{L^\theta},\frac{H}{L^\theta},\ldots\right)-\ldots$$

where all variables are intensive.



–Classical short-range-interacting many-body Hamiltonian systems

(i.e., $\alpha > d$) $\Rightarrow \theta = 0 \Rightarrow \varepsilon = d$ (textbooks)

–Classical long-range-interacting many-body Hamiltonian systems

(i.e., $0 \leq \alpha < d$) $\Rightarrow \theta = d - \alpha \Rightarrow \varepsilon = 2d - \alpha$ (widely verified in the literature)

–Schwarzschild (3+1)-dimensional black hole $\Rightarrow M_{bh} \propto L \Rightarrow \varepsilon = 1 \Rightarrow \theta = 1 - d$

–Banados-Teitelboim-Zanelli (2+1)-dimensional black hole $\Rightarrow \varepsilon = 2 \Rightarrow \theta = 2 - d$

CONSEQUENCES OF $\varepsilon = \theta + d$:

1) Standard thermodynamical systems $\Rightarrow \boxed{\theta = 0} \Rightarrow \varepsilon = d$ (i.e., extensive energies)

2) Classical long-range-interacting many-body Hamiltonian systems (i.e., $0 \le \alpha < d$)

$\Rightarrow \boxed{\theta = d - \alpha} \Rightarrow \varepsilon = 2d - \alpha$ (widely verified in the literature)

3) Schwarzschild (3+1)-dimensional black hole $\Rightarrow M_{bh} \propto L \Rightarrow \varepsilon = 1 \Rightarrow \boxed{\theta = 1 - d}$

- If the black hole is identified with its event horizon, then $d = 2$, hence $\theta = -1$, which recovers the Bekenstein-Hawking scaling $T \propto 1/L \propto 1/M_{bh}$

  The thermodynamical entropy can be identified with S_{BG} .

- If the black hole is identified with $d = 3$, then $\theta = -2$, i.e., $T \propto 1/L^2 \propto 1/M_{bh}^2$

  The thermodynamical entropy can not be identified with S_{BG} .

4) Banados-Teitelboim-Zanelli (2+1)-dimensional black hole $\Rightarrow \varepsilon = 2 \Rightarrow \boxed{\theta = 2 - d}$

- If the black hole is identified with its event horizon, then $d = 1$, hence $\theta = 1$, i.e., $T \propto L \propto M_{bh}^{1/2}$

  The thermodynamical entropy can be identified with S_{BG} .

- If the black hole is identified with $d = 2$, then $\theta = 0$, which recovers the BTZ scaling $T \propto$ constant (i.e., intensive).

  The thermodynamical entropy can not be identified with S_{BG} .

Nonextensive statistical mechanics

- Connection with thermodynamics

C. T.
Possible generalization of Boltzmann-Gibbs statistics
J Stat Phys **52**, 479 (1988)

E.M.F. Curado and C. T.
Generalized statistical mechanics: connection with thermodynamics
J Phys A **24**, L69 (1991)
[Corrigenda: **24**, 3187 (1991) and **25**, 1019 (1992)]

C. T., R.S. Mendes and A.R. Plastino
The role of constraints within generalized nonextensive statistics
Physica A **261**, 534 (1998)

NONEXTENSIVE STATISTICAL MECHANICS AND THERMODYNAMICS (CANONICAL ENSEMBLE):

Extremization of the functional

$$S_q[p_i] \equiv k \frac{1 - \sum_{i=1}^{W} p_i^q}{q-1}$$

with the constraints

$$\sum_{i=1}^{W} p_i = 1 \qquad \textit{and} \qquad \frac{\sum_{i=1}^{W} p_i^q E_i}{\sum_{i=1}^{W} p_i^q} = U_q$$

yields

$$p_i = \frac{e_q^{-\beta_q (E_i - U_q)}}{\mathbf{Z}_q}$$

with $\beta_q \equiv \frac{\beta}{\sum_{i=1}^{W} p_i^q}$, $\beta \equiv$ *energy Lagrange parameter*, *and* $\mathbf{Z}_q \equiv \sum_{i=1}^{W} e_q^{-\beta_q (E_i - U_q)}$

We can rewrite $$p_i = \frac{e_q^{-\beta'_q E_i}}{Z'_q}$$

with $$\beta'_q \equiv \frac{\beta_q}{1+(1-q)\beta_q U_q}\ , \quad and \quad Z'_q \equiv \sum_{i=1}^{W} e_q^{-\beta'_q E_i}$$

And we can prove

$$(i) \qquad \frac{1}{T} = \frac{\partial S_q}{\partial U_q} \quad with \quad T \equiv \frac{1}{k\beta}$$

$$(ii) \qquad F_q \equiv U_q - TS_q = -\frac{1}{\beta}\ln_q Z_q \quad where \quad \ln_q Z_q = \ln_q \mathbb{Z}_q - \beta U_q$$

$$(iii) \qquad U_q = -\frac{\partial}{\partial \beta}\ln_q Z_q$$

$$(iv) \qquad C_q \equiv T\frac{\partial S_q}{\partial T} = \frac{\partial U_q}{\partial T} = -T\frac{\partial^2 F_q}{\partial T^2},\ \forall q$$

(*i.e., the Legendre structure of Thermodynamics is q-invariant!*)

11. *Theorie der Opaleszenz von homogenen Flüssigkeiten und Flüssigkeitsgemischen in der Nähe des kritischen Zustandes;*
von A. Einstein.

(1) $$S = \frac{R}{N} \lg W + \text{konst.}$$

Daß die zwischen S und W in Gleichung (1) gegebene Beziehung die einzig mögliche ist, kann bekanntlich aus dem Satze abgeleitet werden, daß die Entropie eines aus Teilsystemen bestehenden Gesamtsystems gleich ist der Summe der Entropien der Teilsysteme.

The relation between *S* and *W* given in Eq. (1) is the only reasonable given the proposition that the entropy of a system consisting of subsystems is equal to the sum of entropies of the subsystems.

[Free translation by Tobias Micklitz]