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POSSIBLE GENERALIZATION OF BOLTZMANN-GIBBS STATISTICS

by

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ABSTRACT

Using the quantity normally scaled in multifractals we postulate a generalized form for the entropy, namely $S_q \equiv k\left[1 - \sum_{i=1}^{W} p_i^q\right]/(q-1)$, where $q \in \mathbb{R}$ characterizes the generalization and $\{p_i\}$ are the probabilities associated with W(microscopic) configurations ($W \in \mathbb{N}$). We establish the main properties associated with this entropy, in particular those corresponding to the microcanonical and canonical ensembles. The Boltzmann-Gibbs statistics is recovered as the $q \to 1$ limit.

Key-words: Generalized statistics; Entropy; Multifractals; Statistical ensembles.

Multifractal concepts and structures are quickly acquiring importance in many active areas (e.g., non-linear dynamical systems, growth models, commensurate/incommensurate structures). This is due to their utility as well as to their elegance. Within this framework, the quantity which is normally scaled is p_i^q, where p_i is the probability associated to an event and q any real number [1]. We shall use this quantity to generalize the standard expression of the entropy S in information theory, namely $S = -k\sum_{i=1}^{W} p_i \ln p_i$, where $W \in \mathbb{N}$ is the total number of possible (microscopic) configurations and $\{p_i\}$ the associated probabilities. We *postulate* for the entropy

$$S_q \equiv k\,\frac{1-\sum_{i=1}^{W} p_i^q}{q-1} \qquad (q \in \mathbb{R}) \tag{1}$$

where k is a conventional positive constant and $\sum_{i=1}^{W} p_i = 1$. We immediately verify that

$$S_1 \equiv \lim_{q\to 1} S_q = k\lim_{q\to 1}\frac{1-\sum_{i=1}^{W} p_i e^{(q-1)\ln p_i}}{q-1} = -k\sum_{i=1}^{W} p_i \ln p_i \tag{1'}$$

where we have used the replica-trick type of expansion. We illustrate definition (1) in Fig. 1. S_q may be rewritten as follows:

$$S_q = \frac{k}{q-1}\sum_{i=1}^{W} p_i\left(1-p_i^{q-1}\right) \tag{2}$$

which makes evident that $S_q \geq 0$ in all cases. It vanishes for $W = 1$, $\forall q$, as well as for $W > 1$, $q > 0$ and only one event with probability one (all the others having vanishing probabilities).

Microcanonical ensemble: We want to extremize S_q with the condition $\sum_{i=1}^{W} p_i = 1$. By introducing a Lagrange parameter it is straightforward to obtain that S_q is extremized, *for all values of q*, in the case of *equiprobability*, i.e., $p_i = 1/W, \forall i$, and consequently

$$S_q = k \frac{W^{1-q} - 1}{1-q} \tag{3}$$

We immediately verify that

$$S_1 = k \ln W \tag{3'}$$

thus recovering the celebrated Boltzmann's expression. We illustrate Eq. (3) in Fig. 2. S_q given by Eq. (3) diverges if $q \leq 1$ and saturates (at $S_q = k/(q-1)$) if $q > 1$, in the $W \to \infty$ limit. It is straightforward to prove that the extremum indicated in Eq. (3) is a maximum (minimum) for $q > 0$ ($q < 0$); for $q = 0$, $S_q(\{p_i\}) = k(W-1)$ for all $\{p_i\}$. Finally, Eq. (3) implies

$$\frac{S_q}{k} = \frac{e^{(1-q)S_1/k} - 1}{1-q} \tag{4}$$

Concavity: Let us extend here a property already mentioned, namely that $q > 0$ ($q < 0$) implies that the extremum of S_q is a maximum (minimum). Let $\{p_i\}$ and $\{p_i'\}$ be two sets of probabilities corresponding to a unique set of W possibilities, and λ such that $0 < \lambda < 1$. We define an *intermediate* probability law as follows

$$p_i'' \equiv \lambda p_i + (1-\lambda)p_i' \quad (\forall i) \tag{5}$$

and also

$$\Delta_q \equiv S_q(\{p_i''\}) - \left[\lambda S_q(\{p_i\}) + (1-\lambda)S_q(\{p_i'\})\right] \tag{6}$$

It is straightforward to prove that $\Delta_q \geq 0$ if $q > 0$, $\Delta_q \leq 0$ if $q < 0$ and $\Delta_q = 0$ if $q = 0$. The equalities hold for $q \neq 0$ for $p_i = p_i'$, $\forall i$. The proof follows from Eq. (2) and the discussion of the function $p_i(1-p_i^{q-1})/(q-1)$. Indeed, this function presents, for $p_i \in (0,1)$, a negative, positive or vanishing curvature for $q > 0$, $q < 0$ and $q = 0$ respectively.

Additivity: Let us assume two *independent* systems A and B with ensembles of configurational possibilities $\Omega^A \equiv \{1,2,\ldots,i,\ldots,W_A\}$ and $\Omega^B \equiv \{1,2,\ldots,j,\ldots,W_B\}$ respectively, the corresponding probabilities being $\{p_i^A\}$ and $\{p_j^B\}$. We now consider $A\cup B$, the ensemble of possibilities being $\Omega^{A\cup B} \equiv \{(1,1),(1,2),\ldots,(i,j),\ldots,(W_A,W_B)\}$; we note $p_{ij}^{A\cup B}$ the corresponding probabilities. The independence of the systems means that $p_{ij}^{A\cup B} = p_i^A p_j^B$, $\forall (i,j)$, hence $\sum_{i,j}^{W_A W_B} (p_{ij}^{A\cup B})^q = \left[\sum_{i=1}^{W_A} (p_i^A)^q\right]\left[\sum_{j=1}^{W_B} (p_j^B)^q\right]$, hence ((using Eq. (1)).

$$\bar{S}_q^{A\cup B} = \bar{S}_q^A + \bar{S}_q^B \quad \text{(additivity)} \tag{7}$$

with

$$\bar{S}_q \equiv k\,\frac{\ell n[1+(1-q)S_q/k]}{1-q} \tag{8}$$

In the $q \to 1$ limit, Eq. (7) becomes $S_1^{AUB} = S_1^A + S_1^B$, thus recovering the standard additivity of the entropies of independent systems.

To study the case of *correlated* systems (i.e., p_{ij}^{AUB} is not equal to $(\sum_{i=1}^{W_A} p_{ij}^{AUB})(\sum_{j=1}^{W_B} p_{ij}^{AUB})$ for all (i,j)) it is useful to define $\Gamma_q(\{p_{ij}^{AUB}\}) \equiv \bar{S}_q^{AUB}(\{p_{ij}^{AUB}\}) - \bar{S}_q^A(\{\sum_{j=1}^{W_B} p_{ij}^{AUB}\}) - \bar{S}_q^B(\{\sum_{i=1}^{W_A} p_{ij}^{AUB}\})$. It is clear from Eq. (7) that independency (no correlation) implies $\Gamma_q = 0$, $\forall q$. For arbitrary and fixed $\{p_{ij}^{AUB}\}$ implying correlation, it is easy to prove that $\Gamma_1 < 0$ (*sub-additivity* of the standard entropies of correlated systems) and $\Gamma_o = 0$. For arbitrary values of q, Γ_q presents a great sensitivity to $\{p_{ij}^{AUB}\}$, it might be positive or negative for $q \gg 1$ as well as for $q \ll -1$, and typically exhibits more than one extrema. Extensive and systematic computer verification indicates that, generally speaking, Γ_q varies smoothly with q but presents no particular regularities besides $\Gamma_o = 0$ and $\Gamma_1 \le 0$. When $\{p_{ij}^{AUB}\}$ gradually approach vanishing correlation, Γ_q gradually flattens until eventually achieving $\Gamma_q = 0$, $\forall q$.

Canonical ensemble: We want to extremiza S_q with the conditions $\sum_{i=1}^{W} p_i = 1$ and

$$\sum_{i=1}^{W} p_i \varepsilon_i = U_q \tag{9}$$

where $\{\varepsilon_i\}$ and U_q are known real numbers (the same value ε_i might be associated to more than one possible configuration); we shall refer to them as *generalized spectrum* and *generalized internal energy*. We introduce the α and β Lagrange parameters and define the quantity

$$\phi_q \equiv \frac{S_q}{k} + \alpha \sum_{k=1}^{W} p_i - \alpha\beta(q-1) \sum_{i=1}^{W} p_i \varepsilon_i \tag{10}$$

which has been written this way for future convenience. We impose $\partial\phi_q/\partial p_i = 0$, $\forall i$, and obtain $p_i \propto [1 - \beta(q-1)\varepsilon_i]^{\frac{1}{q-1}}$, hence

$$p_i = \frac{[1 - \beta(q-1)\varepsilon_i]^{\frac{1}{q-1}}}{Z_q} \tag{11}$$

with

$$Z_q \equiv \sum_{\ell=1}^{W} [1 - \beta(q-1)\varepsilon_\ell]^{\frac{1}{q-1}} \tag{12}$$

We immediately verify that, in the $q \to 1$ limit, we recover

$$p_i = e^{-\beta\varepsilon_i}/Z_1 \tag{11'}$$

with

$$Z_1 \equiv \sum_{\ell=1}^{W} e^{-\beta\varepsilon_i} \tag{12'}$$

If A and B are two *independent* systems with probabilities (spectrum) $\{p_i^A\}(\{\varepsilon_i^A\})$ and $\{p_j^B\}(\{\varepsilon_j^B\})$ respectively, the probabilities corresponding to AUB satisfy $p_{ij}^{AUB} = p_i^A p_j^B$, $\forall (i,j)$. This implies

$$1 - \beta(q-1)\varepsilon_{ij}^{AUB} = \left[1 - \beta(q-1)\varepsilon_i^A\right]\left[1 - \beta(q-1)\varepsilon_j^B\right] \tag{13}$$

or equivalently

$$\bar{\varepsilon}_{ij}^{AUB} = \bar{\varepsilon}_i^A + \bar{\varepsilon}_j^B \tag{14}$$

with

$$\bar{\varepsilon} \equiv \frac{\ell n\left[1 + \beta(1-q)\varepsilon\right]}{\beta(1-q)} \tag{15}$$

In the $q \to 1$ limit (and/or $\beta \to 0$ limit), Eq. (14) becomes $\varepsilon_{ij}^{AUB} = \varepsilon_i^A + \varepsilon_j^B$, thus recovering the standard energy additivity. The property (14), together with the factorization of probabilities, replaced in Eq. (9) yields

$$\bar{U}_q^{AUB} = \bar{U}_q^A + \bar{U}_q^B \tag{16}$$

with

$$\bar{U}_q \equiv \frac{\ell n\left[1 + \beta(1-q)U_q\right]}{\beta(1-q)} \tag{17}$$

In the $q \to 1$ limit (and/or the $\beta \to 0$ limit) Eq. (16) becomes $U_1^{AUB} = U_1^A + U_1^B$, thus recovering the standard additivity of the internal energies of independent systems.

Let us now discuss the main characteristics of distribution law (11). First of all we notice that this distribution is *invariant* under the transformation $[1-\beta(q-1)\varepsilon_\ell] \to [1-\beta(q-1)\varepsilon_\ell][1-\beta(q-1)\varepsilon_o]$ for all ℓ, ε_o being an arbitrary fixed real number. In other words, the distribution (11) is invariant under $\bar{\varepsilon}_\ell \to \bar{\varepsilon}_\ell + \bar{\varepsilon}_o$ (this is in fact a trivial consequence from the fact that the distribution can be formally rewritten as $p_i \propto \exp(-\beta\bar{\bar{\varepsilon}}_i)$). For $\beta(q-1) \to 0$, we recover the well known invariance of the Boltzmann-Gibbs statistics under uniform translation of the energy spectrum. We illustrate distribution (11) in Fig. 3. We notice that, for $q > 1$, $p_i = 0$ for all levels such that $\varepsilon_i \geq 1/[\beta(q-1)]$ ($\varepsilon_i \leq -1/[|\beta|(q-1)]$) if $\beta > 0$ ($\beta < 0$), i.e. positive (negative) "temperatures". On the other hand we notice that, for $q < 1$, the levels such that $\varepsilon_i \leq -1[\beta(1-q)]$ ($\varepsilon_i \geq 1/[|\beta|(1-q)]$) are, if $\beta > 0$ ($\beta < 0$), highly occupied, in a way which clearly reminds the Bose-Einstein condensation.

To better realize the unusual properties of the present statistics it is instructive to analyze the following situation. Assume $q > 1$, $\beta > 0$ and $\{\varepsilon_i\}$ such that $0 < \varepsilon_1 < \varepsilon_2 \ldots < \varepsilon_W$ (W might even diverge). When $1/\beta$ is above $(q-1)\varepsilon_W$, all levels have a finite occupancy probability; when $(q-1)\varepsilon_{W-1} < 1/\beta < (q-1)\varepsilon_W$, then $p_1 > p_2 > \ldots > p_{W-1} > p_W = 0$. The probabilities successively vanish while $1/\beta$ decreases. We eventually arrive to $(q-1)\varepsilon_1 < 1/\beta < (q-1)\varepsilon_2$, which implies $p_1 = 1$. Finally, the temperatures $1/\beta$ in the interval $[0,(q-1)\varepsilon_1]$ are physically unaccessible, thus generalizing the non-accessibility of $1/\beta = 0$ in standard thermodynamics. Let us illustrate this and similar facts through a simple example.

Application: We consider two non-degenerate levels with values $\varepsilon_1 \equiv \varepsilon - \delta$ and $\varepsilon_2 \equiv \varepsilon + \delta$ ($\delta > 0$; $\varepsilon \gtrless 0$). The quantity $U_q(\beta)$ is given by $U_q = \varepsilon_1 p_1 + \varepsilon_2 p_2$. A straightforward calculation yields

$$y_q = -\frac{\left[1-(q-1)(\frac{\varepsilon}{\delta}-1)/x\right]^{\frac{1}{q-1}} - \left[1-(q-1)(\frac{\varepsilon}{\delta}+1)/x\right]^{\frac{1}{q-1}}}{\left[1-(q-1)(\frac{\varepsilon}{\delta}-1)/x\right]^{\frac{1}{q-1}} + \left[1-(q-1)(\frac{\varepsilon}{\delta}+1)/x\right]^{\frac{1}{q-1}}} \tag{18}$$

with $x \equiv 1/\beta\delta$ and $y_q = (U_q - \varepsilon)/\delta \in [-1,1]$. Eq. (18) is invariant under $(x, y_q, q-1, \varepsilon/\delta) \to (x, y_q, -(q-1), -\varepsilon/\delta)$ and also under $(x, y_q, q, \varepsilon/\delta) \to (-x, -y_q, q, -\varepsilon/\delta)$. Consequently, it suffices to discuss $q \geq 1$ and $\varepsilon/\delta \geq 0$. In the limit $q \to 1$, we obtain $y_1 = -\text{th}(1/x)$, $\forall\ \varepsilon/\delta$. For $q \neq 1$, $y_q(x)$ depends on ε/δ: see Figs. 4 and 5.

Let us conclude by recalling that, using the quantity normally scaled for multifractals, we have postulated an expression for the entropy which generalizes the usual one (recovered for the parameter $q \to 1$). By preserving the standard variational principle we have established the microcanonical and canonical distributions, as well as several other properties. Some of the emerging peculiar characteristics are illustrated through a simple example. One of the most interesting is the fact that the unaccessible "temperatures" might belong to a *finite* interval which shrinks on the $T=0$ point in the $q\to$ limit. Finally, the fact that S_q/k, $\beta\varepsilon_i$ and βU_q are *additive under one and the same functional form* (namely $f(x) \equiv \ln[1+(1-q)x]/(q-1)$) opens the door to the generalization of standard Thermodynamics through the introduction of appropriate generalized thermodynamic potentials. Applications of these generalized equilibrium statistics in Physics (e.g., fractals, multifractals), Information Theory or any other branch of knowledge using probabilistic concepts would be extremely welcome.

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CAPTION FOR FIGURES

Fig. 1 - $S_q(\{p_i\})$ for $W=2$ and typical values of q (numbers on curves).

Fig. 2 - Value of the entropy at its extremum for typical values of q (numbers on curves). The dashed line indicates the $W \to \infty$ asymptotic of S_2/k.

Fig. 3 - The distribution law of Eq. (11) as a function of $\beta\varepsilon_i$. The curves are parametrized by q. (i) $q=1$: standard exponential law; (ii) $q>1$: the distribution presents a cut-off at $\beta\varepsilon_i = 1/(q-1)$ (with a slope which is $0, -1$ and $-\infty$ for $q<2$, $q=2$ and $q>2$ respectively) and diverges for $\beta\varepsilon_i \to -\infty$; (iii) $q<1$: the distribution diverges at $\beta\varepsilon_i = -1/(1-q)$ (the dashed line indicates the asymptote for $q=0$) and vanishes for $\beta\varepsilon_i \to +\infty$.

Fig. 4 - $q=2$ reduced internal "energy" as a function of the reduced "temperature" (see the text) for a non-degenerate two level system and typical values of ε/δ. The dashed region in (d) indicates the unaccessible "temperatures".

Fig. 5 - Reduced internal "energy" as a function of the reduced "temperature" (see the text) for a non-degenerate two level system and typical values of q (numbers on curves).

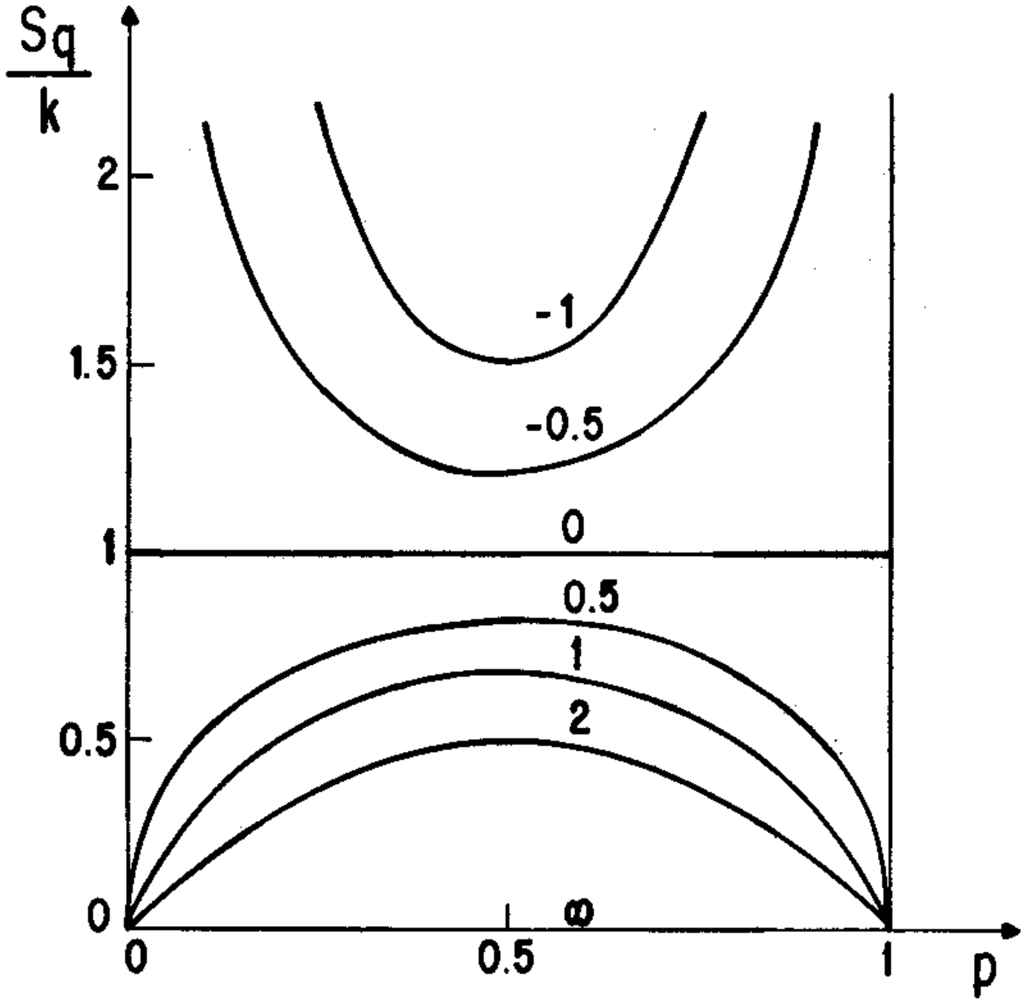

FIG.1

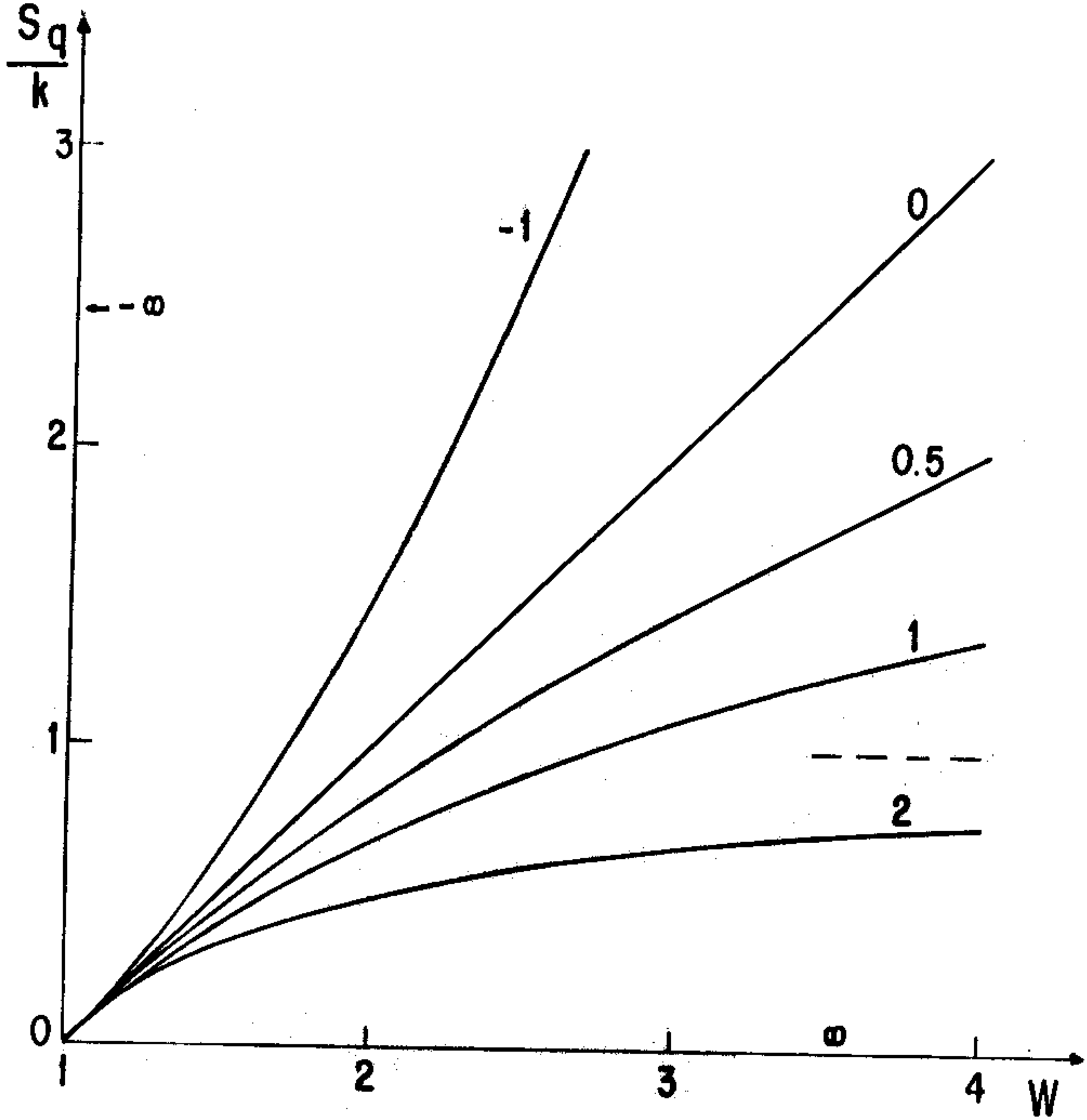

FIG. 2

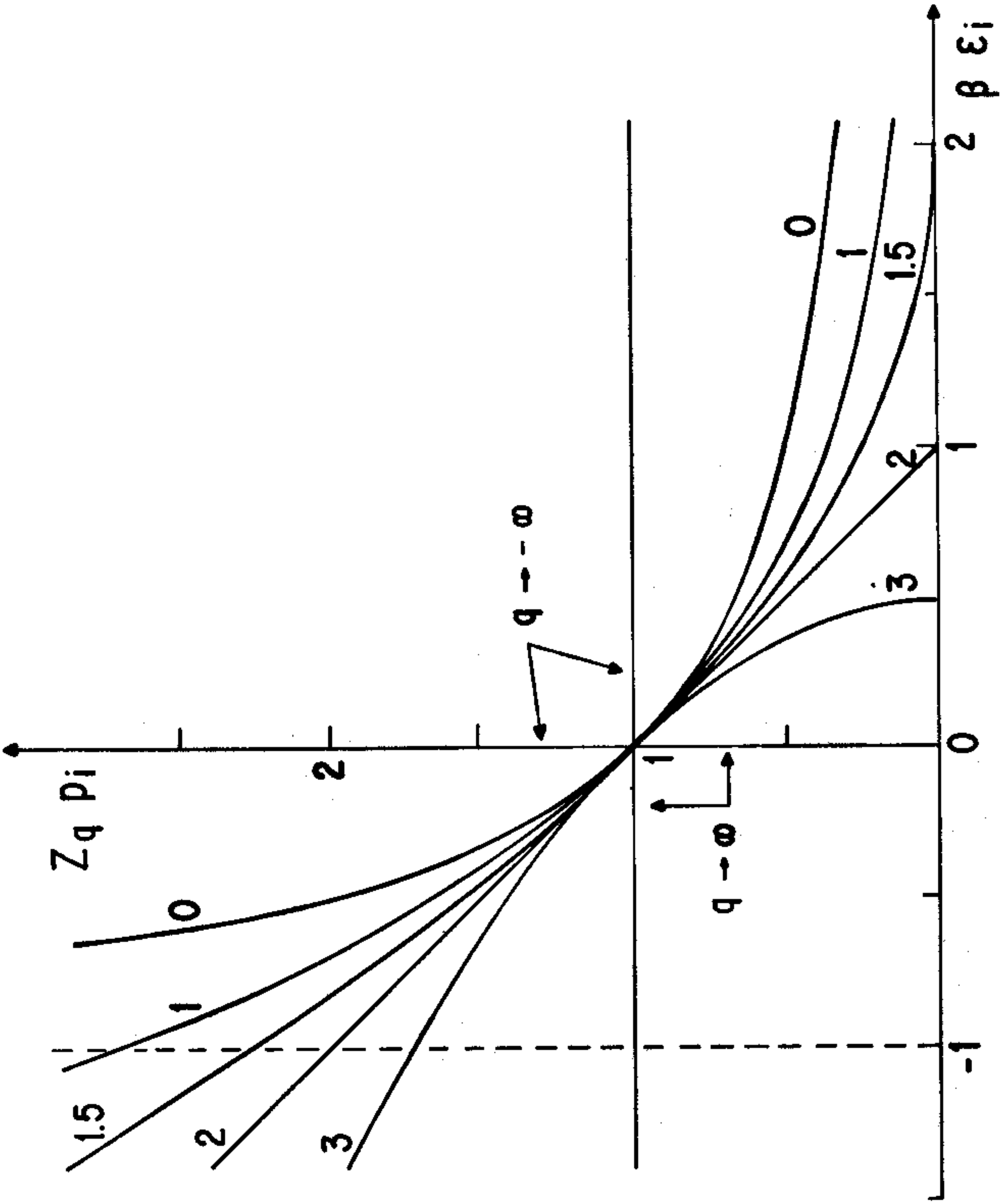

FIG. 3

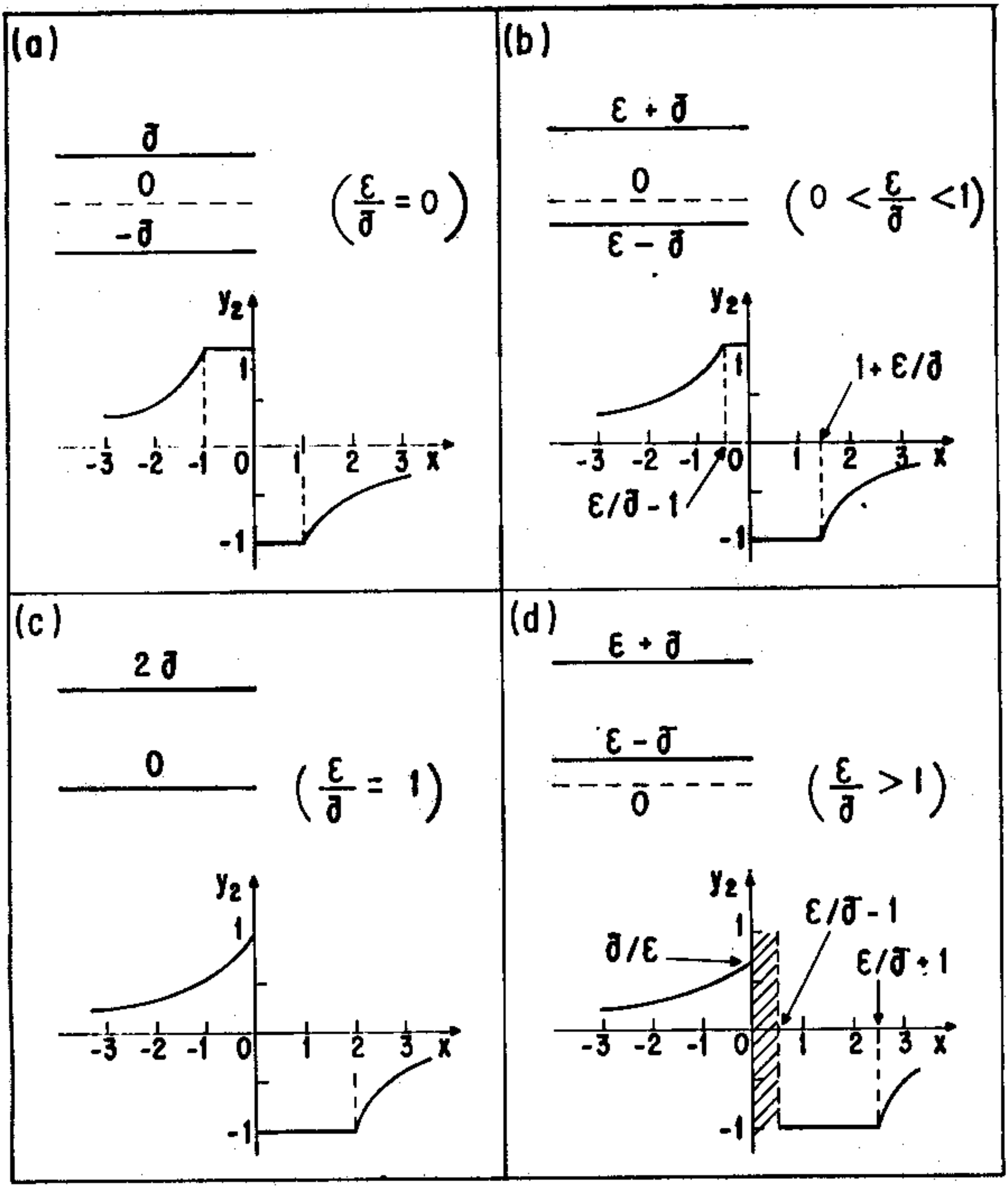
(a)
∂
0
-∂
(ε/∂ = 0)
y2
1
-3 -2 -1 0 1 2 3 x
-1
(b)
ε + ∂
0
ε − ∂
(0 < ε/∂ < 1)
y2
1
1+ ε/∂
-3 -2 -1 0 1 2 3 x
ε/∂ - 1
-1
(c)
2 ∂
0
(ε/∂ = 1)
y2
1
-3 -2 -1 0 1 2 3 x
-1
(d)
ε + ∂
ε − ∂
0
(ε/∂ > 1)
y2
1
ε/∂ - 1
∂/ε
ε/∂ + 1
-3 -2 -1 0 1 2 3 x
-1

FIG.4

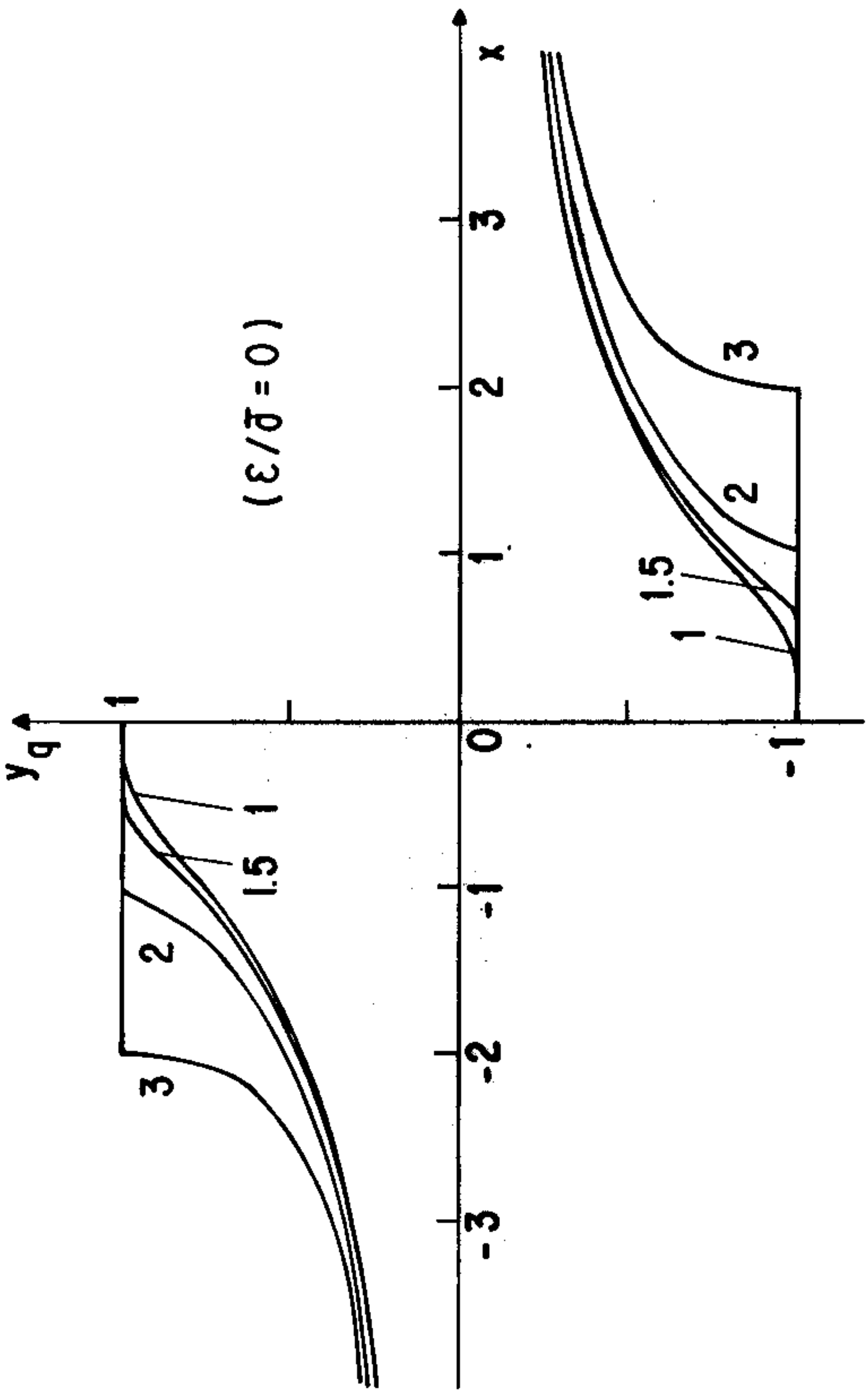

FIG.5

REFERENCES

[1] - H.G.E. Hentschel and I. Procaccia, Physica D 8, 435 (1983); T.C. Halsley, M.H. Jensen, L.P. Kadanoff, I. Procaccia and B.I. Shraiman, Phys. Rev. A 33, 1141 (1986).