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Majorization and disorder Majorization and disorder in generalized thermal states in generalized thermal

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Majorization and disorder in generalized thermal states

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Majorization Theory

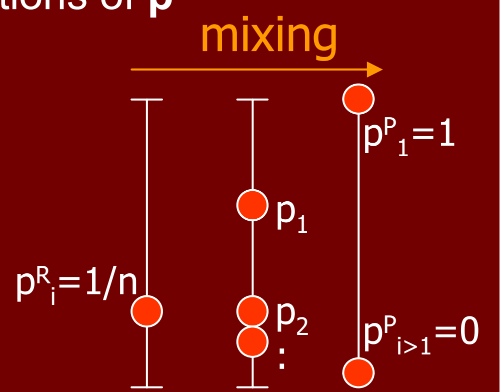
n-dimensional quantum system
density matrix ρ
eigenvalues p_i : $\sum_{i=1}^{n} p_i = 1, \quad p_i \in [0,1]$

(decreasing order: **p**↓) $1 \geq p_1 \geq p_2 \geq \ldots \geq p_n \geq 0$
"cumulants" : $s_j \equiv p_1 + p_2 + \ldots + p_j \qquad (s_n = 1)$

$$\rho \prec \rho' \;\Leftrightarrow\; s_j \leq s'_j \quad \forall j = 1, \ldots, n-1$$

ρ is **more mixed** than ρ'
p is **majorized** by **p'**

p can be written as a probabilistic (convex) combination of permutations of **p'**
In this sense: **p** is **more disordered** than **p'**



Trivial examples

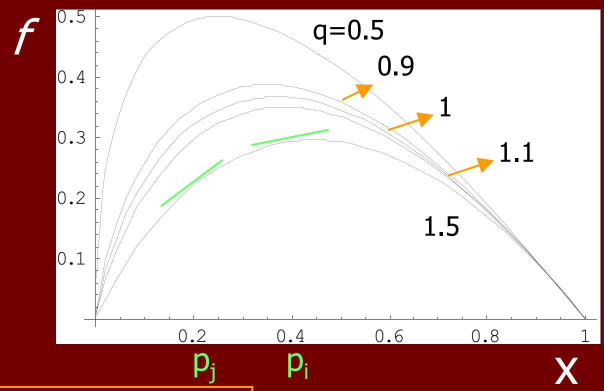
Tot.random state: $\mathbf{p}^R=(1/n,1/n,\ldots,1/n)$, $s^R_j=j/n$ $\quad \rho^R \prec \rho$
Any state: $\quad \rho^R \prec \rho \prec \rho^P$
Pure state: $\mathbf{p}^P = (1,0,\ldots,0)$, $s^P_j=1$ $\quad \rho \prec \rho^P$

Majorization and Entropy

general trace-form entropies : $S_f(\hat{\rho}) = \mathrm{Tr} f(\hat{\rho}) = \sum_{i=1}^{n} f(p_i)$

with f: [0,1] → R , $f(0)=f(1)=0$, smooth, strictly concave

$(\ f'' < 0 \quad \text{i.e.} \quad f'(p_i) < f'(p_j) \ \text{ if } \ p_i > p_j \ )$



Examples

- von Neumann : $f(x) = -x \ln(x)$
- Tsallis (q > 0) : $f(x) = (x - x^q) / (q-1) = x \ln_q(1/x)$

  where $\ln_q(x) = (x^{1-q} - 1)/(q-1)$

$\rho \prec \rho' \ \Rightarrow \ S_f(\rho) \geq S_f(\rho')$ for ANY f

but

$S_f(\rho) \geq S_f(\rho')$ for a GIVEN f $\not\Rightarrow$ $\rho \prec \rho'$

however

$S_f(\rho) \geq S_f(\rho')$ for ANY f $\ \Rightarrow \ \rho \prec \rho'$

*Majorization gives stronger idea of **disorder** than a given entropy form.*
Increasing mixedness is characterized by a universal entropy increase.

Mixing parameter

Let $\rho = \rho(\lambda)$ where λ is a continuous parameter

$$\lambda = \text{mixing parameter for } \rho(\lambda) \quad \Leftrightarrow \quad \rho(\lambda) \prec \rho(\lambda') \text{ if } \lambda \geq \lambda'$$

Iff $s_j(\lambda) \leq s_j(\lambda')$, i.e. s_j is a decreasing function of λ for all j. Then

$$\lambda = \text{mixing parameter for } \rho(\lambda) \quad \Leftrightarrow \quad \frac{d\, s_j}{d\, \lambda} \leq 0 \quad \forall\ j = 1, \ldots, n-1$$

*The system becomes **more mixed** as the parameter increases (in certain interval).*

Consequences:

a) ANY increasing function $\tilde{\lambda}(\lambda)$ is a *mixing parameter* for ρ

b) *The general entropy S_f is a <u>non-decreasing</u> function of λ for ANY concave f* :

$$\frac{d\ S_f[\hat{\rho}(\lambda)]}{d\ \lambda} = \sum_{j=1}^{n-1} \underbrace{[f'(p_j) - f'(p_{j+1})]}_{f'(p_j) \leq f'(p_{j+1}) \quad \text{if } p_j \geq p_{j+1} \text{ and } f \text{ concave}} \frac{d\ s_j}{d\ \lambda} \quad \geq \quad 0$$

Example: escort densities

given density matrix ρ ⟹ associated escort densities ρ_q (q real)

$$\rho_q \equiv \frac{\rho^{\,q}}{Z_q}, \qquad Z_q = \mathrm{Tr}\ \rho^{\,q}$$

Let λ = 1/q :

$$s_{q,j} \equiv \sum_{i=1}^{j} p_{q,i} = \sum_{i=1}^{j} \frac{p_i^{\,q}}{Z_q} \qquad \rightarrow \qquad \frac{\partial s_{q,j}}{\partial \lambda} = -q^2 \sum_{i=1}^{j} \sum_{k=j+1}^{n} p_{q,i}\, p_{q,k} \ln \frac{p_i}{p_k} \ \leq\ 0$$

$p_{q,i} \geq p_{q,j}$ if $i \leq j$, for all q>0

Then

λ = 1/q

(as well as ANY decreasing function of q)
is a *mixing parameter* for ρ_q if q > 0 :

$$\hat{\rho}_q \prec \hat{\rho}_{q'} \quad \text{if} \quad \frac{1}{q} \geq \frac{1}{q'} > 0$$

As q decreases, escort densities of ρ describe more mixed states

Hamiltonian systems

hamiltonian $\hat{H}$

eigenvalues ϵ_i : $\epsilon_1 \le \epsilon_2 \le \ldots \le \epsilon_n$ (increasing order)

Assume

1) $\rho(\lambda)$:

$$\begin{cases} [\rho, H] = 0 \\ p_i \ge p_j \text{ if } i \le j \quad (p = \text{non-increasing with energy}) \\ \lambda \in (\lambda_m, \lambda_M) \text{ is a mixing parameter for } \rho(\lambda) \end{cases}$$

2) $w(H)$:

$$\begin{cases} w(\epsilon_i) \le w(\epsilon_j) \text{ if } i < j \quad (w = \text{non-decreasing with energy}) \\ w = \lambda\text{-independent} \end{cases}$$

Then

$$\frac{\partial \langle w(\hat{H}) \rangle_{\hat{\rho}}}{\partial \lambda} = \sum_{j=1}^{n-1} [w(\epsilon_j) - w(\epsilon_{j+1})] \frac{\partial s_j}{\partial \lambda} \quad \ge \quad 0$$

ANY non-decreasing function w of H is a non-decreasing function of λ

Examples:

- Average energy : <H>$_\rho$ = Tr $\rho(\lambda)$ H increases with λ
- Generalized "specific heat" : $c_\lambda \equiv \partial \langle \hat{H} \rangle_{\hat{\rho}} / \partial \lambda \ \ge \ 0$ (non-negative)

Thermal behaviour

Assume also

3) $\rho(\lambda)$: $\begin{cases} \to \hat{I}_1/n_1 \quad \text{(ground state)} & \text{if } \lambda \to \lambda_m \\ \to \hat{I}/n \quad \text{(totally random state)} & \text{if } \lambda \to \lambda_M \end{cases}$

Then $\rho(\lambda)$ has a "thermal-like behaviour" : $\rho(\lambda)$ becomes more mixed *monotonously* as λ increases, evolving from the g.s. to the totally random state

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Example: BG canonical distribution (ρ minimizes $\langle H\rangle_\rho$ - T S[ρ])

$$\rho_{BG}(\lambda \equiv T) = \frac{e^{-H/T}}{Z(T)}, \qquad Z(T) = \mathrm{Tr} e^{-H/T} \qquad (k_B = 1)$$

S [ρ_{BG}(T)] is known to be an <u>increasing</u> function of T

Moreover $$\frac{\partial s_j}{\partial T} = \sum_{i=1}^{j} \sum_{k=j+1}^{n} p_i p_k \frac{(\epsilon_i - \epsilon_k)}{T^2} \leq 0, \qquad p_i = e^{-\epsilon_i/T}/Z(T)$$

then $\rho_{BG}(T) \prec \rho_{BG}(T') \quad \text{if} \quad T \geq T' > 0$

λ = T ε (0,∞) is a <u>mixing parameter</u> for ρ_{BG}(T)

Also S_f [ρ_{BG}(T)] is an <u>increasing</u> function of T, for ANY concave *f*

Mixing for general densities

Assume $$\rho_g(\lambda) = \frac{g(H,\lambda)}{Z(\lambda)}, \qquad Z(\lambda) = \mathrm{Tr}\, g(H,\lambda)$$

with g(ε, λ) smooth, positive and non-increasing for ε in [ε_1, ε_n] ; [ρ (λ), H] = 0

Compute $$\underbrace{\frac{\partial s_j}{\partial \lambda}}_{\leq 0\ \forall j} = \sum_{i=1}^{j} \sum_{k=j+1}^{n} p_i p_k \underbrace{\left(\frac{\partial \ln g}{\partial \lambda}(\epsilon_i) - \frac{\partial \ln g}{\partial \lambda}(\epsilon_k) \right)}_{\leq 0 \text{ (i.e., } \frac{\partial \ln g}{\partial \lambda} \text{ non-decreasing with } \epsilon)}, \qquad p_i = \frac{g(\epsilon_i,\lambda)}{Z(\lambda)}$$

$\leq 0\ \forall j$ IF ≤ 0 (i.e., $\frac{\partial \ln g}{\partial \lambda}$ non-decreasing with ϵ)

Examples: $g(\epsilon, T) = e^{-\epsilon/T}$ gives $\frac{\partial \ln g}{\partial T} = \epsilon/T^2$ increasing with ϵ ;

$g_r(\epsilon,\lambda) = e^{-[(\epsilon-\epsilon_1)/\lambda]^r}, r > 0$ gives $\frac{\partial \ln g_r}{\partial \lambda} = \frac{r}{\lambda^2}\left(\frac{\epsilon-\epsilon_1}{\lambda}\right)^{r-1}$ increasing with ϵ, if $\lambda > 0$

Sufficient condition : If $\frac{\partial}{\partial \epsilon}\left(\frac{\partial \ln g}{\partial \lambda}\right) \geq 0$, then λ is a mixing parameter for ρ_g (λ)

ALSO for its associated escort distributions for positive values of q

Similar considerations apply for a *set* of λ-parameters : $\frac{\partial}{\partial \epsilon}\vec{\nabla}_{\vec{\lambda}} \ln g(\epsilon, \vec{\lambda})$

Power-law distributions

Consider the 2-parameters power-law distribution (in q-exponential form) :

$$\rho(q,T^*) = \frac{[I-(1-q)\bar{H}/T^*]_+^{1/(1-q)}}{Z(q,T^*)} = \frac{e_q(-\bar{H}/T^*)}{Z(q,T^*)}$$

with $[x]_+ = (x+|x|)/2$ and $\bar{H} = H - \varepsilon_1 I$ (excitation spectrum or $\varepsilon_1 := 0$)

Tsallis index q

effective temperature T*

$\rho(q,T) \xrightarrow{q \to 1} \rho_{BG}(T)$

For all q real and T* > 0, $\rho(q,T^*)$ satisfies :

- positivity
- commutativity with H
- non-increasing eigenvalues p_i as functions of (excitation) energy $\varepsilon_i - \varepsilon_1$

Indeed
- for q > 1 : p_i are strictly decreasing with ε_i
- for q < 1 : p_i are non-increasing with ε_i due to *high-energy cutoff.*
  $p_i = 0$ if $\varepsilon_i - \varepsilon_1 \geq T^*/(1-q)$

q and T* as mixing parameters for ρ (q,T*)

Let $$g(\bar{\epsilon}, q, T^*) \equiv [1-(1-q)\bar{\epsilon}/T^*]_+^{1/(1-q)} = e_q(-\bar{\epsilon}/T^*)$$

Then ($\bar{\varepsilon} \geq 0$) :

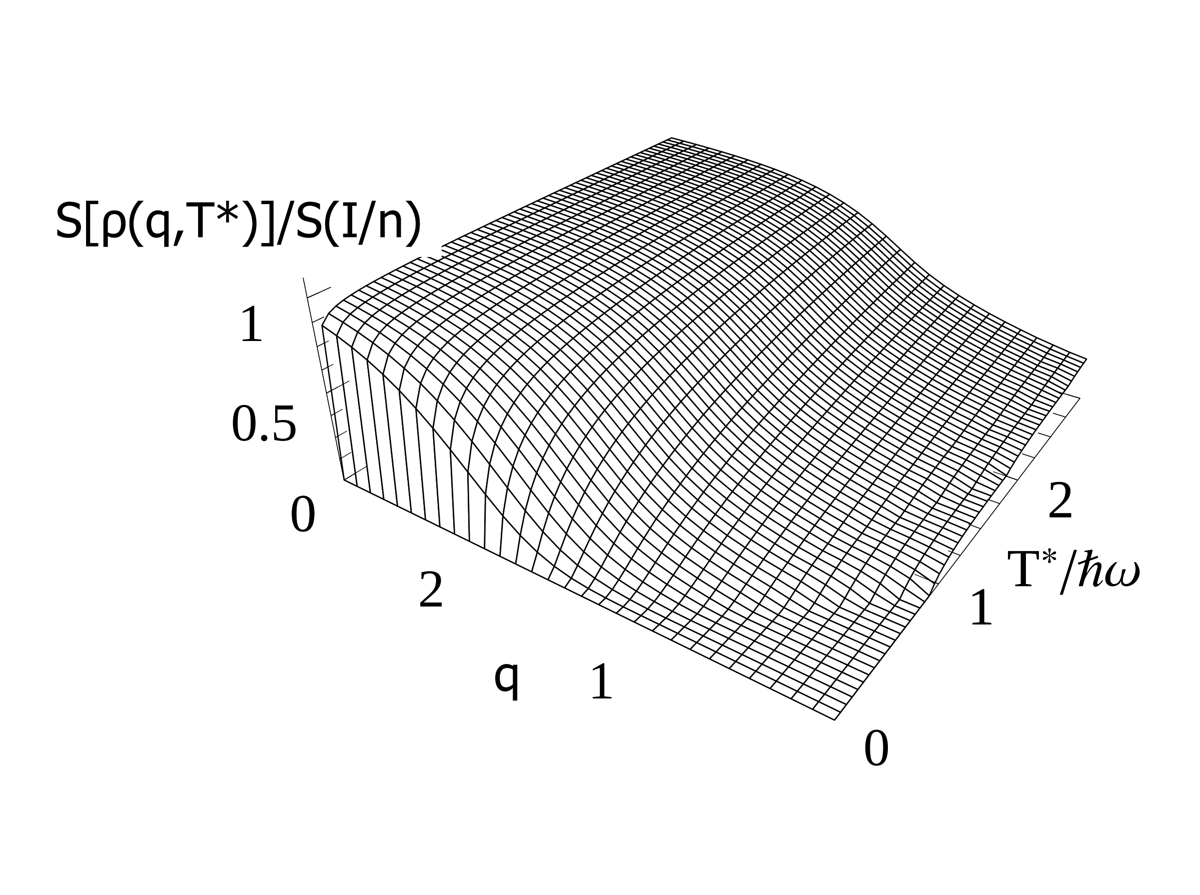
$$\frac{\partial}{\partial \bar{\epsilon}} \left(\frac{\partial \ln g}{\partial q} \right) = \frac{\bar{\epsilon}}{[T^* - (1-q)\bar{\epsilon}]^2} \geq 0$$

$$\frac{\partial}{\partial \bar{\epsilon}} \left(\frac{\partial \ln g}{\partial T^*} \right) = \frac{1}{[T^* - (1-q)\bar{\epsilon}]^2} \geq 0$$

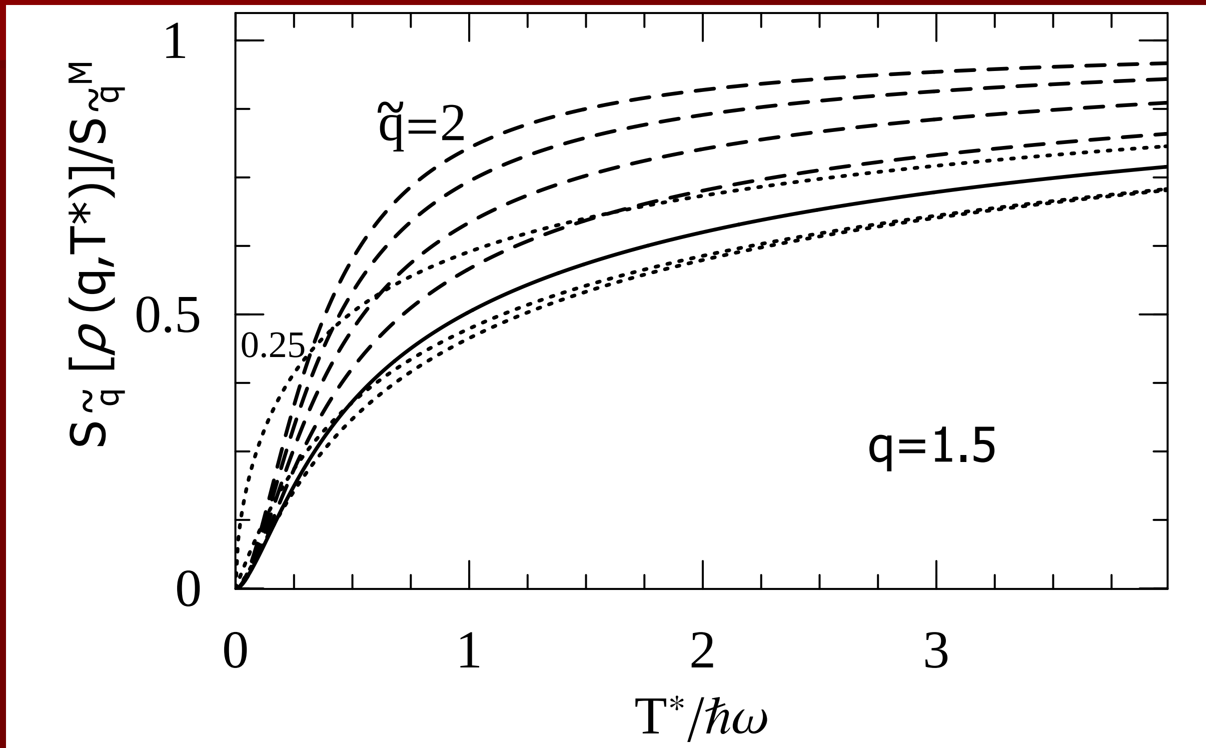
$$\rho(q, T^*) \prec \rho(q', T^*) \quad \text{if} \quad q \geq q'$$

$$\rho(q, T^*) \prec \rho(q, T^{*\prime}) \quad \text{if} \quad T^* \geq T^{*\prime} > 0$$

q-exponential states ρ (q,T*) have the fundamental property
of becoming *more mixed* as λ_1 = q OR λ_2 = T*>0 increases
AND
ANY general trace-form entropy S_f [ρ (q,T*)] (e.g. $S_{\tilde{q}}$[ρ (q,T*)], $\tilde{q}$>0)
is *non-decreasing* wrt q and wrt T*>0

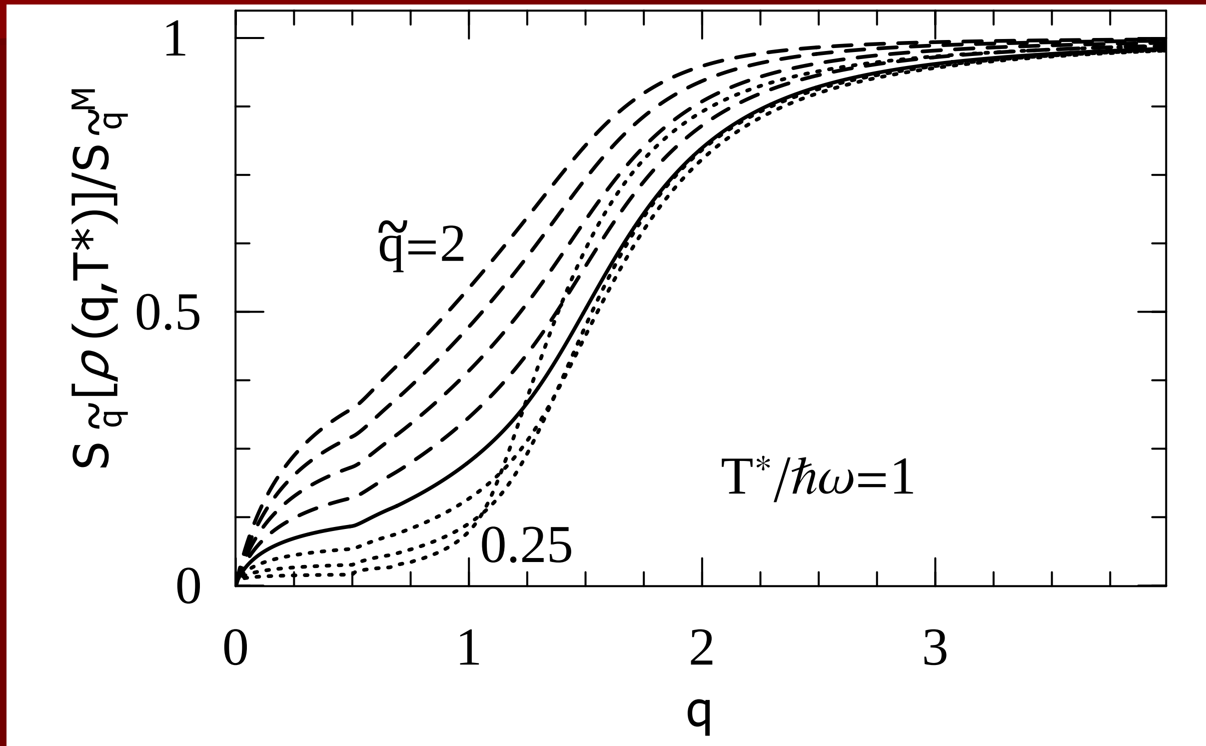


Scaled von Neumann entropy for power-law distributions as (increasing) function of both q and T*, for a system of n=100 equally spaced levels



Scaled Tsallis entropies $S_{\tilde{q}}[\rho\,(q,T^*)]$ as (increasing) functions of T*

for different values of $\tilde{q}$, for a system of n=100 equally spaced levels



Scaled Tsallis entropies $S_{\tilde{q}}[\rho(q,T^*)]$ as (increasing) functions of q

for different values of $\tilde{q}$, for a system of n=100 equally spaced levels

Tsallis NExt thermal distributions

Tsallis q-entropy S_q for a given $q > 0$
+
generalized free energy ($F_q = \langle H \rangle_{\rho_q} - T\, S_q[\rho]$) minimization

↓

$$\rho^{(q)}(T) = \rho(q,T) \quad \text{with} \quad T = [T^* - (1-q)\langle \bar{H} \rangle_{\rho_q}]/Z_q$$

For $q > 1$, and also for $0 < q < 1$ (taking absolute minimum of F_q),
it is proven that T is a non-decreasing function of T*

Therefore T is also a *mixing parameter* for the q-MaxEnt state, with q>0 :

$$\rho^{(q)}(T) \prec \rho^{(q)}(T') \quad \text{if} \quad T \geq T' \ (q > 0)$$

Conclusions

- Study of the disorder properties of generalized thermal states.

- Application of <u>majorization theory</u> to identify *rigorous sufficient mixing (disorder) conditions*, for general mixed states.

- Analysis of mixing properties for power law distributions [in q-exp. form: $\rho(q,T^*)$]:
  q (real) and T^* (postive) are two fundamental mixing parameters.
  → *Universal entropy (S_f) increase* with both q and T^* for any concave *f*.

- Tsallis non-extensive thermal distribution corresp. to a given fixed q>0 [$\rho^{(q)}(T)$] :
  becomes *more mixed* with increasing T (like for BG thermal state).
  → *Universal entropy (S_f) increase* with temperature for any concave *f*
  (particularly, generalized Tsallis entropies with any positive index $\tilde{q}$).

- Extension to density matrices derived from two or more *non-commuting observables* is feasible

N.Canosa, R.Rossignoli & MP, Physica A **368**, 435 (2006); Physica A (2006)