

# Divergences in the 2-qubits' Space: Werner and Thermal States

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## Abstract

We revisit the notion of using divergences, or relative-entropies, as measures of the distance between two mixed states, with special emphasis on power-law entropies. We analyze the Csiszár and Bregman-type  $q$ -divergences with reference to i) Werner states, and ii) thermal states obtained using a one-dimensional Heisenberg two-spin chain with a magnetic field  $B$  along the  $z$ -axis. In both cases, we find that the  $q$ -Jensen-Shannon divergence enlarges the range of permissible power-law exponents, as compared to results of previous literature. It is also shown that this divergence-measure serves as a good indicator for critical phenomena in the Heisenberg model.

**Keywords:** Jensen-Shannon divergence, Heisenberg model

# 1 Introduction

The discernibility of quantum states is a basic question for quantum-information purposes and it is obviously associated to the concept of distance between different quantal distributions in the same Hilbert space. These distances play an important role in several problems, like different preparations of the same system [1], purification of a mixed state for quantum error correction [2, 3, 4], the geometric properties of the quantum evolution sub-manifold [5], or for ascertaining the quality of approximate treatments [6].

In classical information theory the distance between two probability distributions is usually discussed using the Kullback-Leiber divergence (i.e. the ordinary, Shannon relative entropy) [7]. Regrettably enough, this quantity cannot be employed, in a quantum mechanics context, for measuring the degree of purification by comparing a mixed state density matrix  $\rho$  with a pure reference-state  $\sigma$  [9, 10]. It is important to note that the Kullback-Leiber divergence is well defined *only* when the support of  $\sigma$  is equal or larger than that of  $\rho$ .

The situation can be remedied by recourse to non-logarithmic information measures. These are also called by many authors power-law entropies, generalized, or “ $q$ -entropies”, and have indeed become rather fashionable nowadays, with multiple applications to different scientific disciplines (see, for instance, [11] and references therein). They were introduced long ago in the cybernetic-information communities by Harvda-Charvat [12] and Vadja [13] in 1967-68, being rediscovered by Daroczy in 1970 [14] with several echoes mostly in the field of image processing. For a historic summary and the pertinent references see [15]. In astronomy, physics, economics, biology, etc., these non-logarithmic information measures are often rebaptized as Tsallis entropies since 1988 [16]. The quantum  $q$ -divergence, defined as the *generalized* relative power-law-entropy associated with the quantum-mechanical version of the Harvda-Charvat-Tsallis [11, 16] information measure, avoids the problem of the  $\sigma$  support. The generalized versions of the relative entropy can be obtained as well from the so-called  $f$ -divergences (Csiszár-type) [17] or by an alternative expression which uses the derivative of  $f$ , called divergence of the Bregman-type [18, 19] in the mathematics literature. It has been shown that the quantum  $q$ -divergence of Csiszár-type is always well defined and no conditions are required on the supports of  $\rho$  and  $\sigma$  if the index  $q \in (0, 1)$  [9].

In the present effort we will systematically explore the use of  $q$ -divergences of both Csiszár’s and Bregman’s type within the context of Werner states  $\rho_W$  [20], that play a paradigmatic role in information theory. They determine a family of mixed states that includes both entangled and separable ones and model a decoherence process occurring on a singlet state travelling along a noisy channel. Thus, they are often employed in the quantum-communication

literature to investigate distillation and concentration processes and thereby as a “model” for assessing the value various types of theoretical treatment.

It will be shown that a Bregman-type divergence is well defined for all  $q > 1$ . For the two types of divergences we will construct a useful *generalization* of the Kullback-Leibler one, called the Jensen-Shannon divergence (JSD) [21], a measure originally introduced by Rao [21] and currently used by several authors (see, for example, [22, 23]). We will show that the symmetric JSD of the mixed Werner state [20] with respect to a pure Bell-reference state is positively defined for all  $q > 0$ -values. The result holds for our two types of  $q$ -divergences, thereby considerably enlarging the range of validity in which one can apply the standard quantum  $q$ -divergence as a purification-measure of  $\rho_W$ , with respect to the above mentioned  $(0, 1)$ -interval. Additionally, the Jensen-Shannon divergence obtained for our two types of quantum  $q$ -divergences will also be utilized to compute the distance between quantum *thermal* states obtained from the 1D-Heisenberg spin chain under the influence of a magnetic field  $B$  oriented along the  $z$ -axis.

The paper is organized as follows: In section II we present the quantum  $q$ -divergences of both of Csiszár's and Bregman's type. Section III is devoted to the application of these types of divergences and also of the JSD measure, to the Werner state. Distances between two-qubits thermal states are considered in section IV and, finally, some conclusions are drawn in section V.

## 2 Quantum divergences

Quantum divergences, or quantum relative-entropies, measure the “distance” between two mixed states. We concentrate here on the generalized  $q$ -divergences of the preceding section and start by reminding the reader that (in what would be here the case  $q = 1$ ) the Kullback-Leibler divergence writes [8]

$$K(\rho, \sigma) = Tr[\rho(\ln \rho - \ln \sigma)], \quad (1)$$

which is positive and well defined if the support of  $\sigma$  is larger or equal to that of  $\rho$ . The quantum  $q$ -divergences obtained as the generalized relative entropy associated to the Harvda-Charvat-Tsallis (HCT) information measure [11, 16] relieves one from taking into account this condition for certain values of the  $q$ -entropic parameter. We consider here two-types of  $q$ -divergences that often appear nowadays in the literature:

- 1) Csiszár-type, developed in [10] for (normalized) density matrices. For two classical probability distributions  $\rho_c$  and  $\sigma_c$  the so-called  $f$ -divergence writes [18, 17]

$$C(\rho_c, \sigma_c) = Tr[\rho_c f(\rho_c/\sigma_c)], \quad (2)$$

with  $f$  a convex function defined for  $x > 0$ . Using for  $f$  the corresponding HCT- information measure and replacing  $\rho_c$  and  $\sigma_c$  by the corresponding quantum density matrices  $\rho$  and  $\sigma$ , we obtain

$$C_q(\rho, \sigma) = \frac{1}{q-1} [\text{Tr}(\rho^q \sigma^{1-q}) - 1]. \quad (3)$$

By means of the spectral decomposition of our density matrices

$$\rho = \sum_a r(a) |a\rangle\langle a|; \quad \sigma = \sum_b s(b) |b\rangle\langle b|, \quad (4)$$

we get [10]

$$\begin{aligned} C_q(\rho, \sigma) &= \frac{1}{1-q} \sum_{a,b} |\langle a|b\rangle|^2 r(a)^q [r(a)^{1-q} - s(b)^{1-q}] = \\ &= \frac{1}{1-q} \sum_{a,b} |\langle a|b\rangle|^2 r(a) [1 - \{s(b)/r(a)\}^{1-q}], \end{aligned} \quad (5)$$

that can be shown to be positive definite, so that no restrictions are needed on the support of  $\rho$  and  $\sigma$  if  $q \in (0, 1)$  [10].

- 2) Bregman-type [18, 19] is based upon the derivative of  $f$ , and for two densities  $\rho$  and  $\sigma$  reads

$$B(\rho, \sigma) = \text{Tr}[f(\rho) - f(\sigma) - (\rho - \sigma)f'(\sigma)], \quad (6)$$

and we realize that both (2) and (6) coincide in the Shannon-case  $f(x) = x \log x$ . When the HCT-information measure is used for  $f$  one obtains

$$B_q(\rho, \sigma) = \frac{1}{q-1} [\text{Tr}(\rho^q) - \text{Tr}(\rho \sigma^{q-1})] + [\text{Tr}(\sigma^q) - \text{Tr}(\rho \sigma^{q-1})], \quad (7)$$

to be discussed below in the quantal cases of interest here.

### 3 Werner states

The so-called Bell basis is spanned by four vectors that in the canonical basis write

$$\begin{aligned} |1\rangle &\equiv |\Phi^+\rangle = \frac{1}{\sqrt{2}} |++\rangle + |--\rangle; & |2\rangle &\equiv |\Phi^-\rangle = \frac{1}{\sqrt{2}} |++\rangle - |--\rangle, \\ |3\rangle &\equiv |\Psi^+\rangle = \frac{1}{\sqrt{2}} |+-\rangle + |-+\rangle; & |4\rangle &\equiv |\Psi^-\rangle = \frac{1}{\sqrt{2}} |+-\rangle - |-+\rangle. \end{aligned} \quad (8)$$

To these vectors one associates the four density operators (projectors)

$$\begin{aligned} |\Psi^+\rangle\langle\Psi^+|; \quad & |\Psi^-\rangle\langle\Psi^-|, \\ |\Phi^+\rangle\langle\Phi^+|; \quad & |\Phi^-\rangle\langle\Phi^-|, \end{aligned} \tag{9}$$

respectively. We will cast in terms of these Bell projectors the Werner density matrix, that will be the protagonist of our present discussion. It mixes, with a parameter,  $x$  the pure state  $|\Psi^-\rangle\langle\Psi^-|$  with the totally mixed state  $I/4$  and reads [20]

$$\begin{aligned} \rho_W &= x|\Psi^-\rangle\langle\Psi^-| + [(1-x)I]/4 \equiv \\ &\equiv F|\Psi^-\rangle\langle\Psi^-| + [(1-F)/3] [|\Psi^+\rangle\langle\Psi^+| + |\Phi^-\rangle\langle\Phi^-| + |\Phi^+\rangle\langle\Phi^+|] \equiv \\ &\equiv [(1-F)/3] [|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|] + F|4\rangle\langle 4|, \end{aligned} \tag{10}$$

where we have introduced the fidelity  $F$  of  $\rho_W$  with respect to the pure state  $|\Psi^-\rangle\langle\Psi^-|$

$$F = (3x + 1)/4; \quad (1/4 \leq F \leq 1). \tag{11}$$

The state (10) is separable (unentangled) if the mixing coefficient  $x \leq 1/3$  ( $F \leq 1/2$ ) [20]. For  $x > 1/3$  ( $F > 1/2$ ) the Werner state is entangled [25, 26, 27]. As in [9] we obtain for the divergence (3)

$$\begin{aligned} C_q(\rho_W, |4\rangle\langle 4|) &= (1-q)^{-1} (1-F^q), \\ C_q &\geq 0 \text{ iff } 0 < q < 1, \end{aligned} \tag{12}$$

which is not linear in  $F$  and yields a measure of the “distance” between the mixed state  $\rho_W$  and the pure (entangled) projector-state  $|4\rangle\langle 4|$ . In this instance the support of  $\sigma \equiv |4\rangle\langle 4|$  is smaller than that of  $\rho$  and the Csiszár  $q$ -divergence is only positive definite for  $q \in (0, 1)$ .

A situation of special interest is that of  $q = 1/2$  [24]. We consider it below in some detail because it leads to an interesting picture. Let us first of all define

$$d_2 \equiv C_2(\rho_W, |4\rangle\langle 4|) = 2(1 - \sqrt{F}), \tag{13}$$

entailing

$$F = (1 - d_2/2)^2. \tag{14}$$

We thus obtain

$$\rho_W = \frac{1 - (1 - d_2/2)^2}{3} [ |1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3| ] + (1 - d_2/2)^2 |4\rangle\langle 4|, \quad (15)$$

so that we have entanglement for  $d_2 \leq (2 - \sqrt{2})$ . We can picture a kind of hyper-sphere centered around  $|4\rangle\langle 4|$  in the 2-qubits space with hyper-radius  $= d_2$ . You find entangled Werner states within the “hyper-sphere”. Outside it one encounters only separable Werner states. We are thus associating in geometric fashion entanglement with “distance”.

Consider now, for arbitrary  $q$ , the distance  $C_q$  from the Werner state to the totally mixed one

$$\begin{aligned} C_q(\rho_W, I/4) &= \frac{1}{q-1} [Tr(\rho_W^q (I/4)^{1-q}) - 1] = \\ &= \frac{1}{q-1} [(1/4)^{1-q} (3 \left(\frac{1-F}{3}\right)^q + F^q) - 1]. \end{aligned} \quad (16)$$

One easily ascertains that

$$C_q(\rho_W, I/4) \geq 0 \quad \text{iff} \quad q > 0 \quad (17)$$

As expected, when the  $\sigma$  support is larger than the one of  $\rho$ , (3) is positive definite for  $q > 0$ .

Let us evaluate now the other divergence, namely  $B_q$ . Traces are to be computed, for convenience, in the Bell-basis  $\{|1\rangle; |2\rangle; |3\rangle; |4\rangle\}$ . The eigenvalues of  $\rho_W$ , are, respectively,  $\{(1-F)/3; [(1-F)/3]; [(1-F)/3]; F\}$ . In such way one obtains

$$\begin{aligned} B_q(\rho_W, |4\rangle\langle 4|) &= \frac{1}{q-1} \left[ 3 \left( \frac{1-F}{3} \right)^q + F^q - F \right] + 1 - F, \quad \text{so that} \\ &B_q \geq 0 \quad \text{iff} \quad q > 1, \end{aligned} \quad (18)$$

and the distance from the Werner state to the maximally mixed one reads

$$\begin{aligned} B_q(\rho_W, I/4) &= \frac{1}{q-1} \left\{ F_1^q + 3 \left( \frac{1-F_1}{3} \right)^q + (q-1)4^{1-q} - q [F_1 4^{1-q} + (1-F_1)4^{1-q}] \right\}, \\ &\text{with } B_q \geq 0 \quad \text{iff} \quad q > 0. \end{aligned} \quad (19)$$

Using (3) and (7) we can compute the distances between two Werner states using our two divergence-measures. Let us call

$$\rho_{W1} = [(1 - F_1)/3] [ |1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3| ] + F_1 |4\rangle\langle 4|, \quad (20)$$

and

$$\rho_{W2} = [(1 - F_2)/3] [|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|] + F_2|4\rangle\langle 4|. \tag{21}$$

According to (3), the corresponding Kullback-Leibler divergence between the two states writes

$$\begin{aligned} C_q(\rho_{W1}, \rho_{W2}) &= \frac{1}{q-1} [Tr(\rho_{W1}^q \rho_{W2}^{1-q}) - 1] = \\ &= \frac{1}{q-1} [F_1^q F_2^{1-q} + (1 - F_1)^q (1 - F_2)^{1-q} - 1]. \end{aligned} \tag{22}$$

Notice that for  $F_2 = 1$  we recover the distance to the maximally entangled Bell-state  $|4\rangle\langle 4|$  (12) and for  $F_2 = 1/4$  the distance to the maximally mixed state  $I$  (16). As depicted in Fig. 1a, the Csiszár-type distance to the maximally entangled state is only positive in the interval  $0 < q < 1$  and increases with growing  $q$ -values. The distance to the maximally mixed state (Fig. 1b) also increases with  $q$ , but remains positive for *all*  $q > 0$ . In this last case, large  $q$ -values imply also a strong dependence of the distance on  $F$ .

Consider now the symmetrized Kullback-Leibler between  $\rho_{W1}$  and  $\rho_{W2}$ . It reads

$$\begin{aligned} CS_q(\rho_{W1}, \rho_{W2}) &= C_q(\rho_{W1}, \rho_{W2}) + C_q(\rho_{W2}, \rho_{W1}) = \\ &= \frac{1}{q-1} [F_1^q F_2^{1-q} + F_2^q F_1^{1-q} + \\ &+ (1 - F_1)^q (1 - F_2)^{1-q} + (1 - F_2)^q (1 - F_1)^{1-q} - 2]. \end{aligned} \tag{23}$$

Using it we can construct the so-called  $q$ -quantum Jensen-Shannon divergence ( $q$ -QJS), which assigns “weights”  $\pi_i$  to each  $\rho_{Wi}$ . In the special case  $q = 1$  and for weight-values  $\pi_1 = \pi_2 = 1/2$  one recovers the quantum Jensen-Shannon divergence (QJS) of [28]. The  $q$ -QJS measure writes

$$\begin{aligned} JS_q^{\pi_1, \pi_2}(\rho_{W1}, \rho_{W2}) &= \\ &= \pi_1 C_q(\rho_{W1}, \pi_1 \rho_{W1} + \pi_2 \rho_{W2}) + \pi_2 C_q(\rho_{W2}, \pi_1 \rho_{W1} + \pi_2 \rho_{W2}) = \\ &= \frac{\pi_1}{q-1} [F_1^q (\pi_1 F_1 + \pi_2 F_2)^{1-q} + (1 - F_1)^q (\pi_1 (1 - F_1) + \pi_2 (1 - F_2))^{1-q} - 1] \\ &\quad + \frac{\pi_2}{q-1} [F_2^q (\pi_1 F_1 + \pi_2 F_2)^{1-q} + \\ &\quad + (1 - F_2)^q (\pi_1 (1 - F_1) + \pi_2 (1 - F_2))^{1-q} - 1], \end{aligned} \tag{24}$$

which, for  $\pi_1 = \pi_2 = 1/2$ , specializes to

$$\begin{aligned}
JS_q^{1/2,1/2}(\rho_{W1}, \rho_{W2}) &= \frac{1}{2(q-1)} \left[ (F_1^q + F_2^q) \left( \frac{F_1 + F_2}{2} \right)^{1-q} + \right. \\
&\quad \left. + \left( (1-F_1)^q + (1-F_2)^q \right) \left( \frac{2-F_1-F_2}{2} \right)^{1-q} - 2 \right] \quad (25)
\end{aligned}$$

We have systematically explored (see Fig. 2) the behavior of (25) as a function of  $q$ , selecting as  $\rho_{W2}$  either the maximally entangled state (Fig. 2a) or the maximally mixed one (Fig. 2b). In both instances  $JS_q$  turns out to be positive for  $q > 0$  and increases with  $q$  for all  $F$  values.

We pass now to the consideration of the distance between two Werner states using the Bregman-type parametrization (7) and write [18, 19]

$$\begin{aligned}
(q-1)B_q(\rho_{W1}, \rho_{W2}) &= [Tr(\rho_{W1}^q) + (q-1)Tr(\rho_{W2}^q) - qTr(\rho_{W1}\rho_{W2}^{q-1})] = \mathbf{X} \\
\mathbf{X} &= F_1^q + 3\left(\frac{1-F_1}{3}\right)^q + \\
&\quad + (q-1)\left(F_2^q + 3\left(\frac{1-F_2}{3}\right)^q\right) - q\left[F_1F_2^{q-1} + (1-F_1)\left(\frac{1-F_2}{3}\right)^{q-1}\right], \quad (26)
\end{aligned}$$

The Bregman-type distance to the maximally entangled state is positive only for  $q > 1$  and decreases (non-monotonically) as  $q$  grows. For large  $q$  values a saturation limit is reached and the distance becomes constant for all  $F$  values, dropping off abruptly to zero for  $F = 1$ . If  $\rho_{W2}$  is the maximally mixed state, (26) is positive for all  $q > 0$ . The distance increases with  $q$  in the interval  $0 < q < 1$  and diminishes for  $q$ -values larger than 1, but without reaching a saturation limit-value. As in the case of the Csiszár-type distance, the dependence of the distance on  $F$  is strong for large  $q$ -values.

The associated symmetrized Bregman-quantity reads

$$\begin{aligned}
BS_q(\rho_{W1}, \rho_{W2}) &= B_q(\rho_{W1}, \rho_{W2}) + B_q(\rho_{W2}, \rho_{W1}) = \\
&= \frac{q}{q-1} \left[ Tr(\rho_{W1}^q) + Tr(\rho_{W2}^q) - \left( Tr(\rho_{W1}\rho_{W2}^{q-1}) + Tr(\rho_{W2}\rho_{W1}^{q-1}) \right) \right] = \\
&= \frac{q}{q-1} \left[ F_1^q + 3\left(\frac{1-F_1}{3}\right)^q + F_2^q + 3\left(\frac{1-F_2}{3}\right)^q - \right. \\
&\quad \left. - \left( F_1F_2^{q-1} + (1-F_1)\left(\frac{1-F_2}{3}\right)^{q-1} + F_2F_1^{q-1} + (1-F_2)\left(\frac{1-F_1}{3}\right)^{q-1} \right) \right] = \\
&= \frac{q}{q-1} (F_1 + F_2) \left[ F_1^{q-1} - F_2^{q-1} + \left(\frac{1-F_2}{3}\right)^{q-1} - \left(\frac{1-F_1}{3}\right)^{q-1} \right], \quad (27)
\end{aligned}$$

and the  $q$ -Bregman-Jensen Shannon defined with the  $B$  distance thus becomes



$$\begin{aligned}
 & (q-1)JS_{B_q}^{\pi_1, \pi_2}(\rho_{W_1}, \rho_{W_2}) = \\
 & = (q-1)[\pi_1 B_q(\rho_{W_1}, \pi_1 \rho_{W_1} + \pi_2 \rho_{W_2}) + \pi_2 B_q(\rho_{W_2}, \pi_1 \rho_{W_1} + \pi_2 \rho_{W_2})] = \\
 & = \left\{ \pi_1 \left( F_1^q + 3 \left( \frac{1-F_1}{3} \right)^q \right) + \pi_2 \left( F_2^q + 3 \left( \frac{1-F_2}{3} \right)^q \right) + \right. \\
 & \left. + \left( (q-1)(\pi_1 + \pi_2) - q \right) \left[ (\pi_1 F_1 + \pi_2 F_2)^q + 3 \left( \pi_1 \left( \frac{1-F_1}{2} \right) + \pi_2 \left( \frac{1-F_2}{2} \right) \right)^q \right] \right\} \quad (28)
 \end{aligned}$$

which, for  $\pi_1 = \pi_2 = 1/2$ , writes

$$\begin{aligned}
 JS_{B_q}^{1/2, 1/2}(\rho_{W_1}, \rho_{W_2}) = & \frac{1}{q-1} \left\{ \frac{1}{2} \left[ F_1^q + 3 \left( \frac{1-F_1}{3} \right)^q + F_2^q + 3 \left( \frac{1-F_2}{3} \right)^q \right] - \right. \\
 & \left. - \left[ \left( \frac{F_1+F_2}{2} \right)^q + 3 \left( \frac{2-F_1-F_2}{6} \right)^q \right] \right\} \quad (29)
 \end{aligned}$$

The Jensen-Shannon divergence obtained from the Bregman type divergence is positive definite for all  $q$ -positive values and exhibits the same type of qualitative behavior as the standard  $q$ -divergence (26). When we consider the distance to the maximally entangled state the saturation limit is here reached already for small  $q$ -values, the distance becoming constant for all  $F$  values up to  $F = 1$ . Figs. 3a and 3b depict our two Bregman-type divergences respect to the maximum entangled state and the maximum mixed state as a function of  $F$ . We appreciate the existence of “crossings” between different  $q$ -curves. This fact indicates that  $q$ -based divergences of the Bregman kind seem not physically acceptable as measures of quantum distances, since “ $q$ -single-valuedness” is violated.

## 4 Thermal states

In this Section we consider the Hamiltonian  $H$  of the 1D Heisenberg spin chain with a magnetic field of intensity  $B$  along the  $z$ -axis, as given by Arnesen *et al.* [29] with the idea of studying *thermal entanglement*.  $H$  is of the form

$$H = \sum_{i=1}^N (B\sigma_z^i + J_H \vec{\sigma}^i \vec{\sigma}^{i+1}), \quad (30)$$

where  $\sigma_{x,y,z}^i$  stand for the Pauli matrices associated with spin  $i$  and periodic boundary conditions are imposed ( $\sigma_{\mu}^{N+1} = \sigma_{\mu}^1$ ).  $J_H$  is the strength of the spin-spin repulsive interaction (only the anti-ferromagnetic ( $J_H > 0$ ) instance is

discussed). If we limit ourselves to the case  $N = 2$ , we will be dealing with two spinors, i.e., with a two-qubits system. For “thermal equilibrium” one should consider [29] the thermal state

$$\rho(T) = \frac{\exp(-\frac{H}{k_B T})}{Z(T)}, \quad (31)$$

with  $Z(T)$  the partition function. Expressing both  $H$  and  $\rho(T)$  in the computational basis  $|00\rangle, |01\rangle, |10\rangle, |11\rangle$  we obtain

$$H = \begin{pmatrix} 2J_H + 2B & 0 & 0 & 0 \\ 0 & -2J_H & 4J_H & 0 \\ 0 & 4J_H & -2J_H & 0 \\ 0 & 0 & 0 & 2J_H - 2B \end{pmatrix}. \quad (32)$$

After defining, for convenience's sake,

$$e_{wmy} = \exp(-2w - 2y);$$

$$e_{wp} = \exp(-2w) + \exp(6w);$$

$$e_{wm} = \exp(-2w) - \exp(6w);$$

$$e_{wpy} = \exp(-2w + 2y),$$

with  $w = J_H/k_B T$  and  $y = B/k_B T$ , we also get

$$\rho(T) = \frac{1}{Z(T)} \begin{pmatrix} e_{wmy} & 0 & 0 & 0 \\ 0 & e_{wp}/2 & e_{wm}/2 & 0 \\ 0 & e_{wm}/2 & e_{wp}/2 & 0 \\ 0 & 0 & 0 & e_{wpy} \end{pmatrix}, \quad (33)$$

Entanglement is measured by the concurrence of  $\rho(T)$ , that reads [29]

$$\begin{aligned} C &= 0; & \text{for } T \geq T_c \text{ (or } e^{8w} \leq 3), \\ C &= \frac{e^{8w} - 3}{1 + e^{-2y} + e^{2y} + e^{8w}}; & \text{for } T < T_c \text{ (or } e^{8w} > 3), \end{aligned} \quad (34)$$

For our purposes we must emphasize that there is no entanglement beyond a certain critical temperature  $T_c = 8J_H/(k_B \ln 3)$  [29]. Our interest here is aroused by the following consideration: on the one hand, it is well-known that entanglement vanishes for a high enough degree of mixing. On the other one, in the present scenario, “thermal entanglement” decreases as we increase  $T$ . It is tempting then to suggest that temperature plays a “mixing role”, as verified in Ref. [30].

Notice that  $T_c$  is independent of  $B$  and thus an intrinsic structural property. Also, there is a change in the structure of the ground state of hamiltonian (30) at  $B_c = 4J_H$ . In what follows we consider  $J_H = 1$ . For our present purposes it

is worth remarking that the ground state ( $T = 0$ ) of  $H$  has no entanglement for all  $B > B_c$  [30].

Remarkably enough, *the Werner states (10) and the thermal states (31) of the 1D Heisenberg model for  $N = 2$  can be put, for  $B \leq B_c$ , into a one-to-one correspondence via a mapping fidelity-temperature  $F \Leftrightarrow T$  as demonstrated [30], (see their Eq. (18)). Notice that, by recourse to (11), this mapping writes  $F = \frac{C+1}{2}$ , with  $C$  depending on the temperature as stipulated in Eq. (34). Here we analyze, by recourse to the Jensen-Shannon divergence, the distance between*

- $\rho(T)$  and
- $\rho(T = 0)$
- for the three cases  $B < B_c$ ,  $B = B_c = 4$ , and  $B > B_c$ .

Both Csiszár's and Bregman's types of divergence are used. In all cases the Jensen-Shannon divergence is well defined for positive  $q$ -values. For  $T \rightarrow \infty$  a saturation limit corresponding to the distance between  $\rho(0)$  and the maximally mixed state is attained.

In Fig. 4 we show the  $q$ -JSD (Csiszár type) of  $\rho(T)$  with respect to  $\rho(0)$  for  $q = 0.25$  (Fig.4a) and  $q = 2.5$  (fig.4b) and several values of the magnetic field. The saturation limit reached by the Jensen-Shanon divergence increases with the value of the  $q$ -parameter. For values of the magnetic field above or below the critical value, the saturation is reached for smaller  $T$ -values than in the case of  $B = B_c$ . The values of this limit are similar when the magnetic field strength is either greater or smaller than the critical strength-value  $B_c$  and, in both cases, are larger than those for the  $B = B_c$  instance. The same comments apply to the  $q$ -JSD measure obtained from the Bregman-type  $q$ -divergence. However, in this case the distance between the density matrices decreases as  $q$ -increases (see Figs. 5a and 5b).

In both Figs. 4 and 5 a rather surprising fact is to be registered. For any  $q$ -value, the curve corresponding to  $B = B_c$  "separates" nitidly out of all the other curves, generating a noticeable "gap". For example, the curves for  $B = 3.9$  and  $B = 4.1$  fall in-between those actually drawn in the figures for  $B = 6$  and  $B = 2$ . This gap between the  $B_c$ -curve and the curves for *all* other  $B$ -values indicates that our distance-measures are excellent "detectors" of the critical field-strengths.

## 5 Conclusions

We have performed a rather exhaustive study of several types of distance between quantum density matrices of Werner and thermal states. Our main

results are:

1. We were able to associate in geometric fashion entanglement with “distance” in Section III.
2. Our distance-measures are excellent “detectors” of the critical field-strengths in the Heisenberg model, as evidenced by the gap between the  $B_c$ -curve and the curves for *all* other  $B$ -values.
3. We appreciate the existence of “crossings” between different  $q$ -curves for distances associated to the Bregman family, indicative of the fact that they seem not physically acceptable as measures of quantum distances, since “ $q$ -single-valuedness” is violated.
4. In the two analyzed cases, the Jensen-Shannon divergence obtained from the Csiszár and Bregman quantum  $q$ -divergences are well defined for all positive  $q$ -values. As a consequence, they can be applied to confidently compute distance between two-qubit mixed states and no conditions are needed on the supports of the two density matrices that we compare in this way. In particular the  $q$ -JSD can be used as a measure of the purification of the Werner state. Clearly, the Jensen-Shannon divergences enlarges the validity range of the standard quantum  $q$ -divergences for the Werner and thermal states, usually employed as a “models” in quantum communication.

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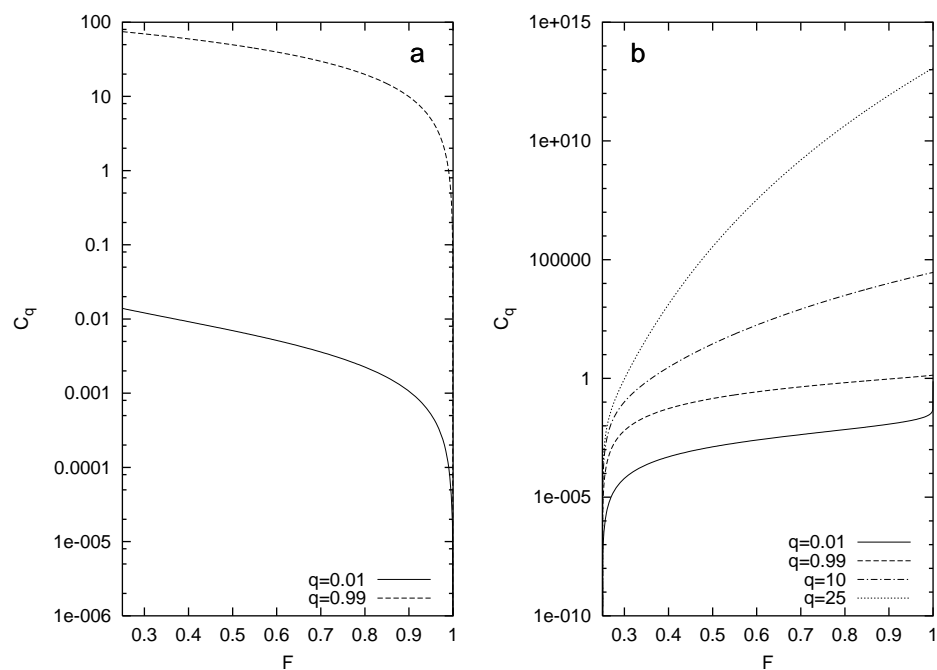


Figure 1: a) Csiszár type quantum  $q$ -divergence ( $C_q$ ) of  $\rho_W$  with respect to the maximally entangled state and to the b) maximally mixed state.

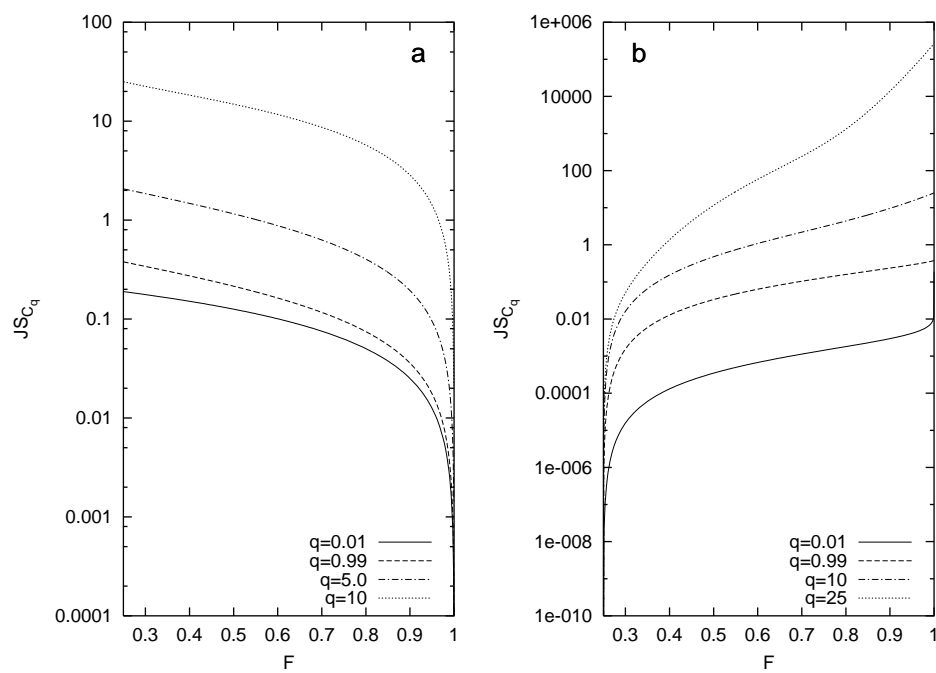


Figure 2: a) Jensen-Shannon divergence (25) of  $\rho_W$  with respect to the maximally entangled state and b) to the maximally mixed state.



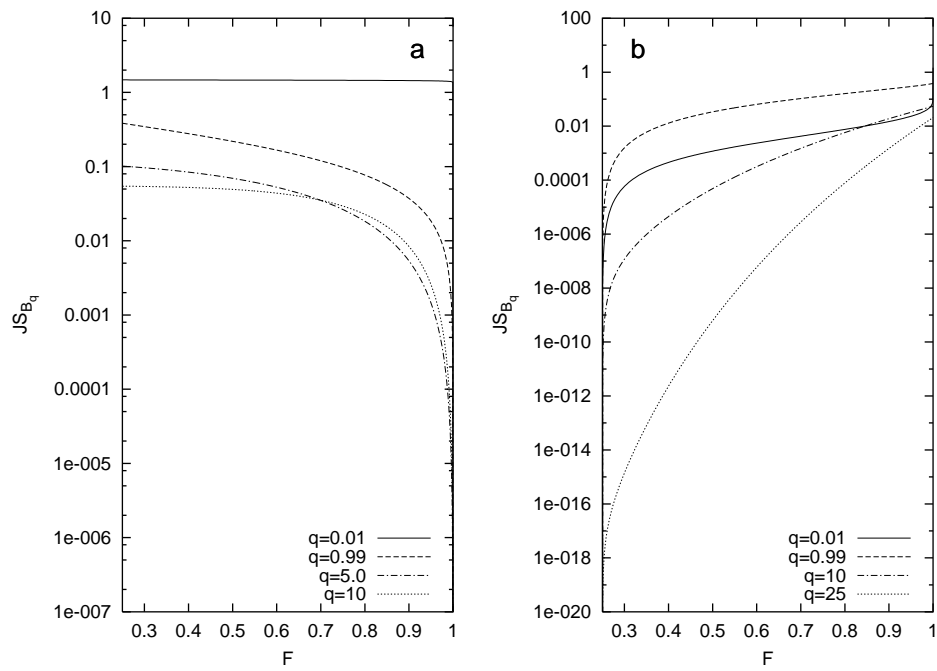


Figure 3: a) Jensen-Shannon divergence (29) of  $\rho_W$  with respect to the maximally entangled state and b) to the maximally mixed state.

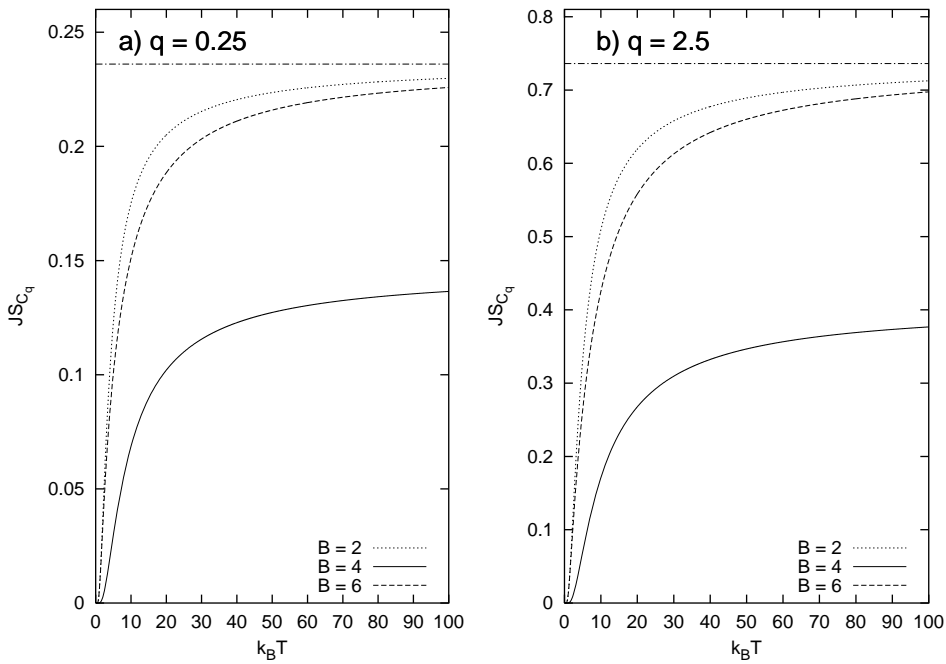


Figure 4: a) Jensen-Shannon divergence (25) of  $\rho(T)$  with respect to  $\rho(0)$  for  $B < B_c$ ,  $B = B_c$  and  $B > B_c$  and parameter  $q = 0.25$ . b) Same result for  $q = 2.5$ . In both cases horizontal dot-dashed line is the limit  $T \rightarrow \infty$  for  $B = 2$ .

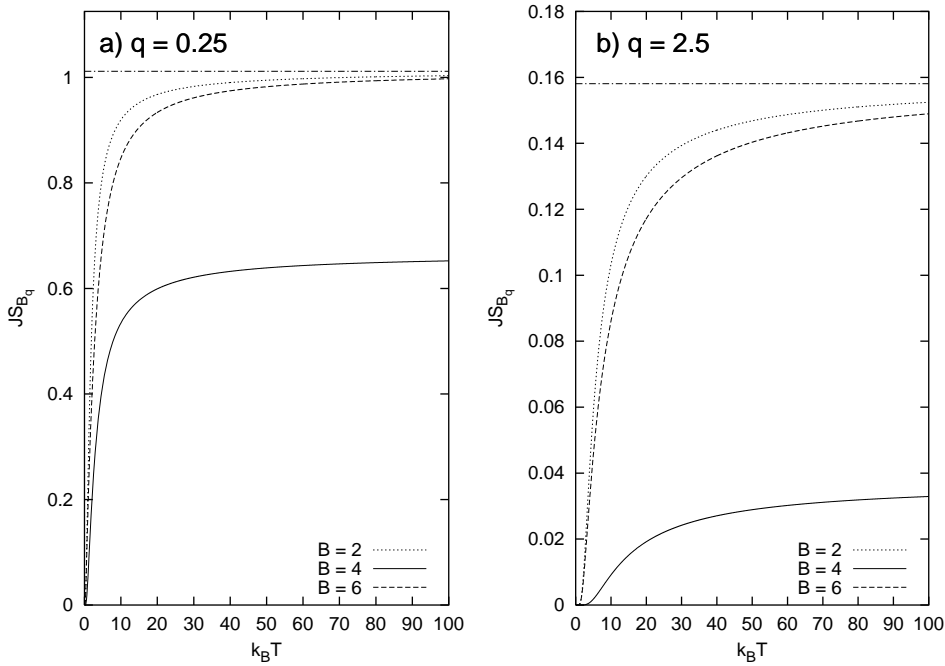


Figure 5: a) Jensen-Shannon divergence (29) of  $\rho(T)$  with respect to  $\rho(0)$  for  $B < B_c$ ,  $B = B_c$  and  $B > B_c$  and parameter  $q = 0.25$ . b) Same result for  $q = 2.5$ . In both cases horizontal dot-dashed line is the limit  $T \rightarrow \infty$  for  $B = 2$ .