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QUANTUM DISCORD AND RELATED MEASURES OF QUANTUM CORRELATIONS IN FINITE *XY* CHAINS

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We examine the quantum correlations of spin pairs in the ground state of finite XY chains in a transverse field, by evaluating the quantum discord as well as other related entropic measures of quantum correlations. A brief review of the latter, based on generalized entropic forms, is also included. It is shown that parity effects are of crucial importance for describing the behavior of these measures below the critical field. It is also shown that these measures reach full range in the immediate vicinity of the factorizing field, where they become independent of separation and coupling range. Analytical and numerical results for the quantum discord, the geometric discord and other measures in spin chains with nearest neighbor coupling and in fully connected spin arrays are also provided.

Keywords: Quantum discord; quantum correlations; spin chains.

1. Introduction

The last decades have witnessed the great progress experienced by the interdisciplinary field of quantum information science,[1–3] which began with the recognition of the potential of quantum systems and quantum correlations for information processing tasks. While it is well known that quantum entanglement is essential for quantum teleportation,[4] superdense coding[5] and also for achieving exponential speed-up in pure state based quantum algorithms,[6,7] the mixed state based quantum algorithm of Knill and Laflamme[8] showed that such speedup could in principle be achieved in this case without a substantial presence of entanglement.[9] This has oriented the attention to alternative definitions and measures of quantum correlations for mixed states, like the quantum discord.[10–13] While coinciding with the entanglement entropy for pure states, the quantum discord differs essentially from the entanglement of formation in the case of mixed states, being nonzero in most separable mixed states and vanishing just for states which are strictly classically correlated at least with respect to one of the constituents, i.e., diagonal in a standard or conditional product basis.[10–12] The result of Ref. 15 showing the existence of a finite discord between the control qubit and the remaining qubits in the circuit of Ref. 8, unleashed a great interest on this measure and several investigations on its fundamental properties,[16–19] on its evaluation on spin chains and specific states[20–28] as well as on related measures,[29–34] have been recently made (see Ref. 35 for a recent review). Distinct quantum capabilities of states with nonzero discord have also been recently investigated.[36–39]

Our aim here is to describe the remarkable behavior of the quantum discord and of other related entropic measures of quantum correlations, in the exact ground state of finite XY chains in a transverse field.[24] We first provide in Secs. 2–5 a brief review of the quantum discord and of the generalized entropic measures of quantum correlations discussed in Refs. 33 and 34. The latter comprise as particular cases the one-way information deficit[36,40,41] and the geometric measure of discord of Ref. 32, embedding them in a unified formalism based on majorization[42–44] and general entropic forms.[45] While their basic features are similar to those of the quantum discord, the possibility of using simple entropic forms permits an easier evaluation, allowing for analytical expressions in some cases, as occurs with the geometric discord of general two qubit states.[32]

We then use these measures to investigate, in Secs. 6–8, the quantum correlations of spin pairs in the exact ground state of finite XY chains in a transverse field. We review the main results of Ref. 24 on the behavior of the quantum discord in these chains and also add new results concerning the behavior of the geometric discord and other related measures in such chains. The exact ground state of a finite XY chain in a transverse field has a definite spin parity and this fact will be seen to deeply affect the discord and the previous measures for fields lower than the critical field B_c. We will show that the essential results in this sector can be interpreted in terms of the discord of mixtures of aligned pairs.

Moreover, these chains can exhibit a *factorizing field* B_s,[46–57] where they have a completely separable ground state. For transverse fields, such eigenstate actually breaks the previous parity symmetry and is hence degenerate, coinciding B_s in a finite chain with the last crossing of the two lowest opposite parity levels.[51] A related remarkable effect is that in the immediate vicinity of B_s, pairwise entanglement, though weak, reaches *full range*,[49–51] regardless of the coupling range. Here we will show that the quantum discord as well as the entropic measures of quantum correlations also reach full range at this point, exhibiting universal features such as being independent of separation and coupling range.[24] Moreover, the value reached by them at this point is nonnegligible and does not decrease with size, in contrast with the pairwise entanglement, since these measures are not restricted by the monogamy property[58,59] which affects the latter (limiting the concurrence[60,61] to order n^{-1} in an n spin chain if all pairs are equally entangled). Consequently, the behavior of these measures with the applied field and separation will deviate significantly from that of the concurrence or entanglement of formation for $|B| < B_s$. Conclusions are finally discussed in Sec. 9.

2. Quantum Discord

The quantum discord was originally defined[10–14] as the difference between two distinct quantum versions of the mutual information, or equivalently, the conditional entropy. For a classical bipartite system $A + B$ described by a joint probability distribution $p_{ij} = p(A = i, B = j)$, the conditional entropy is defined as the average lack of information about A when the value of B is known: $S(A|B) = \sum_j p_j^B S(A|B = j)$, where $p_j^B = \sum_i p_{ij}$ is the probability of outcome j in B and $S(A|B = j) = -\sum_i p_{i/j} \log p_{i/j}$ is the Shannon entropy of the conditional distribution $p_{i/j} = p_{ij}/p_j^B$. It is a nonnegative quantity, and can also be expressed in terms of the joint entropy $S(A, B) = -\sum_{i,j} p_{ij} \log p_{ij}$ and the marginal entropy $S(B) = -\sum_j p_j^B \log p_j^B$ as $S(A|B) = S(A, B) - S(B)$. Positivity of $S(A|B)$ then implies $S(A, B) \geq S(B)$ (and hence $S(A, B) \geq S(A)$) for any classical system.

The last expression for $S(A|B)$ allows a direct quantum generalization, namely

$$S(A|B) = S(\rho_{AB}) - S(\rho_B)\,, \tag{1}$$

where $S(\rho) = -\mathrm{Tr}\,\rho \log_2 \rho$ is now the von-Neumann entropy and ρ_{AB} the system density matrix, with $\rho_B = \mathrm{Tr}_A\, \rho_{AB}$ the reduced state of subsystem B. It is well known, however, that Eq. (1) can be negative,[42] being for instance negative in any entangled pure state: If $\rho_{AB}^2 = \rho_{AB}$, $S(\rho_{AB}) = 0$ and $S(A|B) = -E(A, B)$, where $E(A, B) = S(A) = S(B)$ is the entanglement entropy.[62,63] The positivity of Eq. (1) provides in fact a basic separability criterion for general mixed states[64]: ρ_{AB} separable $\Rightarrow S(A|B) \geq 0$, a criterion which can actually be extended to more general entropies.[65–67] We recall that ρ_{AB} is separable if it can be written as a convex combination of product states, i.e., $\rho_{AB} = \sum_\alpha q_\alpha \rho_A^\alpha \otimes \rho_B^\alpha$, with $q_\alpha \geq 0$, $\sum_\alpha q_\alpha = 1$.[68]

A second quantum version of the conditional entropy, closer in spirit to the first classical expression, can be defined[10–12] on the basis of a complete local projective measurement M_B on system B (von-Neumann measurement), determined by one dimensional orthogonal local projectors $\Pi_j = |j_B\rangle\langle j_B|$. The conditional entropy after such measurement is:

$$S_{M_B}(A|B) = \sum_j p_j^B S(\rho_{A/j}) = S(\rho'_{AB}) - S(\rho'_B)\,, \tag{2}$$

where $p_j^B = \mathrm{Tr}\,\rho_{AB}\Pi_j^B$, with $\Pi_j^B = I_A \otimes \Pi_j$, is the probability of outcome j, $\rho_{A/j} = \mathrm{Tr}_B\,(\rho_{AB}\Pi_j^B)/p_j^B$ is the reduced state of A after such outcome and

$$\rho'_{AB} = \sum_j p_j^B \rho_{A/j} \otimes \Pi_j = \sum_j \Pi_j^B \rho_{AB} \Pi_j^B\,, \tag{3}$$

is the average joint state after such measurement, with $\rho'_B = \mathrm{Tr}_A\,\rho'_{AB} = \sum_j p_j^B \Pi_j$. Equation (2) represents the average lack of information about A after the measurement M_B in B is performed and is clearly nonnegative, in contrast with Eq. (1).

For a classical system, both quantities (1)–(2) are, however, equivalent. We also mention that for general local measurements, defined by a set of positive operators E_j ($\sum_j E_j = I$), the first expression in (2) is to be used for $S_{M_B}(A|B)$ (with $\Pi_j \to E_j$).

The quantum discord[10–15] can then be defined as the minimum difference between Eqs. (1) and (2):

$$D^B(\rho_{AB}) = \operatorname*{Min}_{M_B}[S_{M_B}(A|B)] - S(A|B)\,, \tag{4}$$

where the minimization is over all local measurements M_B. Due to the concavity of the von-Neumann conditional entropy (1) with respect to ρ_{AB},[42] Eq. (4) is nonnegative,[10–12] vanishing just for classically correlated states with respect to B, i.e., states which are already of the general form (3) (a particular case of separable state) and which remain then unchanged under a specific unread local measurement. Such states are diagonal in a "conditional" product basis $\{|i_j j\rangle \equiv |i_{j\,A}\rangle \otimes |j_B\rangle\}$, with $|i_{j\,A}\rangle$ the eigenstates of $\rho_{A/j}$.

Equation (4) is then nonzero not only in entangled states but also in separable states not of the form (3), i.e., those which involve convex mixtures of noncommuting product states, for which the entanglement of formation[69] vanishes. It is then a measure of all quantum-like correlations between A and B. The distinction with entanglement arises nonetheless just for mixed states: For pure states $\rho^2_{AB} = \rho_{AB}$, $S(\rho_{AB}) = 0$ and $S(\rho'_{AB}) = S(\rho'_B)$ for any von-Neumann measurement, reducing the quantum discord exactly to the entanglement entropy: $D^A = D^B = E(A, B)$.

Equation (4) can be of course also understood[13,14] as the minimum difference between the *quantum mutual information*[42] $I(A : B) = S(A) - S(A|B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB})$, which measures all correlations between A and B ($I(A : B) \geq 0$, with $I(A : B) = 0$ if and only if $\rho_{AB} = \rho_A \otimes \rho_B$) and the "classical" mutual information $I_{M_B}(A : B) = S(A) - S_{M_B}(A|B)$, which measures the correlations after the local measurement M_B.

3. Generalized Entropic Measures of Quantum Correlations

Let us now discuss an alternative approach for measuring quantum correlations,[33] which allows the direct use of more general entropic forms. We consider a complete local projective measurement M_B (von-Neumann type measurement) on part B of a bipartite system initially in a state ρ_{AB}, such that the post-measurement state is given by Eq. (3) if the result is unread. A fundamental property satisfied by the state (3) is the majorization relation[1,42–44]

$$\rho'_{AB} \prec \rho_{AB}\,, \tag{5}$$

where $\rho' \prec \rho$ means, for normalized mixed states ρ, ρ' of the same dimension n,

$$\sum_{j=1}^{i} p'_j \leq \sum_{j=1}^{i} p_j\,, \quad i = 1, \ldots, n-1\,.$$

Here p'_j, p_j denote, respectively, the eigenvalues of ρ' and ρ sorted in *decreasing* order ($p_j \geq 0$, $\sum_j p_j = 1$). Equation (5) implies that ρ'_{AB} is always *more mixed* than ρ_{AB}: If Eq. (5) holds, ρ'_{AB} can be written as a convex combination of unitaries of ρ_{AB}: $\rho'_{AB} = \sum_\alpha q_\alpha U_\alpha \rho_{AB} U_\alpha^\dagger$, with $q_\alpha > 0$, $\sum_\alpha q_\alpha = 1$ and $U_\alpha^\dagger U_\alpha = I$.[1,42–44]

Equation (5) not only implies that $S(\rho'_{AB}) \geq S(\rho_{AB})$ for the von-Neumann entropy, but also:

$$S_f(\rho'_{AB}) \geq S_f(\rho_{AB}) \tag{6}$$

for *any* entropy of the form[45]

$$S_f(\rho) = \mathrm{Tr}\, f(\rho)\,, \tag{7}$$

where $f : [0,1] \to \Re$ is a smooth strictly concave function satisfying $f(0) = f(1) = 0$. As in the von-Neumann case, recovered for $f(\rho) = -\rho \log \rho$, these entropies also satisfy $S_f(\rho) \geq 0$, with $S_f(\rho) = 0$ if and only if ρ is a pure state ($\rho^2 = \rho$), and $S_f(\rho)$ maximum for the maximally mixed state $\rho = I_n/n$. Hence, Eq. (5) implies a strict disorder increase by measurement which cannot be fully captured by considering just a single choice of entropy ($S(\rho') \geq S(\rho)$ does not imply $\rho' \prec \rho$). More generally, Eq. (5) actually implies $F(\rho') \geq F(\rho)$ for any Schur concave function F of ρ.[43,44] Nonetheless, entropies of the form (7) are *sufficient* to characterize Eq. (5), in the sense that if Eq. (6) holds for *all* such S_f, then $\rho' \prec \rho$.[67]

We may now consider the generalized information loss due to such measurement,[33]

$$I_f^{M_B} = S_f(\rho'_{AB}) - S_f(\rho_{AB})\,, \tag{8}$$

which is always *nonnegative* due to Eqs. (5)–(6), vanishing only if $\rho'_{AB} = \rho_{AB}$ due to the strict concavity of f. Equation (8) is a measure of the information contained in the off-diagonal elements $\langle ij|\rho_{AB}|i'j'\rangle$ ($j \neq j'$) of the original state, lost in the measurement. The minimum of $I_f^{\mathrm{M_B}}$ among all complete local measurements,[33]

$$I_f^B(\rho_{AB}) = \underset{M_B}{\mathrm{Min}}\, S_f(\rho'_{AB}) - S_f(\rho_{AB})\,, \tag{9}$$

provides then a measure of the quantum correlations between A and B present in the original state and destroyed by the local measurement in B: $I_f^B \geq 0$, vanishing, as the quantum discord (4), only if ρ_{AB} is already of the form (3), i.e., only if it is diagonal in a standard or conditional product basis.

Again, in the case of a pure state $\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|$, it can be shown[33] that Eq. (9) reduces to the *generalized entanglement entropy*: $I_f^A = I_f^B = E_f(A,B)$ if $\rho_{AB}^2 = \rho_{AB}$, where $E_f(A,B) = S_f(\rho_A) = S_f(\rho_B)$. The minimizing measurement in this case is the local Schmidt basis for $|\Psi_{AB}\rangle$: $M_B = \{|k^B\rangle\langle k^B|\}$, if $|\Psi_{AB}\rangle = \sum_k \sqrt{p_k}|k^A\rangle \otimes |k^B\rangle$.[33]

In the case of the von-Neumann entropy ($S_f(\rho) = S(\rho)$), Eq. (9) becomes the one-way information deficit,[36,40,41] which coincides with the different version of discord given in Ref. 12 (and denoted as thermal discord in Ref. 35). It can be rewritten in this case in terms of the relative entropy[42,70] $S(\rho\|\rho') = -\mathrm{Tr}\,\rho(\log\rho' - \log\rho)$ (a nonnegative quantity) as:

$$I^B(\rho_{AB}) \equiv \underset{M_B}{\mathrm{Min}}\, S(\rho'_{AB}) - S(\rho_{AB}) = \underset{M_B}{\mathrm{Min}}\, S(\rho_{AB}\|\rho'_{AB})\,, \tag{10}$$

where we have used the fact that the diagonal elements of ρ_{AB} and ρ'_{AB} in the basis where the latter is diagonal are obviously coincident. We also note that for these measurements, the quantum discord (4) can be expressed as $D^B = \mathrm{Min}_{M_B}[I^{M_B}(\rho_{AB}) - I^{M_B}(\rho_B)]$, coinciding then with I^B when the minimizing measurements in (10) and (4) are the same and such that $\rho'_B = \rho_B$.

In the case of the *linear entropy* $S_2(\rho) = 1 - \mathrm{Tr}\,\rho^2$, obtained for $f(\rho) = \rho(1-\rho)$ (i.e., using the linear approximation $\log\rho \to \rho - I$ in $-\rho\log\rho$), Eq. (9) becomes[33]

$$I_2^B(\rho_{AB}) \equiv \underset{M_B}{\mathrm{Min}}\; \mathrm{Tr}(\rho_{AB}^2 - \rho'^2_{AB}) = \underset{M_B}{\mathrm{Min}}\, \|\rho'_{AB} - \rho_{AB}\|^2\,, \tag{11}$$

where $\|O\|^2 = \mathrm{Tr}\,O^\dagger O$ is the squared Hilbert Schmidt norm. This quantity becomes then equivalent to the geometric measure of discord introduced in Ref. 32. The latter is defined as the last expression in Eq. (11) with minimization over all states diagonal in a product basis, but the minimum corresponds to a state of the form (3).[33] For pure states, I_2^B becomes proportional to the squared *concurrence* C_{AB}^2,[60,61] as for pure states C_{AB}^2 is proportional to the linear entropy of any of the subsystems.[71]

Finally, in the case of the Tsallis entropy[72,73] $S_q(\rho) = (1 - \mathrm{Tr}\,\rho^q)/(q-1)$, $q > 0$, which corresponds to $f(\rho) = (\rho - \rho^q)/(q-1)$, Eq. (9) becomes[34]

$$I_q^B(\rho_{AB}) = \underset{M_B}{\mathrm{Min}}\, S_q(\rho'_{AB}) - S_q(\rho_{AB}) \propto \underset{M_B}{\mathrm{Min}}\, \mathrm{Tr}(\rho^q_{AB} - \rho'^q_{AB})\,, \tag{12}$$

with I_q reducing to the one way information deficit for $q \to 1$ (as $S_q(\rho) \to S(\rho)$), and to the geometric discord for $q = 2$. This entropy allows then a simple continuous shift between different measures.

When considering qubit systems, we will normalize entropies such that $S_f(\rho) = 1$ for a maximally mixed two-qubit state ρ (i.e., $2f(1/2) = 1$), implying that all I_f^B will take the value 1 in a maximally entangled two-qubit state (Bell state). This implies setting $\log \equiv \log_2$ in the von-Neumann entropy, $S_2(\rho) = 2(1 - \mathrm{Tr}\,\rho^2)$ in the linear case (such that $I_2^B = 2\mathrm{Min}_{M_B}\|\rho'_{AB} - \rho_{AB}\|^2$) and $S_q(\rho) = (1 - \mathrm{Tr}\,\rho^q)/(1 - 2^{1-q})$ in the Tsallis case.

4. General Stationary Conditions for the Least Disturbing Measurement

The stationary condition $\delta I_f^{M_B}(\rho_{AB}) = 0$ for the quantity (8), obtained by considering a general variation $\delta|j_B\rangle = (e^{i\delta h_B} - I)|j_B\rangle \approx i\delta h|j_B\rangle$ of the local measurement basis, where h_B is an hermitian local operator, reads[34]

$$\mathrm{Tr}_A[f'(\rho'_{AB}), \rho_{AB}] = 0\,, \tag{13}$$

i.e., $\sum_i [f'(p^i_j)\langle i_j j|\rho_{AB}|i_j k\rangle - f'(p^i_k)\langle i_k j|\rho_{AB}|i_k k\rangle] = 0$, where f' denotes the derivative of f and $\langle i_j j|\rho_{AB}|i'_j j\rangle = \delta_{ii'}p^i_j$. In the case of the geometric discord, $f'(\rho) \propto I - 2\rho$ and Eq. (13) reduces to $\mathrm{Tr}_A[\rho'_{AB}, \rho_{AB}] = 0$. In the case of the quantum discord (4), Eq. (13) should be replaced for these measurements by[34]:

$$\mathrm{Tr}_A[f'(\rho'_{AB}), \rho_{AB}] - [f'(\rho'_B), \rho_B] = 0\,, \tag{14}$$

with $f(\rho) = -\rho \log \rho$, due to the extra local term.

Equations (13)–(14) allow us to identify the stationary measurements, from which the one providing the absolute minimum of $I_f^{M_B}$ (least disturbing measurement) is to be selected. For instance, if there is a standard product basis where $\langle ij|\rho_{AB}|ij'\rangle = \delta_{jj'}p^i_j$ and $\langle ij|\rho_{AB}|i'j\rangle = \delta_{ii'}p^i_j$, such that the only off-diagonal elements are $\langle ij|\rho_{AB}|i'j'\rangle$ with $i \neq i'$ and $j \neq j'$, a measurement in the basis $\{|j_B\rangle\}$ is clearly stationary for *all* I_f^B, as Eq. (13) is trivially satisfied, leading to a *universal stationary point*.[34] It will also be stationary for the quantum discord.

An example of such basis is the Schmidt basis for a pure state, $|\Psi_{AB}\rangle = \sum_{k=1}^{n_s} \sqrt{p_k}|kk\rangle$, with $|kk\rangle \equiv |k_A\rangle \otimes |k_B\rangle$ and n_s the Schmidt rank, since $\langle kl|\rho_{AB}|k'l'\rangle = \delta_{kl}\delta_{k'l'}\sqrt{p_k p_{k'}}$ for $\rho_{AB} = |\Psi_{AB}\rangle\langle\Psi_{AB}|$. The same holds for a mixture of a pure state with the maximally mixed state,

$$\rho_{AB}(x) = x|\Psi_{AB}\rangle\langle\Psi_{AB}| + \frac{1-x}{n} I_n\,, \tag{15}$$

where $n = n_A n_B$ and $x \in [0,1]$. The Schmidt basis provides in fact the *actual minimum* of $I_f^B(x) \equiv I_f^B(\rho_{AB}(x))\ \forall\ x \in [0,1]$, as shown in Ref. 33. This implies the existence in this case of a universal least disturbing measurement, and of a concomitant *least mixed* post measurement state, such that ρ'_{AB} majorizes any other post-measurement state. We can then obtain a closed evaluation of I_f^B for this case $\forall\ S_f$,[33] which shows some of its main features:

$$I_f^B(x) = \sum_{k=1}^{n_s} f\left(\frac{x(np_k - 1) + 1}{n}\right) - f\left(\frac{x(n-1)+1}{n}\right) - (n_s - 1) f\left(\frac{1-x}{n}\right). \tag{16}$$

If $n_s > 1$, it can be shown that $I_f^B(x) > 0$ for $x > 0$, being a strictly increasing function of x for $x \in [0,1]$ if $f(p)$ is strictly concave. Moreover, a series expansion for small x leads to $I_f^B(x) \approx \alpha x^2(1 - \sum_{k=1}^{n_s} p_k^2)$, where $\alpha = -f''(1/n)/2 \geq 0$, indicating a *universal quadratic increase* with increasing x if $f''(1/n) \neq 0$.[33] This behavior is then similar to that of the quantum discord[10–12] and quite distinct from that of the entanglement of formation, which requires a finite threshold value of x for acquiring a nonzero value.

5. The Two Qubit Case

Let us now examine the particular case of a two qubit system. A general two-qubit state can be written as:

$$\rho_{AB} = \frac{1}{4}(I + \mathbf{r}_A \cdot \boldsymbol{\sigma}_A + \mathbf{r}_B \cdot \boldsymbol{\sigma}_B + \boldsymbol{\sigma}_A^t J \boldsymbol{\sigma}_B)\,, \tag{17}$$

where $I \equiv I_2 \otimes I_2$ denotes the identity, $\boldsymbol{\sigma}_A = \boldsymbol{\sigma} \otimes I_2$ and $\boldsymbol{\sigma}_B = I_2 \otimes \boldsymbol{\sigma}$. Due to the orthogonality of the Pauli matrices, we have $\mathbf{r}_A = \langle \boldsymbol{\sigma}_A \rangle$, $\mathbf{r}_B = \langle \boldsymbol{\sigma}_B \rangle$ and $J = \langle \boldsymbol{\sigma}_A^t \boldsymbol{\sigma}_B \rangle$, i.e., $J_{\mu\mu'} = \langle \sigma_{A\mu}\sigma_{B\mu'} \rangle$, where $\mu, \mu' = x, y, z$ and $\langle O \rangle = \mathrm{Tr}\, \rho_{AB}\, O$.

A general local projective measurement in this system is just a spin measurement along a unit vector $\mathbf{k}$, and is represented by the orthogonal projectors $(1/2)(I \pm \mathbf{k}\cdot\boldsymbol{\sigma})$. Therefore, the most general post-measurement state (3) reads

$$\rho'_{AB} = \frac{1}{4}(I + \mathbf{r}_A \cdot \boldsymbol{\sigma}_A + (\mathbf{r}_B \cdot \mathbf{k})\mathbf{k}\cdot\boldsymbol{\sigma}_B + (\boldsymbol{\sigma}_A^t J\mathbf{k})(\mathbf{k}\cdot\boldsymbol{\sigma}_B))\,, \tag{18}$$

and corresponds in matrix notation (setting $\mathbf{r}$ and $\mathbf{k}$ as column vectors) to $\mathbf{r}_B \to \mathbf{k}\mathbf{k}^t\mathbf{r}_B$ and $J \to J\mathbf{k}\mathbf{k}^t$. The general stationary condition (13) can be shown to lead to the equation[34]

$$\alpha_1 \mathbf{r}_B + \alpha_2 J^t \mathbf{r}_A + \alpha_3 J^t J\mathbf{k} = \lambda\mathbf{k}\,, \tag{19}$$

i.e., $\mathbf{k} \times (\alpha_1 \mathbf{r}_B + \alpha_2 J^t \mathbf{r}_A + \alpha_3 J^t J\mathbf{k}) = \mathbf{0}$, which determines the possible values of the minimizing measurement direction $\mathbf{k}$. Here $(\alpha_1, \alpha_2, \alpha_3) = (1/4) \sum\limits_{\nu,\nu'=\pm 1} f'(p_\nu^{\nu'})(\nu, \nu\nu'/\lambda_\nu, \nu'/\lambda_\nu)$, with $p_\nu^{\nu'} = (1/4)(1 + \nu\mathbf{r}_B\cdot\mathbf{k} + \nu'\lambda_\nu)$ the eigenvalues of (18) and $\lambda_\nu = |\mathbf{r}_A + \nu J\mathbf{k}|$. In the case of the quantum discord (4), the additional local term leads to the modified equation[34]

$$(\alpha_1 - \eta)\mathbf{r}_B + \alpha_2 J^t \mathbf{r}_A + \alpha_3 J^t J\mathbf{k} = \lambda\mathbf{k}\,, \tag{20}$$

where $f(p) = -p\log p$ and $\eta = (1/2)\sum_{\nu=\pm 1} \nu f'(p_\nu) = (1/2)\log(p_-/p_+)$, with $p_\nu = \sum_{\nu'} p_\nu^{\nu'} = (1/2)(1 + \nu\mathbf{r}_B\cdot\mathbf{k})$ the eigenvalues of ρ'_B. A different approach was provided in Ref. 28.

General analytic solutions of these equations can be obtained in a few cases. For instance, a closed evaluation of I_f^B for any S_f is directly feasible for any two-qubit state with *maximally mixed marginals*, i.e.,

$$\rho_{AB} = \frac{1}{4}(I + \boldsymbol{\sigma}_A J \boldsymbol{\sigma}_B)\,, \tag{21}$$

for which Eq. (19) reduces to $J^t J\mathbf{k} = \lambda\mathbf{k}\ \forall\ I_f$, indicating that $\mathbf{k}$ should be an eigenvector of $J^t J$. Moreover, it can be shown[34] that the minimum corresponds to $\mathbf{k}$ directed along the eigenvector with the largest eigenvalue of $J^t J\ \forall S_f$ (universal least disturbing measurement), such that the post-measurement state (3)–(18) conserves the largest component: By suitable local rotations, $\boldsymbol{\sigma}_A J \boldsymbol{\sigma}_B$ can be written as $\sum_{\mu=x,y,z} J_\mu \sigma_{A\mu}\sigma_{B\mu}$, where J_μ are the eigenvalues of $J^t J$ (the same as those of JJ^t), and the least disturbing measurement leads then to $\rho'_{AB} = (1/4)(I + J_{\tilde{\mu}}\sigma_{A\tilde{\mu}}\sigma_{B\tilde{\mu}}$, where $J_{\tilde{\mu}} = \mathrm{Max}[J_x, J_y, J_z]$. The final result for I_f^B (obviously identical to I_f^A for this state) is[34]:

$$I_f^B(\rho_{AB}) = 2f\left(\frac{p_1 + p_2}{2}\right) + 2f\left(\frac{p_3 + p_4}{2}\right) - f(p_1) - f(p_2) - f(p_3) - f(p_4)\,, \tag{22}$$

where (p_1, p_2, p_3, p_4) are the eigenvalues of ρ_{AB} sorted in decreasing order ($p_{1,2} = (1 + J_z \pm (J_x - J_y))/4$, $p_{3,4} = (1 - J_z \pm (J_x + J_y))/4$ if $|J_z| \geq |J_x| \geq |J_y|$ and

$J_z \geq 0$, $J_x \geq 0$). It is verified that $I_f^B = 0$ only if $p_1 = p_2$ *and* $p_3 = p_4$, in which case $\rho_{AB} = \rho'_{AB}$ is a classically correlated state.[34] In the von-Neumman case, Eq. (22) is just the quantum discord for this state, as in this case it coincides with the one-way information deficit ($\rho'_B = \rho_B$ are maximally mixed). In the case of the linear entropy, Eq. (22) yields the geometric discord and reduces to[34] $I_2^B(\rho_{AB}) = (p_1 - p_2)^2 + (p_3 - p_4)^2$.

The linear entropy case (11) is obviously the most simple to evaluate, and in this sense the most convenient. A full analytic evaluation for a general two-qubit state was achieved in Ref. 32. Since $\mathrm{Tr}\sigma_\mu\sigma_{\mu'} = 2\delta_{\mu\mu'}$, one easily obtains in this case

$$I_2^{\mathbf{k}} = S_2(\rho'_{AB}) - S_2(\rho_{AB}) = \frac{1}{2}(\mathrm{tr}\, M_2 - \mathbf{k}^t M_2 \mathbf{k})\,, \quad M_2 = \mathbf{r}_B \mathbf{r}_B^t + J^t J\,, \tag{23}$$

where $\|J\|^2 = \mathrm{tr}J^tJ$, $|\mathbf{r}|^2 = \mathbf{r}\cdot\mathbf{r}$ and M_2 is a positive semidefinite symmetric matrix. The minimum of $I_2^{\mathbf{k}}$ is then obtained when $\mathbf{k}$ is directed along the eigenvector associated with the maximum eigenvalue λ_1 of M_2, leading to[32]:

$$I_2^B = \underset{\mathbf{k}}{\mathrm{Min}}\, I_2^{\mathbf{k}} = \frac{1}{2}(\mathrm{tr}\, M_2 - \lambda_1)\,. \tag{24}$$

It is easily seen that Eq. (19) reduces in this case to the eigenvalue equation $M_2\mathbf{k} = \lambda\mathbf{k}$, such that the stationary directions are those of the eigenvectors of M_2.

Similarly, the $q = 3$ case in the Tsallis entropy, $S_3(\rho) \propto (1 - \mathrm{Tr}\,\rho^3)$, can also be fully worked out analytically.[34] We obtain:

$$I_3^{\mathbf{k}} = S_3(\rho'_{AB}) - S_3(\rho_{AB}) = \frac{1}{4}(\mathrm{tr}\, M_3 - 2\mathrm{det}\, J - \mathbf{k}^t M_3 \mathbf{k})\,, \tag{25}$$

$$M_3 = \mathbf{r}_B \mathbf{r}_B^t + J^t J + \mathbf{r}_B \mathbf{r}_A^t J + J^t \mathbf{r}_A \mathbf{r}_B^t\,, \tag{26}$$

where M_3 is again a positive semidefinite symmetric matrix, with $\mathrm{tr}M_3 = |\mathbf{r}_B|^2 + \|J\|^2 + 2\mathbf{r}_A^t J \mathbf{r}_B$. Its minimum corresponds then to $\mathbf{k}$ along the eigenvector with the maximum eigenvalue λ_1 of M_3, which leads to[34]

$$I_3^B = \underset{\mathbf{k}}{\mathrm{Min}}\, I_3^{\mathbf{k}} = \frac{1}{4}(\mathrm{tr}\, M_3 - 2\mathrm{det}\, J - \lambda_1)\,. \tag{27}$$

It is again verified that Eq. (19) leads here to the same eigenvalue equation $M_3\mathbf{k} = \lambda\mathbf{k}$, as $(\alpha_1, \alpha_2, \alpha_3) = (\mathbf{r}_B^t\mathbf{k} + \mathbf{r}_A^t J\mathbf{k}, \mathbf{r}_B^t\mathbf{k}, 1)$. In the case of the state (21), we obtain[34] $I_3^B = (p_1 - p_2)^2(p_1 + p_2) + (p_3 - p_4)^2(p_3 + p_4)$.

It should be stressed that for the case of two qubits, these two entropies, S_2 and S_3, lead to *the same entanglement monotone*,[74] since for an arbitrary single qubit state they become identical:[33,34] $S_2(\rho_A) = S_3(\rho_A) = 1 - |\mathbf{r}_A|^2$ for $\rho_A = (1/2)(I_2 + \mathbf{r}_A \cdot \boldsymbol{\sigma})$. Both quantities I_2^B and I_3^B reduce then to the standard squared concurrence[60,61] C_{AB}^2 in the case of a pure two-qubit state.

6. The Case of a Mixture of Two Aligned States

We are now in a position to examine the important case of a mixture of two aligned spin 1/2 states,[24] which will allow us to understand the behavior of the quantum discord of spin pairs in finite ferromagnetic XY chains, particularly in the vicinity of the transverse factorizing field.[24,46–57] We consider the bipartite state

$$\rho_{AB}(\theta) = \frac{1}{2}(|\theta\theta\rangle\langle\theta\theta| + |-\theta-\theta\rangle\langle-\theta-\theta|) \tag{28}$$

$$= \frac{1}{4}(I + \cos\theta(\sigma_{Az} + \sigma_{Bz}) + \cos^2\theta\,\sigma_{Az}\sigma_{Bz} + \sin^2\theta\,\sigma_{Ax}\sigma_{Bx})\,, \tag{29}$$

where $|\theta\rangle = e^{-i\theta\sigma_y/2}|0\rangle$ denotes the state with its spin aligned along $\mathbf{k} = (\sin\theta, 0, \cos\theta)$, and (29) corresponds to the spin 1/2 case, where $|\theta\rangle = \cos(\theta/2)|0\rangle + \sin(\theta/2)|1\rangle$ and we have used the notation of Eq. (17). It is a particular case of X state,[26,27] i.e., states that commute with the S_z parity $P_z = -e^{i\pi(\sigma_{Az}+\sigma_{Bz})/2}$.[34]

The state (28) arises, for instance, as the reduced state of *any* pair in the n-qubit pure states

$$|\Theta_\pm\rangle = \frac{|\theta\theta\cdots\theta\rangle \pm |-\theta\cdots-\theta\rangle}{\sqrt{2(1\pm\langle-\theta|\theta\rangle^n)}}\,, \tag{30}$$

if the complementary overlap $\langle-\theta|\theta\rangle^{n-2}$ ($\langle-\theta|\theta\rangle = \cos\theta$ for spin 1/2) can be neglected (i.e., n large and θ not too small). As will be seen in the next sections, the states (30) are the actual exact ground states of such chains in the immediate vicinity of the factorizing field.

The state (28) is clearly separable, i.e., a convex combination of product states,[68] but is classically correlated, i.e., diagonal in a product basis, just for $\theta = 0$ or $\theta = \pi/2$. Accordingly, both the quantum discord and all measures (9), including the geometric discord, will be nonzero just for $\theta \in (0, \pi/2)$. As seen in Fig. 1, they all exhibit similar qualitative features, although significant differences concerning the minimizing measurement arise. Due the symmetry of the state, it is apparent that $D^A = D^B = D$ and $I_f^A = I_f^B = I_f\,\forall\,\theta$.

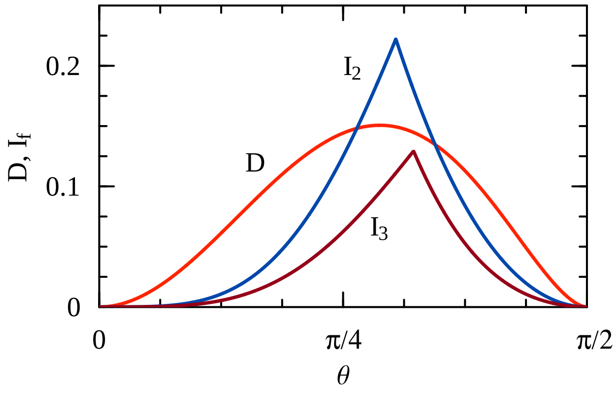

Fig. 1. Quantum correlation measures in the mixture of aligned states (28): The quantum discord D, the geometric discord I_2 and the "cubic" discord I_3, as a function of the angle θ. Normalization is such that all measures take the value 1 in a maximally entangled two-qubit state. Due to the symmetry of the state, $D = D^A = D^B$ and $I_f = I_f^A = I_f^B\,\forall\,f$.

It is rapidly seen from Eq. (19) that for this state (as well as any other X state), spin measurements along x, y or z *are stationary*, for both the quantum discord and all measures I_f.[34] In the case of the quantum discord, the minimizing measurement for this state (which is of rank 2, and hence minimized through a standard von-Neumann measurement[35]) is in fact along $x\,\forall\,\theta \in (0, \pi/2)$, in which case the eigenvalues of ρ'_{AB} become $p_{\nu}^{\nu'} = (1/4)(1 + \nu'\sqrt{\cos^2\theta + \sin^4\theta})$, being twofold degenerate. The final result for the quantum discord can then be expressed as[24]:

$$D = \sum_{\nu=\pm 1}\left[2f\left(\frac{1+\nu\sqrt{1-\frac{1}{4}\sin^2 2\theta}}{4}\right) - f\left(\frac{1+\nu\cos^2\theta}{2}\right) + f\left(\frac{1+\nu\cos\theta}{2}\right)\right] - 1\,, \tag{31}$$

where $f(p) = -p\log_2 p$. It is maximum at $\theta \approx 1.15\pi/4$. For $\theta \approx 0$, D vanishes quadratically ($D \propto \theta^2$) whereas for $\theta \to \pi/2$, $D \propto (\pi/2-\theta)^2(-\log_2(\pi/2-\theta)^2 + c)$.

On the other hand, the geometric discord (11) and the "cubic" discord ($q = 3$ in Eq. (12)) can be directly evaluated using Eqs. (24)–(27). We obtain[34]:

$$I_2 = \begin{cases} \frac{1}{2}\sin^4\theta & \theta < \theta_{c2} \\ \frac{1}{2}\cos^2\theta + \cos^4\theta & \theta > \theta_{c2}\,, \end{cases} \tag{32}$$

$$I_3 = \begin{cases} \frac{1}{4}\sin^4\theta & \theta < \theta_{c3} \\ \frac{1}{4}(\cos^2\theta + 3\cos^4\theta) & \theta > \theta_{c3}\,, \end{cases} \tag{33}$$

where $\cos^2\theta_{c2} = 1/3$ ($\theta_{c2} \approx 0.61\pi/2$) and $\cos^2\theta_{c3} = (\sqrt{17}-3)/4$ ($\theta_{c3} \approx 0.64\pi/2$), the minimizing measurement direction changing abruptly from z to x at $\theta = \theta_c$ as θ increases, in contrast with the quantum discord. Both I_2 and I_3 exhibit therefore a cusp like maximum at $\theta = \theta_c$, as seen in Fig. 1. It is also seen from Eqs. (32)–(33) that these quantities vanish as θ^4 for $\theta \to 0$, whereas for $\theta \to \pi/2$ they vanish quadratically ($\propto (\pi/2-\theta)^2$). For completeness, it should also be mentioned that the behavior of the least disturbing local measurement for this state depends actually on the choice of entropy. For instance, in the von-Neumann case [where Eq. (9) becomes the one-way information deficit (10)], we obtain instead a smoothed $z \to x$ transition for the minimizing measurement direction, which evolves continuously from z to x in a small intermediate interval.[34]

7. XYZ Spin Chains and Transverse Factorizing Field

Let us now use the previous measures and results to analyze the quantum correlations between spin pairs in a chain of spins s_i. We will consider finite chains with XYZ couplings of arbitrary range immersed in a transverse magnetic field, not necessarily uniform, such that the Hamiltonian reads:

$$H = \sum_i B^i s_{iz} - \frac{1}{2}\sum_{\mu=x,y,z}\sum_{i,j} J_\mu^{ij} s_{i\mu}s_{j\mu}\,, \tag{34}$$

where $s_{i\mu}$ denote the components of the local spin $\mathbf{s}_i$ (assumed dimensionless). We first remark that the Hamiltonian (34) always commutes with the total S_z parity or phase flip

$$P_z = \otimes_{i=1}^n \exp[-i\pi(s_{iz}-s_i)]\,, \tag{35}$$

irrespective of the coupling range, anisotropy, geometry or dimension of the array. Hence, nondegenerate eigenstates will have a definite parity. In fact, the ground state of finite chains will typically exhibit a series of parity transitions as the field increases from 0, before ending in an almost aligned state for sufficiently large fields.

A related remarkable effect in these chains is the possibility of exhibiting *a completely separable* exact eigenstate at a *factorizing field*. The existence of a factorizing field was first discussed in Ref. 46, and its properties together with the general conditions for its existence were recently analyzed in great detail by several authors.[24,47–57] At the *transverse* factorizing field, finite XYZ chains actually exhibit a *pair* of completely separable and degenerate parity breaking exact eigenstates,[51,54,55] which can be ground states under quite general conditions. In such a case the transverse factorizing field corresponds to a ground state parity transition (typically the last parity transition[51,54,55]), where the lowest energy levels of each parity subspace cross and enable the formation of such eigenstates. Let us notice that while these lowest levels become practically degenerate in a large chain for fields $|B|<B_c$, they are not exactly degenerate in a finite chain, except at crossing points.[51,54,55,75,76]

Let us then first describe the general conditions for which a separable parity breaking state of the form:

$$|\Theta\rangle = |\theta_1\cdots\theta_n\rangle = \otimes_{j=1}^n \exp[-i\theta_j s_{jy}]|0_j\rangle\,, \tag{36}$$

where $s_{jz}|0_j\rangle = -s_j|0_j\rangle$, can be an *exact* eigenstate of (34). By inserting (36) in the equation $H|\Theta\rangle = E|\Theta\rangle$, it can be shown that such conditions are[54,55]:

$$J_y^{ij} = J_x^{ij}\cos\theta_i\cos\theta_j + J_z^{ij}\sin\theta_i\sin\theta_j\,, \tag{37}$$

$$B^i\sin\theta_i = \sum_j\left(s_j - \frac{1}{2}\delta_{ij}\right)(J_x^{ij}\cos\theta_i\sin\theta_j - J_z^{ij}\sin\theta_i\cos\theta_j)\,, \tag{38}$$

which are valid for arbitrary spins s_i. They determine, for instance, the values of J_y^{ij} and B^i in terms of J_x^{ij}, J_z^{ij}, s_i and θ_i. A careful engineering of couplings and fields can then always produce a chain with such eigenstate, for any chosen values of θ_i. It is also apparent that this eigenstate is degenerate, since $P_z|\Theta\rangle = |-\Theta\rangle = \otimes_{j=1}^n \exp[i\theta_j s_{jy}]|0_j\rangle$ will have the same energy (and differ from $|\Theta\rangle$ if

$\sin\theta_j \neq 0$ for some j), indicating that these fields necessarily correspond to the crossing of two opposite parity levels. Each local state in the product (36) is a local coherent state. We also note that any state $\otimes_{j=1}^n e^{-i\boldsymbol{\theta}_j\cdot\boldsymbol{s}_j}|0_j\rangle$ can be written, except for a normalization factor, in the form (36) by allowing a complex θ_j.[54,55] Equation (37)–(38) are then generally valid for such type of states.

The second equation (38) cancels the matrix elements of H between $|\Theta\rangle$ and one spin excitations, and is then a "mean field-like" equation, i.e., that which arises when minimizing the average energy $\langle\Theta|H|\Theta\rangle$ with respect to the θ_i, for fixed fields and couplings. The first equation (37) ensures that the minimizing separable state is an exact eigenstate, by canceling the residual matrix elements of H connecting $|\Theta\rangle$ with the remaining states (two-spin excitations). It can also be shown[54,55] that in the ferromagnetic-type case

$$|J_y^{ij}| \leq J_x^{ij}\ \forall\, i,j\,, \tag{39}$$

where all off-diagonal elements of H in the standard basis of s_z eigenstates are real and negative, the state (36) is necessarily a *ground state* if $\theta_j \in (0,\pi/2)\ \forall\, j$, as the exact ground state must have (or can be chosen to have if degenerate) expansion coefficients of the same sign in this basis (different signs will not decrease $\langle H\rangle$), and hence cannot be orthogonal to $|\Theta\rangle$.[51,54,55]

In particular, a uniform solution $\theta_j = \theta\ \forall\, j$, leading to $|\Theta\rangle = |\theta\cdots\theta\rangle$, is feasible if the coupling anisotropy:

$$\chi = \frac{J_y^{ij} - J_z^{ij}}{J_x^{ij} - J_z^{ij}}\,, \tag{40}$$

is *constant* $\forall\ i,j$ and nonnegative.[54,55] Of course, if $\chi > 1$ we can change it to $\chi \in (0,1)$ by swapping $x \leftrightarrow y$ through a rotation of $\pi/2$ round the z axis. In such a case, Eqs. (37)–(38) lead to:

$$\cos^2\theta = \chi\,, \tag{41}$$

$$B^i = \sqrt{\chi}\sum_j (J_x^{ij} - J_z^{ij})\left(s_j - \frac{1}{2}\delta_{ij}\right), \tag{42}$$

where Eq. (42) holds for $\sin\theta \neq 0$.

Equations (41)–(42) allow, for instance, the existence of a factorizing field for uniform first neighbor couplings $J_\mu^{ij} = J_\mu\delta_{j,i\pm 1}$ in a finite linear spin s chain if $\chi = (J_y - J_z)/(J_x - J_z) > 0$, both in the cyclic case ($J_\mu^{1n} = J_\mu$), where the factorizing field is completely *uniform*,

$$B^i = B_s = 2s\sqrt{\chi}(J_x - J_z)\,, \tag{43}$$

as well as in the open case ($J_\mu^{1n} = 0$), where $B^i = B_s$ at inner sites but $B^1 = B^n = B_s/2$ at the borders.[54,55] A fully and equally connected spin s array with $J_\mu^{ij} = 2J_\mu/(n-1)\ \forall\, i \neq j$ (Lipkin model[77–79]) will also exhibit a uniform transverse factorizing field at $B = B_s$ if $\chi > 0$.[51,80,81] The ensuing state $|\Theta\rangle$ can be ensured to be a *ground state* in all these cases if $|J_y| \leq J_x$ (when $\chi \in [0,1]$). Other possibilities, like solutions with alternating angles,[54,55] can also be considered.

8. Quantum Correlations in the Definite Parity Ground States

Let us now focus on finite spin chains which exhibit a separable parity breaking exact eigenstate $|\Theta\rangle$ at the factorizing field B_s. It will of course be degenerated with $|-\Theta\rangle = P_z|\Theta\rangle$. The important point is that the definite parity states

$$|\Theta_\pm\rangle = \frac{|\Theta\rangle \pm |-\Theta\rangle}{\sqrt{2(1 \pm \langle -\Theta|\Theta\rangle)}}\,, \tag{44}$$

i.e., the states (30) in the uniform case, will also be exact ground states at B_s. Moreover, since the exact ground state of a finite chain will actually be nondegenerate away from the factorizing field (and the other crossing points), it will have a definite parity. Hence, the actual ground state side-limits at $B = B_s$ will be given by the definite parity states (44) (rather than $|\pm\Theta\rangle$). A ground state parity transition $- \to +$ will then take place as the field increases across B_s.[51,54,55]

While the ground states of each parity sector become degenerate in the large n limit for fields $|B| < B_s$, in finite chains the degeneracy is lifted and the actual ground state will exhibit important correlations arising just from the definite parity effect. For instance, in the immediate vicinity of B_s, the pairwise correlations, rather than vanish, will approach the values determined by the states (44). They will then depend on θ_i and θ_j for a pair i, j, irrespective of the separation $i-j$. In the uniform case, such correlations will then be *independent of the separation*, since the states (44) will be completely symmetric and will lead to a separation independent pair reduced state $\rho_{ij} = \mathrm{Tr}_{\overline{ij}}|\Theta_\pm\rangle\langle\Theta_\pm|$ ($\overline{ij}$ denotes the rest of the chain). Such state is given exactly by[24]

$$\rho_{ij}^{\varepsilon}(\theta) = \frac{|\theta\theta\rangle\langle\theta\theta| + |-\theta-\theta\rangle\langle-\theta-\theta| + \varepsilon(|\theta\theta\rangle\langle-\theta-\theta| + |-\theta-\theta\rangle\langle\theta\theta|)}{2(1+\varepsilon\langle\theta\theta|-\theta-\theta\rangle)}\,, \tag{45}$$

where $\varepsilon = \pm\cos^{n-2}\theta$ for $s = 1/2$. This parameter is then small for not too small n and θ. In the $\varepsilon \to 0$ limit one recovers the mixture (28).

The concurrence of the state (45) (a measure of its entanglement[60,61]) depends essentially on ε and is therefore small, vanishing for $\varepsilon \to 0$ (as in this limit the state (45) becomes separable). It is given explicitly by[24,51,54,55]:

$$C = \frac{|\varepsilon|\sin^2\theta}{1+\varepsilon\cos^2\theta}\,, \tag{46}$$

which is parallel (antiparallel)[49,50] for $\varepsilon > 0$ (< 0). Its maximum value is $2/n$ (in agreement with the monogamy property[58,59]), reached for $\theta \to 0$ in the negative parity case, where the state (30) approaches an W-state.[51]

In contrast, we have seen that the quantum and geometric discord, as well as the other measures of quantum correlations (9), do acquire finite and nonnegligible values in the mixture (28) (Fig. 1), i.e., in the state (45) even for $\varepsilon \to 0$, entailing

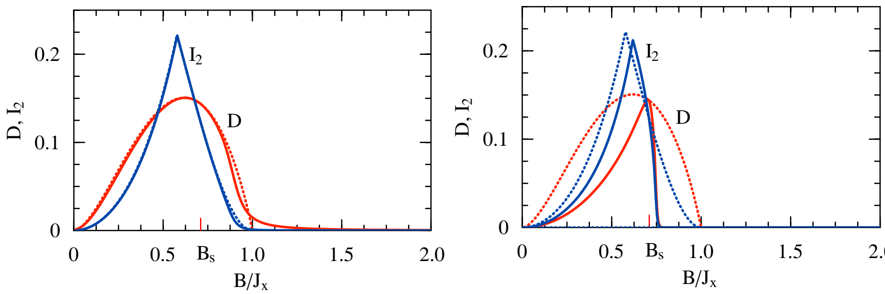

Fig. 2. Left: The quantum discord D and the geometric discord I_2 between spin pairs in the exact ground state of a fully connected XY spin 1/2 array of $n = 50$ spins with coupling anisotropy $\chi = J_y/J_x = 0.5$, as a function of the scaled transverse applied field B. The dotted lines depict the result for the mixture of aligned states (28) at the mean field angle $\cos\theta = B/J_x$, which is almost coincident with the exact result for $|B| < J_x$ and exactly coincident at the factorizing field $B_s = \sqrt{\chi}J_x$. Right: Same quantities for a cyclic chain of $n = 50$ spins with first neighbor XY couplings with the same anisotropy, for a distant pair ($L = 25$). The dotted lines depict again the results for the mixture of aligned states (28) at the mean field angle, which now coincide with the exact results only at the factorizing field B_s.

simultaneous and coincident finite values for all pairs in the state (30).[24] This implies in turn *infinite range* of pairwise quantum correlations, as measured by D or I_f, at least in the immediate vicinity of the factorizing field B_s, where they will be described by the state (28) and will therefore be *independent of both separation and coupling range*. Hence, B_s plays the role of a quantum critical point in the small finite chain.

As illustration, we first depict in Fig. 2 the quantum discord and the geometric discord of spin 1/2 pairs for XY couplings ($J_z^{ij} = 0\ \forall\, i, j$) in the ground state of the fully connected array (Lipkin-type model) and of the nearest-neighbor cyclic chain, for anisotropy $J_y/J_x = 0.5$ in the ferromagnetic type case ($J_x > 0$). The emergence of a finite appreciable value of these quantities for $|B| < B_c$, persisting for pairs with large separation even in the case of first neighbor couplings, is then a direct consequence of the definite parity effect. The exact results for $n = 50$ spins were computed by direct diagonalization of H in the Lipkin case (where the ground state belongs to the completely symmetric representation having total spin $S = n/2$), while in the nearest neighbor chain they were obtained through the exact Jordan–Wigner fermionization,[82] taking into account the parity effect exactly in the discrete Fourier transform (see for instance Refs. 51, 75, 76). In both cases the ground state exhibits $n/2$ parity transitions as the field increases from 0, the last one at B_s, although for the case depicted ($N = 50$), their effects on D or I_2 are not visible in the scale of the figure (they become visible for smaller n[24]).

It is verified that at the factorizing field (43), the exact results for D and I_2 in both models coincide with those obtained for the mixture (28), i.e., with Eqs. (31) and (32) for $\cos\theta = \sqrt{\chi}$ [Eq. (41)], being then identical and the same for any pair at this point. Moreover, in the fully connected case the exact results for D and

I_2 are actually practically coincident with those obtained from the mixture (28) (dotted lines) *in the whole region* $|B| < J_x$ if θ is the mean field angle satisfying $\cos\theta = B/J_x$ [Eq. (38)], since the ground state is in this region well approximated by the definite parity states (44) or (30), even away from B_s. The behavior of D and I_2 for $B \in [0, J_x]$ resembles then that obtained for the mixture (28) for $\theta \in [0, \pi/2]$. This is not the case in the chain with first neighbor couplings, where the agreement holds just at B_s, and where D and I_2 become appreciable only for $|B| < B_c = (J_x + J_y)/2$ (which is smaller than the mean field critical field J_x but slightly above the factorizing field $\sqrt{\chi}$). Nonetheless, the values attained by D and I_2 in the whole region $|B| < B_s$ are still quite large, owing to the definite parity effect, although they exhibit the effects of correlations beyond the parity projected mean field description provided by the states (44).

We also depict in Fig. 3 results for D and I_2 for all separations $L = 1, \ldots, n/2$ of the spins of the pair, in the nearest neighbor coupling case (in the fully connected model they are obviously identical $\forall\, L$). It is seen that the values of D and I_2 (and the same for I_3 or other I_f's) rapidly saturate as L increases in the region $|B| < B_c$, reaching here a finite nonnegligible value due to the definite parity effect, whereas for $|B| > B_c$ they are appreciable just for the first few neighbors ($L = 1, 2$). In the last region they can be described perturbatively.[24]

It is apparent from Figs. 2–3 that the same qualitative information can be obtained either from the quantum discord D or the geometric discord I_2, except for the type of maximum. That of I_2 is cusp-like due to the sharp $x \to z$ transition in the minimizing measurement direction that arises as the field increases, which parallels that occurring for the state (28) as θ decreases (see Fig. 1). Such transition reflects the change in the type of pairwise correlation, and resembles that of the concurrence (which changes from antiparallel to parallel at B_s[51]). We also mention that while the behavior of I_3 (not shown) is similar to I_2, other I_f can exhibit a smoothed maximum as the transition from x to $\to z$ in the measurement direction can be continuous.[34]

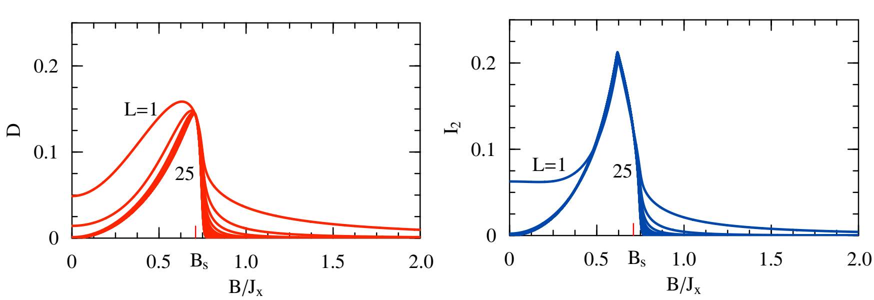

Fig. 3. (left) The quantum discord D and (right) the geometric discord I_2 between spin pairs with separation $L = 1, 2, \ldots, n/2$ in the exact ground state of a cyclic chain of $n = 50$ spins with first neighbor XY couplings and anisotropy $\chi = 0.5$. The results for all separations are simultaneously depicted. They all merge at the factorizing field B_s, where they coincide with the result for the mixture (28) with $\cos\theta = B_s/J_x = \sqrt{\chi}$.

We finally remark that the exact ground state pairwise concurrence in the fully connected case is small (of order n^{-1} and bounded above by $2/n$),[80,81] such that the entanglement monotones associated with D and I_2 (the entanglement of formation and the squared concurrence) are very small in the scale of Fig. 2. The same occurs with the concurrence of largely separated pairs in the nearest neighbor case,[83] which is nonzero (but very small for this anisotropy and size) just in the immediate vicinity of B_s.[51,54,55]

9. Conclusions

We have examined the behavior of pairwise quantum correlations in the exact ground state of finite ferromagnetic-type XY spin chains in a transverse field, by analyzing the quantum discord as well as other generalized measures of quantum correlations. We have first provided a brief review of the latter, which are based on general entropic forms and defined as the minimum information loss due to a local measurement in one of the constituents. They generalize the one-way information deficit and contain the geometric discord as a particular case, preserving at the same time the basic properties of the quantum discord like reducing to the (generalized) entanglement entropy in the case of pure states and vanishing just for classically correlated states. We have shown that all these measures indicate the presence of long range pairwise quantum correlations for $|B| < B_c$ in the exact ground state of these chains, which arise essentially from the definite S_z parity of such state and can be understood in terms of the model based on the mixture of aligned states (28). They all reach full range at the factorizing field, where they acquire a finite nonnegligible constant value which is independent of the pair separation or coupling range and is determined solely by the coupling anisotropy. Such value is exactly described by the states (28) or (45), which also provide a quite reliable description of these correlations for all $|B| < B_c$ for long range couplings, as we have seen in the case of the fully connected model. Parity effects are then seen to be of paramount importance for a proper description of quantum correlations in finite quantum systems. A final comment is that the use of simple entropic forms involving just low powers of the density matrix, like those underlying the geometric discord I_2 and the cubic measure I_3, enables an easier evaluation, offering at the same time an increased sensitivity of the optimizing measurement to changes in the type of correlation.

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