Quantum discord and information deficit in spin chains

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We examine the behavior of quantum correlations of spin pairs in a finite anisotropic XY spin chain immersed in a transverse magnetic field, through the analysis of the quantum discord and the conventional and quadratic one way-information deficits. We first provide a brief review of these measures, showing that the last ones can be obtained as particular cases of a generalized information deficit based on general entropic forms. All these measures coincide with an entanglement entropy in the case of pure states, but can be non-zero in separable mixed states, vanishing just for classically correlated states. It is then shown that their behavior in the exact ground state of the chain exhibits similar features, deviating significantly from that of the pair entanglement below the critical field. In contrast with entanglement, they reach full range in this region, becoming independent of the pair separation and coupling range in the immediate vicinity of the factorizing field. It is also shown, however, that significant differences between the quantum discord and the information deficits arise in the local minimizing measurement that defines them. Both analytical and numerical results are provided.

I. INTRODUCTION

The investigation of non-classical correlations in mixed states of composite quantum systems has attracted strong attention in recent years. While in pure states such correlations can be identified with entanglement [1–5], in the case of mixed states, separable (unentangled) states, defined in general as convex mixtures of product states [6], i.e., as states which can be generated by local operations and classical communication (LOCC), may still exhibit non-classical features. The latter emerge from the possible non-commutativity of the different products and lead, for instance, to a finite value of the quantum discord [7–9] and other recently introduced related quantifiers of quantum correlations [10, 11]. These quantifiers include the one-way information deficit [9, 12, 13], the geometric discord [14], generalized entropic measures [15, 16] and more recently the local quantum uncertainty [17, 18] and the trace distance discord [19–22]. While entanglement is certainly necessary for quantum teleportation [23] and for an exponential speedup in pure state based quantum computation [24], interest on these new measures has been triggered by the existence of mixed state based quantum algorithms like that of [25], able to achieve an exponential speedup over the best classical algorithms for a certain task, with vanishing entanglement [26] but finite quantum discord [27]. And various operational interpretations of the quantum discord and other related measures have been provided [11, 17, 21, 28–33].

In this article we will concentrate on the quantum discord [7–9] and the generalized entropic measures of [15], which include as particular cases the von Neumann based one-way information deficit [9, 12, 13] and the geometric discord [14], and which represent a generalized information deficit. The quantum discord as well as all other related measures require a rather complex minimization over a local measurement or operation which has limited their applicability to small systems or special states. The optimization problem for the quantum discord was in fact recently shown to be NP complete [34]. The advantage of the generalized entropic formalism is, first, the possibility of using simpler entropic forms like the linear entropy, which, as will be discussed in section 2, enables an easier evaluation (it does not require the diagonalization of the density matrix) and a more direct experimental access (it can be determined without a full state tomography). This entails that an explicit solution of the associated optimization problem for certain states can be achieved. The generalized formalism also allows to identify some universal properties, i.e. valid for any entropic form (and not just for a particular choice of entropy) satisfied by the post-measurement state.

We first provide in section 2 an overview of the main concepts and properties associated with these measures. We then apply these measures to examine the quantum correlations of spin pairs in the exact ground state of finite spin 1/2 chains with XY-type couplings in a transverse magnetic field, through their entanglement, quantum discord and information deficit. All separations between the pairs are considered. Several important studies of the quantum discord in spins chains have been made [35–43], but the relation with the generalized information deficit and the differences between their optimizing measurements in these spin pairs have not yet been analyzed in detail. We have recently investigated these aspects for an XX spin chain in [42], and will here extend this analysis to the anisotropic XY case. It is first shown that in contrast with the pair entanglement, the quantum discord and the information deficit exhibit, for the exact ground state of these chains, common features such as an appreciable finite value below the critical field, for all separations. Moreover, they approach a finite *common non-zero value* [37] at the remarkable factorizing field [41, 44–48] that these chains can exhibit in the anisotropic case. On the other hand, we will also show that important differences between the quantum discord on the one side, and the standard and generalized information deficit on the other side, do arise in the minimizing local spin measurement that defines them. While in the quantum discord the direction of the latter is always orthogonal to the transverse field, in the other measures it exhibits a perpendicular to parallel transition as the field increases, which is present for all separations and which reflects significant qualitative changes in the reduced state of the pair. This difference indicates a distinct response of the minimizing measurement of these quantities to the onset of quantum correlations.

II. MEASURES OF QUANTUM CORRELATIONS

A. Quantum Entanglement

We start by providing a brief overview of the basic notions. A pure state $|\Psi_{AB}\rangle$ of a bipartite system $A+B$ is separable iff (if and only if) it is a product state $|\Psi_A\rangle|\Psi_B\rangle$. Otherwise it is entangled. The Schmidt decomposition [3]

$$|\Psi_{AB}\rangle=\sum_{k=1}^{n_s}\sqrt{p_k}\,|k_A\rangle|k_B\rangle\,, \tag{1}$$

where $|k_{A(B)}\rangle$ denote orthonormal states for subsystem $A(B)$ and $p_k\geq 0$, $\sum_{k=1}^{n_s}p_k=1$, allows to easily distinguish separable pure states ($n_s=1$) from entangled states ($n_s\geq 2$). Here n_s is the Schmidt rank of $|\Psi_{AB}\rangle$ ($n_s\leq \mathrm{Min}[d_A,d_B]$, with $d_{A(B)}$ the Hilbert space dimensions of $A(B)$). Pure sate entanglement can be measured by the entanglement entropy [2]

$$E(A,B)=S(\rho_A)=S(\rho_B)=-\sum_{k=1}^{n_s}p_k\log p_k\,, \tag{2}$$

where $\rho_{A(B)}=\mathrm{Tr}_{B(A)}\,\rho_{AB}=\sum_{k=1}^{n_s}p_k|k_{A(B)}\rangle\langle k_{A(B)}|$, with $\rho_{AB}=|\Psi_{AB}\rangle\langle\Psi_{AB}|$, are the reduced states of $A(B)$ and $S(\rho)=-\mathrm{Tr}\,\rho\log\rho$ is the von Neumann entropy. We will set in what follows $\log p\equiv\log_2 p$, such that $E(A,B)=1$ for a maximally entangled two-qubit state ($n_s=2$, $p_1=p_2=1/2$).

On the other hand, a general mixed state ρ_{AB} ($\rho_{AB}\geq 0$, $\mathrm{Tr}\,\rho_{AB}=1$) of a bipartite system $A+B$ is separable iff it can be expressed as a *convex mixture* of product states [6]:

$$\rho_{AB}\text{ separable }\Leftrightarrow\rho_{AB}=\sum_{\alpha}p_\alpha\rho_A^\alpha\otimes\rho_B^\alpha\,,\;\;p_\alpha>0\,, \tag{3}$$

where $\sum_\alpha p_\alpha=1$ and $\rho^\alpha_{A(B)}$ denote mixed states for subsystem $A\,(B)$. Otherwise, it is entangled. The meaning is that a separable state can be created by LOCC, i.e., Alice prepares a state ρ_A^α with probability p_α and tells Bob to prepare a partner state ρ_B^α.

For pure states $\rho_{AB}=|\Psi_{AB}\rangle\langle\Psi_{AB}|$, Eq. (3) is equivalent to the previous definition ($|\Psi_{AB}\rangle=|\Psi_A\rangle|\Psi_B\rangle$), but in the case of mixed states, product states $\rho_{AB}=\rho_A\otimes\rho_B$ are just a very particular case of separable states. The latter also include: a) *classically correlated states*, i.e. states diagonal in a standard product basis $\{|ij\rangle\equiv|i_A\rangle|j_B\rangle\}$,

$$\rho_{AB}=\sum_{i,j}p_{ij}|i_A\rangle\langle i_A|\otimes|j_B\rangle\langle j_B|\,,\;\;p_{ij}\geq 0\,, \tag{4}$$

where $\sum_{i,j}p_{ij}=1$ and $|i_{A(B)}\rangle$ are orthonormal states of $A(B)$, b) *classically correlated states from one of the subsystems*, say B, which are of the form

$$\rho_{AB}=\sum_j p_j\rho_{A/j}\otimes|j_B\rangle\langle j_B|\,,\;\;p_j\geq 0\,, \tag{5}$$

where $\sum_j p_j=1$ and $\rho_{A/j}$ are states of A, and which are then diagonal in a *conditional* product basis $\{|i_jj\rangle\equiv|i_{A/j}\rangle|j_B\rangle\}$ with $|i_{A/j}\rangle$ the eigenstates of $\rho_{A/j}$ (the case (4) recovered when all $\rho_{A/j}$ commute), and c) convex mixtures of product states which are not of the previous forms a) or b). The latter typically possess entangled eigenstates. For this reason, it is much more difficult to determine whether a mixed state is separable or entangled. The well known positive partial transpose criterion [49, 50] ($\rho_{AB}^{t_B}\geq 0$, with $\rho^{t_B}_{ij,kl}=\rho_{il,kj}$ for $\rho_{ilkj}=\langle il|\rho_{AB}|kj\rangle$) provides a necessary criterion for separability, which is sufficient for two-qubit or qubit-qutrit states.

For mixed states, the marginal entropies $S(\rho_A)$, $S(\rho_B)$ no longer provide a measure of entanglement. Instead, it is possible to use the entanglement of formation [51], defined through the convex roof extension of the pure state definition:

$$E(A,B)=\underset{\sum_\alpha p_\alpha|\Psi^\alpha_{AB}\rangle\langle\Psi^\alpha_{AB}|=\rho_{AB}}{\mathrm{Min}}S(\rho_A^\alpha)\,, \tag{6}$$

where the minimization is over all decompositions of ρ_{AB} as convex mixtures of pure states ($p_\alpha\geq 0$, $\sum_\alpha p_\alpha=1$) and $S(\rho_A^\alpha)=S(\rho_B^\alpha)$ is the entanglement entropy of the pure state $|\Psi^\alpha_{AB}\rangle$. Eq. (6) vanishes iff ρ_{AB} is separable, and reduces to the entanglement entropy (2) for pure states. It is an entanglement monotone [52], i.e., it does not increase by LOCC, staying unaltered under local unitary operations $\rho_{AB}\to U_A\otimes U_B\,\rho_{AB}\,U_A^\dagger\otimes U_B^\dagger$. Its evaluation is, however, difficult in general. A general analytic expression has been derived just for the two-qubit case [53], which will be specified in sec. 3.

While the marginal entropies are no longer entanglement indicators, it can still be shown [54] that if $S(\rho_A)>S(\rho_{AB})$ or $S(\rho_B)>S(\rho_{AB})$, ρ_{AB} is entangled, i.e.,

$$\rho_{AB}\text{ separable }\Rightarrow\;S(\rho_A)\leq S(\rho_{AB})\,,\quad S(\rho_B)\leq S(\rho_{AB})\,. \tag{7}$$

Eq. (7) provides an *entropic criterion for separability* [54] (necessary but not sufficient in general), which can be also extended to more general entropic forms [55, 56] and which will be invoked in sec. 2.3.

B. Quantum Discord

For the classically correlated states (4) or in general (5), there is a complete local measurement on B which leaves the state unaltered. This is not the case for entangled states nor for separable states not of the form (4) or (5). Let us recall here that a general positive operator valued measurement (POVM) [3]) on system $A+B$ is defined by a set of operators $\{M_j\}$ satisfying $\sum_j M_j^\dagger M_j = I_{AB} \equiv I_A \otimes I_B$, such that the probability of outcome j and the joint state after such outcome are

$$p_j = \mathrm{Tr}\,\rho_{AB}\,M_j\,, \quad \rho'_{AB/j} = M_j\rho_{AB}M_j^\dagger/p_j\,. \tag{8}$$

The post-measurement state if the outcome is unknown is then

$$\rho'_{AB} = \sum_j p_j\rho'_{AB/j} = \sum_j M_j\rho_{AB}M_j^\dagger\,. \tag{9}$$

Standard projective measurements correspond to the case where the M_j are orthogonal projectors ($M_kM_j = \delta_{jk}M_j$), while a local measurement on B corresponds to $M_j = I_A \otimes M_j^B$. By a complete local measurement on B we will mean one based on rank one orthogonal projectors $M_j^B = P_j^B$. It is then apparent that the states (4) and (5) remain unchanged ($\rho'_{AB} = \rho_{AB}$) after a local measurement on B based on the projectors $P_j^B = |j_B\rangle\langle j_B|$. For the states (4) (but not necessarily (5)) there is also a local measurement on A (that based on the projectors $|i_A\rangle\langle i_A|$) which leaves them unchanged.

The quantum discord [7–9] is a measure of quantum correlations which, unlike the entanglement of formation, can distinguish the classically correlated states (5) from the rest of separable states: It vanishes iff ρ_{AB} is of the form (4) or (5), being positive in the other separable states c), and reduces to the entanglement entropy (2) in the case of pure states. It can be defined as the minimum difference between two distinct quantum versions of the mutual information, or equivalently, of the conditional entropy:

$$\begin{aligned} D(A|B) &= \underset{M_B}{\mathrm{Min}}[I(A,B) - I(A,B_{M_B})] \\ &= \underset{M_B}{\mathrm{Min}}\, S(A|B_{M_B}) - S(A|B)\,, \end{aligned} \tag{10}$$

where the minimization is over all local measurements M_B on B and

$$\begin{aligned} I(A,B) &= S(\rho_A) - S(A|B)\,, \\ S(A|B) &= S(\rho_{AB}) - S(\rho_B)\,, \end{aligned} \tag{11}$$

are, respectively, the standard quantum mutual information and conditional entropy while

$$\begin{aligned} I(A,B_{M_B}) &= S(\rho_A) - S(A|B_{M_B})\,, \\ S(A|B_{M_B}) &= \sum_j p_j S(\rho_{A/j})\,, \end{aligned} \tag{12}$$

are the mutual information and conditional entropy after the local measurement M_B, with $\rho_{A/j} = \mathrm{Tr}_B\,\rho'_{AB/j}$ the reduced state of A after outcome j. Eq. (10) is always non-negative [7, 8], a property which arises from the concavity of the *conditional* von Neumann entropy [57].

In the case of complete local projective measurements M_B we have

$$S(A|B_{M_B}) = S(\rho'_{AB}) - S(\rho'_B)\,, \tag{13}$$

where $\rho'_B = \mathrm{Tr}_A\,\rho'_{AB}$ and ρ'_{AB} is the post-measurement state (9). It is then apparent that if the state is of the form (4) or (5), a measurement M_B based on the projectors $P_j^B = |j_B\rangle\langle j_B|$ leads to $S(A|B_{M_B}) = S(A|B)$ and hence $D(A|B) = 0$. For all other states (i.e., entangled states or separable states not of the form (4) or (5)), $D(A|B) > 0$. In the case of pure states, $S(\rho_{AB}) = 0$ while $S(A|B_{M_B}) = 0$ if M_B is any complete local measurement, entailing $D(A|B) = S(\rho_B) = E(A,B)$. For mixed states, the quantum discord can be related to the entanglement of formation $E(A,C)$ with a third system C purifying the whole system [29–32].

The mutual information $I(A,B)$ is a measure of all correlations between A and B, being non-negative and vanishing just for product states $\rho_{AB} = \rho_A \otimes \rho_B$. The bracket in (10) can then be interpreted as the difference between all correlations (classical+quantum) present in the original state minus the classical correlations left after the local measurement on B, which leaves then the quantum correlations. The evaluation of Eq. (10) is, nevertheless, difficult in the general case, being in fact an NP complete problem [34] due to the minimization over all possible local measurements M_B. Nonetheless, the minimum is always attained for measurements based on rank one projectors P_j^B, not necessarily orthogonal [11, 58].

C. Information Deficit

The one-way information deficit can be considered as an alternative measure of quantum correlations, with basic properties similar to those of the quantum discord. It can be defined as [9, 12, 13, 15]

$$I(A|B) = \underset{M_B}{\mathrm{Min}}\, S(\rho'_{AB}) - S(\rho_{AB})\,, \tag{14}$$

where ρ'_{AB} is the post-measurement state (9) and M_B is here restricted to complete local projective measurements on B, such that ρ'_{AB} is of the form (5). Like the quantum discord, Eq. (14) is a non-negative quantity which also vanishes just for the states (4) or (5), and which also reduces to the entanglement entropy (2) in the case of pure states. These properties will be shown below in a more general context, although they are also apparent from the alternative expression

$$I(A|B) = \underset{M_B}{\mathrm{Min}}\, S(\rho_{AB}||\rho'_{AB})\,, \tag{15}$$

where $S(\rho||\sigma) = \mathrm{Tr}\,\rho(\log\rho - \log\sigma)$ is the relative entropy [57, 59], a quantity satisfying $S(\rho||\sigma) \geq 0$, with

$S(\rho||\sigma) = 0$ iff $\rho = \sigma$. Eq. (15) can be shown by noting that ρ'_{AB} is the diagonal part of ρ_{AB} in the basis defined by the projective measurement (the minimization in (15) can in fact be extended to all ρ'_{AB} of the form (5) [15]). Nevertheless, differences with the quantum discord may arise in the minimizing measurement, as discussed in the next section. We also note that if the minimizing measurement of $D(A|B)$ is projective and in the basis of eigenstates of ρ_B, then $\rho'_B = \rho_B$ and Eqs. (10)–(13) lead to $D(A|B) = I(A|B)$. Otherwise $D(A|B) \leq I(A|B)$, since for projective measurements Eqs. (10)–(13) imply $D(A|B) \leq S(\rho'_{AB}) - S(\rho_{AB}) - [S(\rho'_B) - S(\rho_B)] \leq S(\rho'_{AB}) - S(\rho_{AB})$.

Eq. (14) admits a simple interpretation in terms of the entanglement generated between the system and a measuring apparatus M performing the complete local measurement [13]. The measurement on the local basis $\{|i_B\rangle\}$ can be represented through a unitary operator U_{BM} satisfying $U_{BM}|j_B 0_M\rangle = |j_B j_M\rangle$, where $|0_M\rangle$ is the initial state of the apparatus and $\{|j_M\rangle\}$ an orthogonal basis of M, such that

$$\rho'_{AB} = \mathrm{Tr}_M\, \rho'_{ABM}\,,$$
$$\rho'_{ABM} = (I_A \otimes U_{BM})(\rho_{AB} \otimes |0_M\rangle\langle 0_M|)(I_A \otimes U^\dagger_{BM})\quad(16)$$

Since $S(\rho_{AB}) = S(\rho_{AB} \otimes |0_M\rangle\langle 0_M|) = S(\rho'_{ABM})$, it is seen that Eq. (14) is the difference between the entropy of the subsystem AB and that of the total system ABM after the measurement, and" according to Eq. (7), such difference can be positive only if there is entanglement between AB and M. Thus, a positive $I(A|B)$ indicates that entanglement between AB and M is generated by *any* complete local measurement M_B. On the other hand, if $I(A|B) = 0$, then ρ_{AB} is of the form (5) and for a measurement in the basis $\{|j_B\rangle\}$, $\rho'_{ABM} = \sum_j p_j \rho_{A/j} \otimes |j_B j_M\rangle\langle j_B j_M|$ is clearly separable, so that no entanglement is generated by this measurement. It can be shown [13] that Eq. (14) coincides in fact with the minimum distillable entanglement between AB and M generated by the complete local measurement on B. A similar interpretation for the quantum discord in terms of the minimum partial distillable entanglement can also be obtained [13]. Other operational interpretations can be found in [21, 28, 30–33].

D. Generalized Information Deficit

It is possible in principle to extend Eq. (14) to more general entropic forms, since in contrast with the quantum discord (10), its positivity is not related to specific properties of the von Neumann entropy $S(\rho)$, as shown below. We consider here generalized entropies of the form [60]

$$S_f(\rho) = \mathrm{Tr}\, f(\rho)\,, \quad (17)$$

where $\mathrm{Tr}\, f(\rho) = \sum_i f(p_i)$, with p_i the eigenvalues of ρ and $f(p)$ a smooth strictly concave real function defined for $p \in [0, 1]$ and satisfying $f(0) = f(1) = 0$. These entropies fulfill the same basic properties as the von Neumann entropy, with the exception of additivity: We have $S_f(\rho) \geq 0$, with $S_f(\rho) = 0$ iff ρ is a pure state ($\rho^2 = \rho$), while all $S_f(\rho)$ are maximum for the maximally mixed state $\rho = I/d$, where $d = \mathrm{Tr}\, I$ is the Hilbert space dimension of the system. Moreover, they are strictly concave, i.e., $S_f(\sum_\alpha p_\alpha \rho_\alpha) \geq \sum_\alpha p_\alpha S_f(\rho_\alpha)$, for $p_\alpha > 0$, $\sum_\alpha p_\alpha = 1$, with equality iff all ρ_α are coincident. The von Neumann entropy is obviously recovered for $f(\rho) = -\rho \log \rho$.

Concavity of $S_f(\rho)$ implies the fundamental majorization property

$$\rho' \prec \rho \Rightarrow S_f(\rho') \geq S_f(\rho)\,, \quad (18)$$

where $\rho' \prec \rho$ indicates that ρ' is *majorized* by ρ [57, 61] (also denoted as ρ' *more mixed* than ρ):

$$\rho' \prec \rho \Leftrightarrow \sum_{j=1}^{i} p'_j \leq \sum_{j=1}^{i} p_j\,,\;\; i = 1, \ldots, d-1\,, \quad (19)$$

where p_j, p'_j denote the eigenvalues of ρ and ρ' sorted in *decreasing* order (equality in (19) obviously holds for $i = d$). If the dimensions of ρ and ρ' differ, Eq. (18) still holds (for $f(0) = 0$) after completing with zeros the smallest set of eigenvalues. Conversely, while the reverse of Eq. (18) does not necessarily hold, indicating that majorization provides a more strict concept of mixedness or disorder than that defined by a single choice of entropy, it does hold if $S_f(\rho') \geq S_f(\rho)\ \forall\ f$ of the previous form [56]:

$$S_f(\rho') \geq S_f(\rho)\ \forall\ S_f\ \Rightarrow \rho' \prec \rho\,. \quad (20)$$

Eq. (18) remains actually valid for more general entropic forms (like increasing functions $F(S_f)$ of S_f or in general, Schur concave functions [61]), but Eq. (20) indicates that the forms (17) are already sufficient to capture majorization. Among the various properties implied by majorization, we mention that for states with the same dimension, $\rho' \prec \rho$ iff ρ is a convex mixture of unitary transformations of ρ [57, 61], i.e., iff $\rho' = \sum_\alpha p_\alpha U_\alpha \rho U^\dagger_\alpha$, with U_α unitary and $p_\alpha \geq 0$.

Now, for any projective measurement (local or nonlocal) performed on the system $A + B$, it can be easily shown that $S_f(\rho'_{AB}) \geq S_f(\rho_{AB})\ \forall\ S_f$, i.e.,

$$\rho'_{AB} \prec \rho_{AB}\,. \quad (21)$$

The reason is that the post measurement state ρ'_{AB} conserves just the diagonal elements $p'_\nu = \langle \nu'|\rho_{AB}|\nu'\rangle$ of ρ_{AB} in a certain orthonormal basis $\{|\nu'\rangle\}$ determined by the projectors and hence, $S_f(\rho'_{AB}) = \sum_\nu f(p'_\nu) = \sum_\nu f(\sum_\mu |\langle\mu|\nu'\rangle|^2 p_\mu) \geq \sum_{\mu,\nu} |\langle\mu|\nu'\rangle|^2 f(p_\mu) = S_f(\rho_{AB})$, where p_μ and $|\mu\rangle$ denote here the eigenvalues and eigenvectors of ρ_{AB}. This relation is not restricted to rank one projectors (just choose an orthonormal basis $\{|\nu'\rangle\}$ where ρ'_{AB} is diagonal), so that it holds for local projective measurements. Eq. (21) remains actually valid for any measurement satisfying $\sum_j M_j M^\dagger_j = I_{AB}$, i.e., which leaves the maximally mixed state I_{AB}/d_{AB} unchanged [15].

Note also that strict concavity of S_f implies $S_f(\rho'_{AB}) = S_f(\rho_{AB})$ iff $\rho'_{AB} = \rho_{AB}$, as is apparent from the previous demonstration. In fact, if the off diagonal elements of ρ_{AB} in the measured basis are sufficiently small, a second order expansion of $S_f(\rho_{AB})$ leads to [15]

$$S_f(\rho'_{AB}) - S_f(\rho_{AB}) \approx \sum_{\mu<\nu} \frac{f'(p'_\mu) - f'(p'_\nu)}{p'_\nu - p'_\mu} |\langle\nu'|\rho_{AB}|\mu'\rangle|^2 \,, \tag{22}$$

where the fraction is always positive due to the strict concavity of f (and should be replaced by its limit $-f''(p'_\mu)$ if $p'_\nu \to p'_\mu$). Eq. (22) is essentially the square of a weighted norm of the off-diagonal elements of ρ_{AB} in the measured basis (i.e., of those lost in the measurement), and is therefore non-negative, vanishing (if $f''(p) < 0 \;\forall\; p \in (0,1)$) only if all off-diagonal elements are zero.

We may then define the quantity [15, 16]

$$I_f(A|B) = \operatorname*{Min}_{M_B} S_f(\rho'_{AB}) - S_f(\rho_{AB}) \,, \tag{23}$$

where the minimization is again over all complete local measurements on B. Eq. (23) is non-negative, due to Eq. (21), and vanishes iff $\rho'_{AB} = \rho_{AB}$, i.e., iff ρ_{AB} is already of the classically correlated form (4) or (5). It therefore vanishes only for the states with zero quantum discord. It obviously also remains invariant under local unitary operations.

In the case of pure states, it can be shown [15] that the minimum of Eq. (23) is always attained for a measurement in the basis $\{|k_B\rangle\}$ determined by the Schmidt decomposition (1), i.e., in the basis formed by the eigenstates of ρ_B, which leads to

$$I_f(A|B) = S_f(\rho_A) = S_f(\rho_B) = \sum_{k=1}^{n_s} f(p_k) \,, \quad (\rho_{AB} \text{ pure}) \,. \tag{24}$$

It therefore reduces to the *generalized entanglement entropy* $S_f(\rho_A) = S_f(\rho_B)$ of the pure state. The entanglement entropy can then be identified with the minimum information loss due to a local measurement [15]. It is apparent that for pure states, $I_f(A|B) = I_f(B|A)$, a property which does not hold in the general case.

In the case of the von Neumann entropy, $I_f(A|B)$ becomes the standard information deficit (14) and Eq. (24) implies that for pure states, it will coincide with the standard (von Neumann) entanglement entropy, like the quantum discord. Nevertheless, an important difference arises in the minimizing measurement, since that for the latter becomes undetermined in the case of pure states (it can be any measurement based on rank one projectors [58]), whereas all $I_f(A|B)$, including $I(A|B)$, require a measurement in the basis $\{|k_B\rangle\}$, which is fully undetermined only in the case of maximally mixed marginals.

Like the standard information deficit, $I_f(A|B)$ is also an indicator of the minimum entanglement between the system and the measurement apparatus M generated by a complete local measurement. The von Neumann entropic criterion for separability (7) can actually be extended to any S_f [56]:

$$\rho_{AB} \text{ separable} \;\Rightarrow\; S_f(\rho_A) \le S_f(\rho_{AB}) \,, \quad S_f(\rho_B) \le S_f(\rho_{AB}) \,. \tag{25}$$

The validity of Eq. (25) for all S_f is stronger than the von Neumann based criterion (23) [56], and equivalent to the disorder criterion of separability [55] (ρ_{AB} separable $\Rightarrow \rho_{AB} \prec \rho_{A(B)}$). By the same arguments given below Eq. (16), it follows that a positive $I_f(A|B)$, i.e., $S_f(\rho'_{AB}) > S_f(\rho_{AB}) = S_f(\rho'_{ABM})$, is indicating the existence of entanglement between AB and M after *any* complete local projective measurement on B.

E. Minimizing measurement

Eq. (24) reflects an universal property exhibited by the local measurement minimizing $I_f(A|B)$ for pure states: It is the same for all S_f. Such measurement, i.e., a measurement in the basis $\{|k_B\rangle\}$ determined by the Schmidt decomposition of the pure state, is also optimum, for *all* S_f, for the mixture of the pure state with the maximally mixed state [15],

$$\rho_{AB} = q|\Psi_{AB}\rangle\langle\Psi_{AB}| + (1-q)I_{AB}/d_{AB} \,, \quad q \in [0,1] \,. \tag{26}$$

These states exhibit then an unambiguous *least disturbing local measurement*, in the sense that it minimizes all $I_f(A|B)$ and leads to a "least mixed" post-measurement state

$$\rho'_{AB} = q \sum_{k=1}^{n_s} p_k |k_A\rangle\langle k_A| \otimes |k_B\rangle\langle k_B| + (1-q) I_{AB}/d_{AB} \,,$$

which *majorizes* any other post-measurement state emerging after a local measurement. This property does not hold for an arbitrary initial state ρ_{AB}.

In the general case, the projective measurement $M_B = \{|j_B\rangle\langle j_B|\}$ minimizing $I_f(A|B)$ may depend on the choice of entropy S_f. It can be shown that it must satisfy the necessary stationary condition [16]

$$\mathrm{Tr}_A[f'(\rho'_{AB}), \rho_{AB}] = 0 \,, \tag{27}$$

where f' denotes the derivative of f and ρ'_{AB} is the post-measurement state (9). Eq. (27) implies, explicitly, $\sum_i [f'(p'_{ij})\langle i_j j|\rho_{AB}|i_j k\rangle - f'(p'_{ik})\langle i_k j|\rho_{AB}|i_k k\rangle] = 0$, where $p'_{ij} = \langle i_j j|\rho_{AB}|i_j j\rangle$ and $|i_j j\rangle = |i_{A/j}\rangle|j_B\rangle$, with $|i_{j/A}\rangle$ the eigenstates of $\rho_{A/j}$. The minimizing measurement basis will not coincide in general with the eigenstates of ρ_B, even though this holds for certain states, like pure states and the mixtures (26). Eq. (27) shows that the eigenstates of ρ_B will be stationary for any state ρ_{AB} where the non-zero off-diagonal elements are of the form $\langle ij|\rho_{AB}|kl\rangle$ with $i \neq k$ *and* $j \neq l$, where $|ij\rangle \equiv |i_A\rangle|j_B\rangle$ and $|i_A\rangle$, $|j_B\rangle$ are the eigenstates of ρ_A and ρ_B respectively [16].

In the case of the quantum discord, and for M_B restricted to complete local projective measurements, Eq. (27) is to be replaced by (here $f'(\rho)=-\log\rho$) [16]

$$\mathrm{Tr}_A[f'(\rho'_{AB}),\rho_{AB}]-[f'(\rho'_{AB}),\rho_B]=0\,. \qquad (28)$$

More explicit expressions can be obtained for a two-qubit system, where we may write a general state as

$$\rho_{AB}=\tfrac{1}{4}(I_{AB}+\boldsymbol{r}_A\cdot\boldsymbol{\sigma}_A+\boldsymbol{r}_B\cdot\boldsymbol{\sigma}_B+\boldsymbol{\sigma}_A^tJ\boldsymbol{\sigma}_B)\,, \qquad (29)$$

where $\boldsymbol{\sigma}_A=\boldsymbol{\sigma}\otimes I$, $\boldsymbol{\sigma}_B=I\otimes\boldsymbol{\sigma}$, with $\boldsymbol{\sigma}^t=(\sigma_x,\sigma_y,\sigma_z)$ the Pauli operators, and $I_{AB}=I\otimes I$ the identity. Since $\mathrm{Tr}\,\sigma_\mu=0$ and $\mathrm{Tr}\,\sigma_\mu\sigma_\nu=2\delta_{\mu\nu}$ for $\mu,\nu=x,y,z$, we have ($\langle O\rangle\equiv\mathrm{Tr}\,\rho_{AB}\,O$)

$$\boldsymbol{r}_{A(B)}=\langle\boldsymbol{\sigma}_{A(B)}\rangle,\;\; J=\langle\boldsymbol{\sigma}_A\boldsymbol{\sigma}_B^t\rangle\,. \qquad (30)$$

A complete projective measurement on B corresponds to a spin measurement along the direction of a unit vector $\boldsymbol{k}$, represented by projectors $P_{\pm\boldsymbol{k}}=\frac{1}{2}(I\pm\boldsymbol{k}\cdot\boldsymbol{\sigma})$. After this measurement, Eq. (29) becomes

$$\rho'_{AB}=\tfrac{1}{4}[I+\boldsymbol{r}_A\cdot\boldsymbol{\sigma}_A+(\boldsymbol{r}_B\cdot\boldsymbol{k})\boldsymbol{k}\cdot\boldsymbol{\sigma}_B+(\boldsymbol{\sigma}_A^tJ\boldsymbol{k})\boldsymbol{k}\cdot\boldsymbol{\sigma}_B]\,. \qquad (31)$$

Eq. (27) leads then to the explicit equation [16]

$$\alpha_1\boldsymbol{r}_B+\alpha_2J^t\boldsymbol{r}_A+\alpha_3J^tJ\boldsymbol{k}=\lambda\boldsymbol{k}\,, \qquad (32)$$

where $(\alpha_1,\alpha_2,\alpha_3)=\frac{1}{4}\sum_{\mu,\nu=\pm1}f'(p'_{\mu\nu})(\nu,\frac{\mu\nu}{|\boldsymbol{r}_A+J\boldsymbol{k}|},\frac{\mu}{|\boldsymbol{r}_A+J\boldsymbol{k}|})$, $p'_{\mu\nu}=\frac{1}{4}(1+\nu\boldsymbol{r}_B\cdot\boldsymbol{k}+\mu|\boldsymbol{r}_A+\nu J\boldsymbol{k}|)$ are the eigenvalues of ρ'_{AB}, with $\mu,\nu=\pm1$, and λ is a proportionality factor. In the case of the quantum discord, Eq. (28) leads to a similar equation, with $f(p)\to-p\log p$ and $\alpha_1\to\alpha_1-\frac{1}{2}\log p'_-/p'_+$, where $p'_\pm=\frac{1}{2}(1+\boldsymbol{r}_B\cdot\boldsymbol{k})$ are the eigenvalues of ρ'_B [16].

F. Particular cases

One of the advantages of the generalized information deficit (23) is the possibility of using simple entropic forms which can be more easily evaluated (and measured) than the von Neumann entropy. For instance, if $f(\rho)=2(\rho-\rho^2)$, Eq. (17) becomes the so called linear entropy

$$S_2(\rho)=2(1-\mathrm{Tr}\,\rho^2)\,, \qquad (33)$$

which follows from the linear approximation $\ln\rho\approx\rho-I$ in the von Neumann entropy, but is actually a quadratic function of ρ, i.e., a linear function of the purity $P(\rho)=\mathrm{Tr}\,\rho^2$. It is the simplest entropic form and its evaluation does not require the knowledge of the eigenvalues of ρ (see Eq. (39) below). Moreover, purity, and hence $S_2(\rho)$, can be experimentally determined without a full state tomography [62]. Eq. (33) is actually the $q=2$ case of the Tsallis entropies [63], obtained for $f(\rho)=\frac{\rho-\rho^q}{1-2^{1-q}}$:

$$S_q(\rho)=\frac{1-\mathrm{Tr}\,\rho^q}{1-2^{1-q}}\,,\quad q>0\,. \qquad (34)$$

Eq. (34) approaches the von Neumann entropy $S(\rho)$ for $q\to1$, being strictly concave for $q>0$. We have normalized (33) and (34) such that $S_q(\rho)=1$ for a maximally mixed two-qubit state.

In the case (33), it is first seen that for post-measurements states ρ'_{AB},

$$S_2(\rho'_{AB})-S_2(\rho_{AB})=2\,\mathrm{Tr}\,(\rho_{AB}^2-\rho'^2_{AB})=2||\rho'_{AB}-\rho_{AB}||^2\,, \qquad (35)$$

where $||O||^2=\mathrm{Tr}\,O^\dagger O$. Hence, the local projective measurement minimizing $S_2(A|B)$, which is that maximizing the post-measurement purity $P(\rho'_{AB})$, leads to the post-measurement state with the minimum Hilbert-Schmidt distance to the original state. The associated deficit

$$I_2(A|B)=\underset{M_B}{\mathrm{Min}}\,S_2(\rho'_{AB})-S_2(\rho_{AB})\,, \qquad (36)$$

coincides, apart from a constant factor, with the geometric discord [11, 14, 15]. For pure states, $I_2(A|B)$ will then coincide with the linear marginal entropies:

$$I_2(A|B)=S_2(\rho_A)=S_2(\rho_B)=2(1-\sum_{k=1}^{n_s}p_k^2)\,. \qquad (37)$$

In two qubit systems, Eq. (37) is just the squared *concurrence* [53] of the pure state ρ_{AB}.

While as a measure the geometric discord fails to satisfy some additional properties fulfilled by the quantum discord or the information deficit [64], it offers the enormous advantage of a simple analytic evaluation in qudit-qubit systems [14, 16, 65], as discussed below, also admitting through the purity a more direct experimental access. Moreover, Eq. (22) shows that if ρ_{AB} is close to the maximally mixed state I_{AB}/d_{AB}, all $I_f(A|B)$ will become proportional to $I_2(A|B)$ [15], as in this case $\frac{f'(p'_\mu)-f'(p'_\nu)}{p'_\nu-p'_\mu}\approx-f''(\frac{1}{d_{AB}})$ is nearly constant. In fact, all $S_f(\rho)$ are linearly related to $S_2(\rho)$ in this limit [58].

Any state of a general system $A+B$ can be written in the form (29), replacing the Pauli operators by a complete set of orthogonal operators $\boldsymbol{\sigma}$ in A and B satisfying $\mathrm{Tr}\,\sigma_\mu=0$, $\mathrm{Tr}\,\sigma_\mu\sigma_\nu=d_{A(B)}\delta_{\mu\nu}$:

$$\rho_{AB}=\tfrac{1}{d_Ad_B}(I_{AB}+\boldsymbol{r}_A\cdot\boldsymbol{\sigma}_A+\boldsymbol{r}_B\cdot\boldsymbol{\sigma}_B+\boldsymbol{\sigma}_A^tJ\boldsymbol{\sigma}_B)\,, \qquad (38)$$

where $\boldsymbol{r}_{A(B)}$ and J (now a $d_A\times d_B$ matrix) are again given by Eq. (30). The S_2 entropy can then be readily evaluated as

$$S_2(\rho_{AB})=2[1-\tfrac{1}{d_Ad_B}(1+|\boldsymbol{r}_A|^2+|\boldsymbol{r}_B|^2+||J||^2)]\,, \qquad (39)$$

where $||J||^2=\mathrm{Tr}J^tJ$. If B is now a qubit, the state after a spin measurement along direction $\boldsymbol{k}$ on B, will have the form (31) with $\frac{1}{4}\to\frac{1}{2d_A}$. We then obtain, using Eq. (39),

$$S_2(\rho'_{AB})=2-\frac{1}{d_A}(|\boldsymbol{r}_A|^2+\boldsymbol{k}^tM_2\boldsymbol{k})\,, \qquad (40)$$

where $M_2=\boldsymbol{r}_B\boldsymbol{r}_B^t+J^tJ$ is a 3×3 positive semidefinite symmetric matrix. Hence, $I_2(\boldsymbol{k})=S_2(\rho'_{AB})-S_2(\rho_{AB})=$

$\frac{1}{d_A}(\mathrm{Tr}\, M_2 - \boldsymbol{k}^t M_2 \boldsymbol{k})$. Its minimum $I_2(A|B)$ can then be evaluated analytically as [14, 16]

$$I_2(A|B) = \underset{\boldsymbol{k}}{\mathrm{Min}}\, I_2(\boldsymbol{k}) = \tfrac{1}{d_A}(\mathrm{Tr} M_2 - \lambda_1)\,, \tag{41}$$

where λ_1 is the largest eigenvalue of M_2, the minimizing spin measurement being along the direction of the corresponding eigenvector. Eq. (41) is valid for an arbitrary qudit-qubit state ρ_{AB}. Let us notice that the stationary condition (27) or (32) reduces, for the linear entropy, precisely to the eigenvalue equation $M_2\boldsymbol{k} = \lambda\boldsymbol{k}$, as in this case $f'(\rho'_{AB}) \propto \rho'_{AB}$ and hence, $\alpha_1 = \boldsymbol{r}_B \cdot \boldsymbol{k}$, $\alpha_2 = 0$ and $\alpha_3 = 1$ [16]. This indicates that the stationary measurements are those along the direction of the eigenvectors of M_2.

For arbitrary $q > 0$, we may similarly define the quantities (in what follows $c_q = 1 - 2^{1-q}$)

$$\begin{aligned} I_q(A|B) &= \underset{M_B}{\mathrm{Min}}\, S_q(\rho'_{AB}) - S_q(\rho_{AB}) \\ &= \underset{M_B}{\mathrm{Min}}\, c_q^{-1}\mathrm{Tr}\,(\rho^q_{AB} - \rho'^q_{AB})\,, \end{aligned} \tag{42}$$

$$\begin{aligned} I^R_q(A|B) &= \underset{M_B}{\mathrm{Min}}\, S^R_q(\rho'_{AB}) - S^R_q(\rho_{AB}) \\ &= \underset{M_B}{\mathrm{Min}}\, \frac{1}{1-q}\log\frac{\mathrm{Tr}\,\rho'^q_{AB}}{\mathrm{Tr}\,\rho^q_{AB}} \qquad (43) \\ &= \frac{1}{1-q}\log\left[1 - \frac{c_q I_q(A|B)}{1 - c_q S_q(\rho_{AB})}\right]\,, \qquad (44) \end{aligned}$$

where

$$S^R_q(\rho) = \frac{1}{1-q}\log\,\mathrm{Tr}\,\rho^q = \frac{1}{1-q}\log[1 - c_q S_q(\rho)]\,,\;\; q > 0\,, \tag{45}$$

are the *Renyi* entropies [57], which are just increasing functions of the Tsallis entropies (34) (and also approach the von Neumann entropy for $q \to 1$). Eqs. (42)–(43) are again non-negative, vanishing iff ρ_{AB} is of the form (4) or (5), and approach the von Neumann information deficit (14) for $q \to 1$. Eq. (44) is again just an increasing function of $I_q(A|B)$ (for fixed ρ_{AB}) and does not depend on the addition of an uncorrelated ancilla C to A ($\rho_{AB} \to \rho_C \otimes \rho_{AB}$), as $\mathrm{Tr}\rho^q_C$ cancels out. An analytic expression for $I_3(A|B)$ valid for any two-qubit state can also be obtained [16].

III. APPLICATION: QUANTUM CORRELATIONS OF SPIN PAIRS IN XY CHAINS

A. Model and general expressions

We consider a spin 1/2 system with XYZ couplings of arbitrary range, immersed in a transverse magnetic field B along the z axis. The Hamiltonian reads

$$H = B\sum_i s_{iz} - \tfrac{1}{2}\sum_{\mu=x,y,z}\sum_{i\neq j} J^{ij}_\mu s_{i\mu}s_{j\mu}\,, \tag{46}$$

where $s_{i\mu}$ are the (dimensionless) components of the local spin at site i, and J^{ij}_μ the coupling strengths.

The Hamiltonian (46) commutes with the S_z spin parity operator P_z, irrespective of the coupling range, anisotropy, dimension, or geometry of the system [46, 47],

$$[H, P_z] = 0,\;\; P_z = \exp[i\pi\sum_i(s_{iz} + 1/2)] = \prod_i(-\sigma_{iz})\,, \tag{47}$$

where $\sigma_{iz} = 2s_{iz}$. The non-degenerate eigenstates of H will then have a definite S_z parity $P_z = \pm 1$.

Consequently, the reduced density matrix of an arbitrary spin pair i, j in any non-degenerate eigenstate $|\Psi_\nu\rangle$, $\rho_{ij} = \mathrm{Tr}_{\overline{(i,j)}}\,|\Psi_\nu\rangle\langle\Psi_\nu|$, will then commute with the S_z parity operator of the pair $P^{ij}_z = \sigma_{iz}\sigma_{jz}$: $[\rho_{ij}, P^{ij}_z] = 0$. In the standard basis $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$, ρ_{ij} will therefore be an X-type state of form

$$\rho_{ij} = \begin{pmatrix} a_+ & 0 & 0 & \beta \\ 0 & c_+ & \alpha & 0 \\ 0 & \bar{\alpha} & c_- & 0 \\ \bar{\beta} & 0 & 0 & a_- \end{pmatrix}\,, \tag{48}$$

where the coefficients are all real (since H is real in the full standard basis) and given by ($s_{i\pm} = s_{ix} \pm i s_{iy}$)

$$a_\pm = \tfrac{1}{4} \pm \tfrac{1}{2}\langle s_{iz} + s_{jz}\rangle + \langle s_{iz}s_{jz}\rangle\,, \tag{49}$$

$$c_\pm = \tfrac{1}{4} \pm \tfrac{1}{2}\langle s_{iz} - s_{jz}\rangle - \langle s_{iz}s_{jz}\rangle\,,\;\; \left({\beta \atop \alpha}\right) = \langle s_{i-}s_{j\mp}\rangle \tag{50}$$

with $a_+ + c_+ + c_- + a_- = 1$. It corresponds to $\boldsymbol{r}_A$ and $\boldsymbol{r}_B$ along z in (29) ($r_{A(B)} = a_+ + c_{+(-)} - c_{-(+)} - a_-$), with J *diagonal*, i.e., $J_{\mu\nu} = 4\langle s_{i\mu}s_{j\nu}\rangle = \delta_{\mu\nu} j_\mu$, with $j_{x \atop y} = 2(\alpha \pm \beta)$, $j_z = a_+ + a_- - c_+ - c_-$. Positivity of ρ_{ij} implies $|\alpha| \le \sqrt{c_+c_-}$, $|\beta| \le \sqrt{a_+a_-}$, with $a_\pm$, $c_\pm$ non-negative. The single spin density matrix is

$$\rho_i = \mathrm{Tr}_j\,\rho_{ij} = \begin{pmatrix} a_+ + c_+ & 0 \\ 0 & a_- + c_- \end{pmatrix}\,. \tag{51}$$

Both ρ_{ij} and ρ_i will obviously be typically mixed due to the entanglement with the rest of the chain.

In what follows we will consider translational invariant systems such that $\langle s_{iz}\rangle$ is site independent, i.e., $\langle s_{iz}\rangle = \langle s_{jz}\rangle\ \forall\ i, j$, implying $c_\pm = c = \frac{1 - a_+ - a_-}{2}$. In this situation, $\rho_{ij} = \rho_{ji}$ and $D(A|B) = D(B|A) = D$, $I_f(A|B) = I_f(B|A) = I_f\ \forall\ S_f$.

The entanglement of the pair can be measured by the entanglement of formation (6), which for two qubit states can be evaluated as [53]

$$E = -\sum_{\nu=\pm} q_\nu \log q_\nu\,,\; q_\pm = \tfrac{1}{2}(1 \pm \sqrt{1 - C^2})\,, \tag{52}$$

where C is the concurrence [53]. For the states (48) with $c_\pm = c$, the concurrence of the pair is given by

$$C_{ij} = 2\,\mathrm{Max}[|\beta| - c, |\alpha| - \sqrt{a_+a_-}, 0]\,. \tag{53}$$

The pair entanglement is of parallel type (as in the Bell states $\frac{|00\rangle \pm |11\rangle}{\sqrt{2}}$) if the first entry in (53) is positive and antiparallel (as in $\frac{|01\rangle\pm|10\rangle}{\sqrt{2}}$) if the second entry is positive [45] (just one of them can be positive).

On the other hand, the quantum discord of the pair can be readily evaluated with the expressions (48) and (31) (see [37] for details). The ensuing minimization over the spin measurement direction $\boldsymbol{k}$ (we will consider here just projective measurements) will normally lead to the direction corresponding to maximum correlation, according to general arguments of [58]. In the XY chains which will be considered, i.e., $J_z^{ij}=0$, with $|J_y^{ij}|<J_x^{ij}$ and $J_x^{ij}>0$, the quantum discord for the states (48) will always prefer a measurement along the x axis, irrespective of the field intensity [37].

The information deficit (14) can be evaluated in a similar way. In contrast with the quantum discord, the optimizing measurement direction will be affected by the field intensity, exhibiting a smooth transition from the x to the z direction as the field increases for the systems considered, as discussed below. The angle γ between $\boldsymbol{k}$ and the z axis can be determined from Eq. (32), which leads explicitly to

$$\cos\gamma=\frac{\alpha_1 r_B+\alpha_2 j_z r_A}{\alpha_3(j_x^2-j_z^2)}\,, \tag{54}$$

when $\gamma\neq 0$ [16], which is a transcendental equation (as the α_i depend on γ).

The quadratic information deficit (36) can, however, be analytically evaluated with Eq. (41). Here M_2 is already diagonal, $M_{2\mu\nu}=\delta_{\mu\nu}(\delta_{\mu z}r_B^2+j_\mu)$. Assuming $|j_x|\geq|j_y|$, as will occur in the cases considered, we obtain

$$\begin{aligned}I_2&=\tfrac{1}{2}\mathrm{Min}[j_y^2+j_x^2, j_y^2+r_B^2+j_z^2]\\&=4\mathrm{Min}[\alpha^2+\beta^2, \tfrac{a_+^2+a_-^2}{4}+\tfrac{c^2-(a_+-a_-)c+(\alpha-\beta)^2}{2}]\,,\end{aligned} \tag{55}$$

with the minimizing measurement direction $\boldsymbol{k}$ along the z (x) axis if the first (second) entry is minimum:

$$\boldsymbol{k}=\begin{cases}\boldsymbol{e}_z\,, & j_x^2<r_B^2+j_z^2\\ \boldsymbol{e}_x\,, & j_x^2>r_B^2+j_z^2\end{cases}\,. \tag{56}$$

This entails that as the field B increases from 0, a sharp $x\to z$ transition in the minimizing measurement direction will take place for I_2, reflecting the change in the largest eigenvalue of the matrix M_2. This transition becomes softened in the von Neumann information deficit (14), where $\boldsymbol{k}$ will evolve smoothly from the x to the z axis within a narrow field interval located in the vicinity of the I_2 transition. A measurement transition also occurs for other values of q in the quantities (42)–(43) (see [16] for an example).

B. Results

In Figs. 1–2 we show results for the exact ground state of a finite chain with n spins coupled through cyclic ($n+1\equiv 1$) first neighbor anisotropic XY couplings ($J_z^{ij}=0$, $J_\mu^{ij}=\delta_{j,i\pm1}J_\mu$ for $\mu=x,y$), for which the reduced pair states (48) will depend just on the separation $L=|i-j|$ between the spins of the pair. The exact values of the elements of the density matrix (48) can be obtained, for any size n or separation L, through the Jordan-Wigner fermionization of the model [66] and its analytic parity dependent diagonalization [46, 67, 68] (see Appendix).

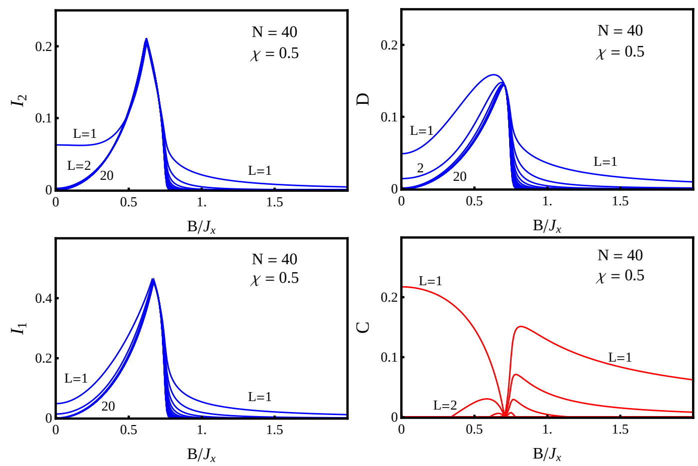

FIG. 1. Left: The one-way information deficits I_2 (Eq. (36), top) and I_1 (Eq. (14), bottom), as a function of the scaled magnetic field B/J_x, for spin pairs with separation $L=1,2,\ldots,n/2$ in the exact ground state of a cyclic chain of $n=40$ spins with first neighbor anisotropic XY couplings ($\chi=J_y/J_x=1/2$). Right: The quantum discord D (Eq. (10), top) and the concurrence C (Eq. (53), bottom) for the same pairs. The results for different separations coincide exactly at the factorization field $B_s=\sqrt{J_yJ_x}\approx 0.71J_x$.

We will set $J_x>0$, with $|J_y|\leq J_x$. This involves no loss of generality as the sign of J_x can be changed by a local rotation of angle π around the z axis at even sites (assuming n even in cyclic chains), which will not affect the value of the correlation measures, and the x axis can be chosen along the direction of maximum coupling.

Fig. 1 depicts the behavior with increasing field B of the one way information deficits $I_1\equiv I$ (Eq. (14)) and I_2 (Eqs. (36)-(55)) of spin pairs in the exact definite parity ground state for the anisotropic case $J_y=J_x/2$, together with that of the quantum discord (14) and the concurrence (53). It is first seen that I_1, I_2 and D exhibit a similar qualitative behavior, acquiring appreciable finite values for *any* separation L in the interval $|B|<B_c=(J_x+J_y)/2$, in marked contrast with the concurrence, which is appreciable just for first and second neighbors (except for the immediate vicinity of the factorizing field, see below). The S_z parity symmetry is essential for this result. In fact, all measures converge to a *finite common value*, independent of the separation L, at the factorizing field [41, 44, 46–48]

$$B_s=\sqrt{J_yJ_x}\,, \tag{57}$$

existing for $0<J_y<J_x$, where the system possesses a pair of degenerate completely separable exact ground

states [41, 46, 47] given by $|\Theta\rangle = |\theta, \ldots, \theta\rangle$ and $|-\Theta\rangle = P_z|\Theta\rangle = |-\theta, \ldots, -\theta\rangle$, where $|\theta\rangle = e^{-i\theta s_y}|\downarrow\rangle$ is the single spin state forming an angle θ with the $-z$ direction and $\cos\theta = B_s/J_x = \sqrt{J_y/J_x}$. Actually, in the finite case this field coincides with *the last parity transition* of the exact (and hence of definite parity) ground state [46], such that the latter approaches, as side limits at $B = B_s$, the definite parity combinations [46, 47]

$$|\Theta_\pm\rangle = \frac{|\Theta\rangle \pm |-\Theta\rangle}{\sqrt{2(1 \pm \langle -\Theta|\Theta\rangle)}}\,. \tag{58}$$

Here $|\Theta_+\rangle$ ($|\Theta_-\rangle$) is the ground state limit for $B \to B_s^+$ ($B \to B_s^-$). Discarding the overlap $\langle -\Theta|\Theta\rangle = \cos^n\theta$, which is negligible if n and θ are not too small ($\cos^n\theta \approx e^{-n\theta^2/2}$ for small θ), Eq. (58) leads to a *common* reduced state for *any* pair i, j, given by [37, 46]

$$\rho_\theta = \tfrac{1}{2}(|\theta\rangle\langle\theta| \otimes |\theta\rangle\langle\theta| + |-\theta\rangle\langle-\theta| \otimes |-\theta\rangle\langle-\theta|)\,. \tag{59}$$

This is a separable mixed state and therefore, it leads to a zero concurrence for any pair, as seen in Fig. 1 (where results at B_s correspond to the side limits (58)). However, it is not of the classically correlated form (4) or (5) if $\langle-\theta|\theta\rangle = \cos\theta \neq 0$ or 1, i.e. if $|\pm\theta\rangle$ are non-orthogonal and distinct, leading then to a common appreciable value of D, I_1, I_2 and in fact all I_f. We also notice that the same reduced state (59) is obtained from the mixture $\frac{1}{2}(|\Theta\rangle\langle\Theta| + |-\Theta\rangle\langle-\Theta|)$, which represents the low temperature limit of the thermal state $\rho \propto \exp[-H/kT]$ at $B = B_s$.

It is then possible to obtain straightforward analytic expressions for the side limits of D [37], I_2 and I_1 at the factorizing field through the state (59), which leads to $a_\pm = \frac{1}{4}(1 \pm \cos\theta)^2$ and $\alpha = \beta = c = \frac{1}{4}\sin^2\theta$ in (48), with $\cos^2\theta = J_y/J_x$. That for I_2 is particularly clean and given by

$$I_2(B_s) = \begin{cases} \frac{(1-\chi)^2}{2}, & \chi \geq 1/3 \\ \frac{\chi(1+\chi)}{2}, & \chi \leq 1/3 \end{cases}, \quad \chi = J_y/J_x\,, \tag{60}$$

with the minimizing measurement at B_s being along z if $\chi > 1/3$ and along x if $\chi < 1/3$. Eq. (60) applies for all separations L.

For small chains, the results are similar but the effects of the parity transitions of the ground state (it undergoes $n/2$ parity transitions as the field increases from 0, the last one at $B = B_s$ [46]) are now appreciable trough the finite discontinuities exhibited by I_2, I_1 and D, as seen in Fig. 2. At the factorizing field, these discontinuities arise from the overlap $\langle-\Theta|\Theta\rangle$, which now cannot be strictly neglected. It leads to an additional term $\propto \pm\cos^{n-2}\theta(|\theta\rangle\langle-\theta| \otimes |\theta\rangle\langle-\theta| + h.c.)$ in Eq. (59), which originates slightly distinct side limits of D [37] and also I_2 and I_1 at B_s. Moreover, it also leads to small but finite and distinct common side limits of the concurrence at $B = B_s$ [46, 47], which was known to reach full range in its vicinity [45]. All these side limits are, nevertheless, still independent of the pair separation L. In the case of I_2, they are given, for $\chi \gtrsim 1/3$, by

$$I_2(B_s^\pm) = \frac{(1-\chi)^2}{2}\frac{1+\chi^{n-2}}{(1 \pm \chi^{n/2})^2}\,, \tag{61}$$

which corrects the upper line in Eq. (60) for finite n (or $\chi \to 1$) and + (−) corresponds to the right (left) side limit. The side limits of the concurrence are $C(B_s^\pm) = \frac{\chi^{n/2-1}(1-\chi)}{1\pm\chi^{n/2}}$, as obtained from (53) [46, 47].

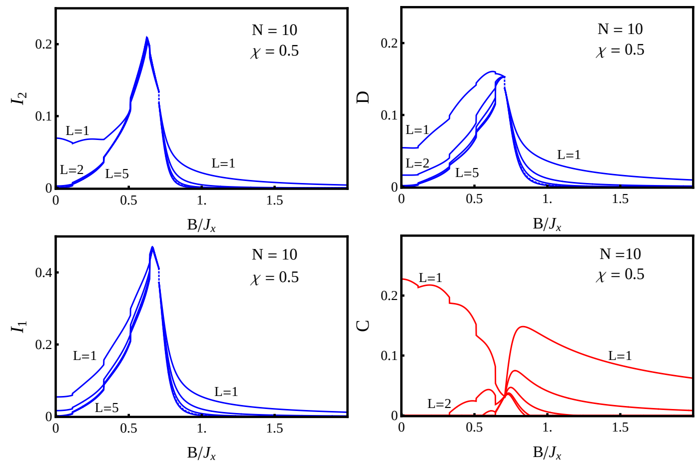

FIG. 2. The same quantities of Fig. 1 for $n = 10$ spins. In this case the parity transitions of the ground state lead to small but appreciable discontinuities in all quantities, with the last transition (indicated by the vertical dotted line) taking place at the factorizing field B_s. For this size the concurrence also presents small but finite side limits at B_s.

The behavior of the quantum discord for longer range ferromagnetic-type couplings is qualitatively similar [37]. Moreover, a factorizing field still exists for longer range couplings with a constant anisotropy $\chi = J_y^{ij}/J_x^{ij}$ [47], in which case the reduced pair state at B_s is again given by Eq. (59) with $\cos\theta = \sqrt{\chi}$, and Eqs. (60)–(61) remain then valid.

In Fig. 3 we compare the behavior of I_2, I_1 and D for first neighbors in the chains of Figs. 1 and 2, with that of the associated entanglement monotone, i.e., the squared concurrence C^2 for I_2 and the entanglement of formation E for I_1 and D, such that both quantities coincide for pure states. It is seen that for strong fields, differences are very small, in agreement with the weak entanglement of the pair with the rest of the chain in this regime ($\rho_{i,i+1}$ is almost pure). The strong differences arise for $B < B_c$, and especially in the vicinity of the factorizing field, due to the arguments exposed above. For $|B| < B_c$ the reduced pair state becomes appreciably mixed in the definite parity ground states, including the states (58) at the factorizing field, due to the entanglement with the rest of the chain. Significant differences between I_f (and D) with the corresponding entanglement monotone become then feasible.

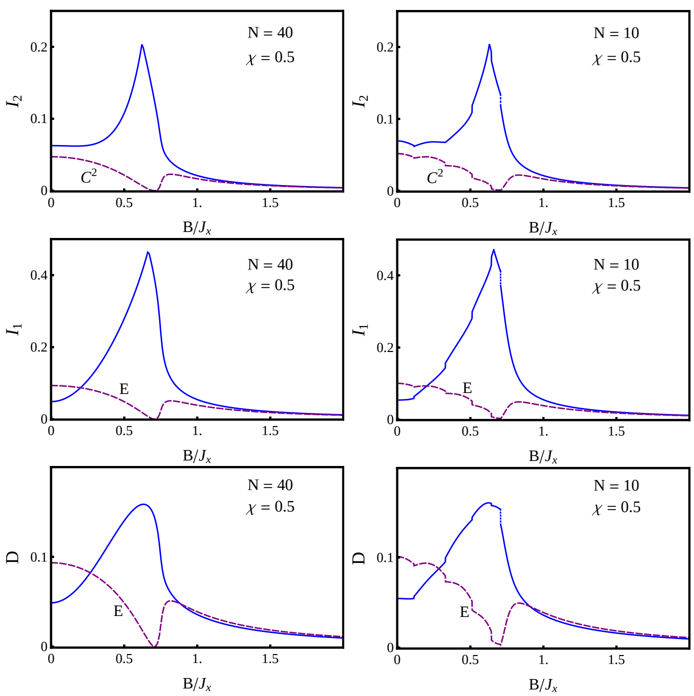

FIG. 3. Plot of I_2 (top), I_1 (center), and D (bottom) together with the associated entanglement monotones for a first neighbor pair ($L = 1$) in the ground state of the chains of Figs. 1 and 2.

It is also seen that I_2 is in this case an upper bound of C^2 for all fields, whereas I_1 is not a upper bound of E for low fields while D is not a upper bound even for strong fields, indicating the lack of an order relationship between D and E even in this regime. In the case of I_2, it is easy to show from Eqs. (53) and (55) that for X states, it is always an upper bound of C^2 when the minimizing measurement is along z [16]. In, fact, for strong fields $|B| \gg J_x$, a perturbative expansion [15] for the present chain leads to $C \approx 2(\eta - \eta^2)$, $I_2 \approx 4\eta^2$, $I_1 \approx \eta^2(\log e - \log \eta^2)$ and $D \approx \eta^2(\log e - \log \eta^2 - 2)$, where

$$\eta = \frac{J_x - J_y}{8B}\,.$$

Hence, in this limit $I_2 - C^2 = O(\eta^3)$ and $I_1 - E = O(-\eta^3 \log \eta^2)$, both positive, whereas $D - E \approx O(-\eta^2)$ becomes negative.

C. Minimizing measurement

Although I_1, I_2 and D show a similar qualitative behavior, both measures I_1, and I_2 exhibit a more pronounced maximum, in comparison to that of the quantum discord, as appreciated in Figs. 1-3. This reflects the transition in the orientation of their local minimizing spin measurements as the field increases, which, as mentioned above, is not present in the quantum discord. The latter prefers in the present system a measurement along the x axis, even for large fields and for any separation between the spins, following the strongest correlation [58]. As seen in Fig. 4 and as previously stated, I_2 exhibits instead a sharp transition from a direction *parallel to the x axis* ($\gamma = \pi/2$) to a direction *parallel to the z axis* ($\gamma = 0$) i.e., parallel to the field. This transition takes place, in the case shown in Fig. 1, for all separations L at $B \approx 0.65 J_x$. In the case of the Information Deficit I_1, the transition becomes smooth, as the angle γ takes all the intermediate values between 0 and $\pi/2$ (as determined by Eq. (54)) for all separations in a narrow field interval centered at the I_2 critical field, as also seen in Fig. 4.

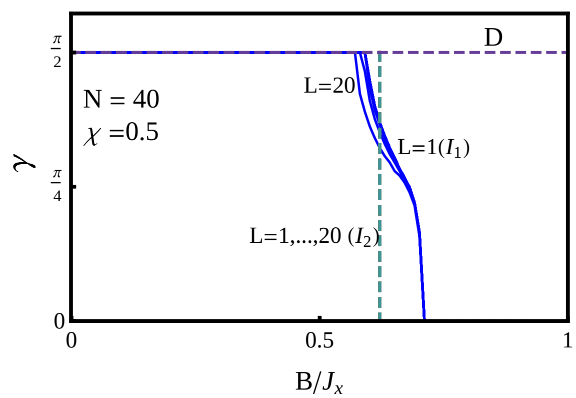

FIG. 4. The angle γ determining the direction of the minimizing local spin measurement for D, I_1 and I_2, as a function of the scaled transverse magnetic field, for a chain of $n = 40$ spins with $J_y = J_x/2$. Results for all separations L of the pair are shown.

The value of the field where the transition in the optimizing local measurement for I_2 occurs, depends on the anisotropy but only slightly on the separation L, except in the XX limit ($J_y \to J_x$), as can be seen in the top panel of Fig. 5. The same holds for the field interval where the "transition" (actually the evolution from $\pi/2$ to 0 of the measurement angle γ) in I_1 takes place (bottom panel of Fig. 5). In the case of I_2, if $\chi = 1/3$ the measurement transition for *all* separations L occurs *exactly* at the factorizing field $B_s = \sqrt{\chi} J_x$, as follows from Eq. (60).

The measurement transition reflects essentially the qualitative change experienced by the reduced state of the pair for increasing fields. Away from the XX limit, the dominant eigenstate of ρ_{ij} (that with the largest eigenvalue) for not too low fields is the entangled state $|\Psi_+\rangle = u|\downarrow\downarrow\rangle + v|\uparrow\uparrow\rangle$ with $v/u = \frac{\beta}{\varepsilon + \sqrt{\varepsilon^2 + \beta^2}}$ and $\varepsilon = \frac{a_- - a_+}{2}$. Above the measurement transition field (i.e., when the optimum measurement is parallel to the field), v/u becomes small ($\lesssim 0.25$), indicating that the pair is approximately aligned with the field. Instead, below the transition field v/u increases, approaching 1 for $B \to 0$ (where $|\Psi_+\rangle$ becomes a parallel Bell state) and the least disturbing measurement is along x. For very low fields

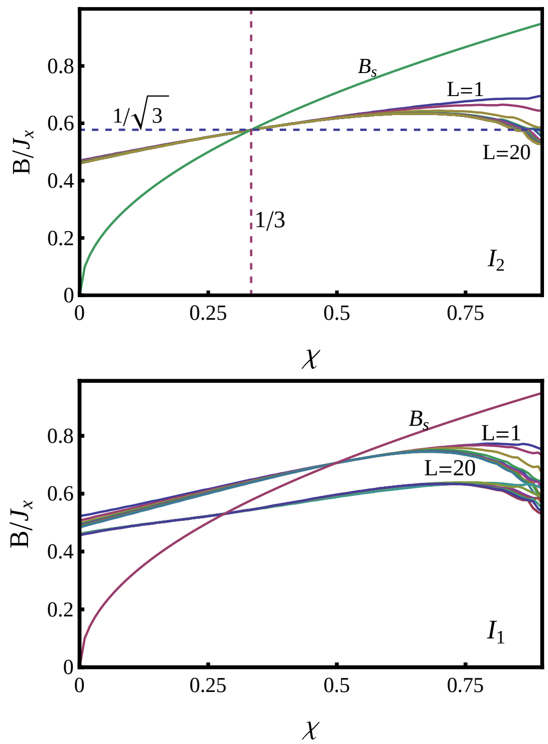

FIG. 5. Top: The field where the transition in the minimizing measurement of I_2 takes place, as a function of the anisotropy $\chi = J_y/J_x$. A direction along the x (z) axis is preferred below (above) the transition field. The factorizing field B_s is also shown. All transition fields coincide with the factorizing field if $\chi = 1/3$ (Eq. (60)). Bottom: The fields delimiting the interval where the smoothed transition in the minimizing measurement of the von Neumann information deficit I_1 takes place.

the dominant eigenstate may shift to the antiparallel Bell state $|\Psi_-\rangle = \frac{|\uparrow\downarrow\rangle+|\downarrow\uparrow\rangle}{\sqrt{2}}$ arising from the central block of (48), and in this case the measurement along x is still preferred. On the other hand, in the XX limit, $\beta = 0$ in (48) and the dominant eigenstate is either $|\Psi_-\rangle$ at low fields, or $|\Psi_+\rangle = |\downarrow\downarrow\rangle$ for strong fields, and the measurement transition of I_2 indicates essentially the field where the sharp transition in the dominant eigenstate (from maximally entangled to separable) takes place [42]. Such measurement transition for increasing fields persists even at finite temperatures [42].

IV. CONCLUSIONS

We have examined the behavior of the quantum discord and the standard and quadratic one-way information deficit of spin pairs in the exact definite parity ground state of a finite anisotropic cyclic XY spin 1/2 chain in a transverse field. We have first provided a brief overview of the quantum discord, the standard von Neumann based one-way information deficit and the generalized information deficit, which contains the standard as well the quadratic deficit as particular cases, and which can be interpreted as a measure of the minimum entanglement generated between the system and the measurement apparatus after a complete local projective measurement. The first important result is that the behavior of all these measures is quite distinct from that of the pair entanglement for fields below the critical field, acquiring finite appreciable values for *all separations* of the spins of the pair. Moreover, they reach (as side limits) a common (independent of the separation) finite value at the factorizing field, which in a finite chain is the field where the last ground state parity transition takes place. These finite limits can be evaluated analytically. The entanglement of pairs also reaches full range in its vicinity, although its value is much smaller and vanishes at this field except for very small samples. Parity effects are of crucial importance for the proper description of these measures in finite systems below the critical field.

The second important result is that the behavior of the optimizing local spin measurement of both the standard and generalized information deficit is quite distinct from that optimizing the quantum discord, exhibiting a transition in the direction of the spin measurement, from that of maximum correlation to that parallel to the field. The details of this transition depend on the choice of entropy (it is sharp for I_2, and smooth for I_1). The quantum discord prefers instead that of maximum correlation even for strong fields. Hence, the quantum discord, which is based on the minimization of a conditional entropy, "detects" in this way this direction [58], while the information deficits, based on the minimization of a total entropy, are more sensible to changes in the structure of the reduced state of the pair.

A final comment is that the generalized formalism permits the use of simple entropic forms involving just low powers of the density matrix, leading to measures of the form (42) or (43) which can be more easily evaluated and optimized, and which are also more easily accessible from the experimental side.

Appendix A: Appendix

We briefly discuss here the exact solution of the *finite* cyclic XY chain with first neighbor couplings, which requires to take into account exactly the parity effects [46, 66–68]. The Jordan Wigner transformation [66] allows to rewrite the Hamiltonian (46) in the XY case ($J_z^{ij} = 0$) for $J_\mu^{ij} = J_\mu \delta_{i,j\pm1}$, $\mu = x, y$, and for each value ±1 of the S_z parity P_z, as a quadratic form in fermion creation and annihilation operators $c_i^\dagger$, c_i defined by $c_i^\dagger = s_{i+} \exp[-i\pi \sum_{j=1}^{i-1} s_{j+}s_{j-}]$, with the reverse transformation given by $s_{i+} = c_i^\dagger \exp[i\pi \sum_{j=1}^{i-1} c_j^\dagger c_j]$. This leads to

$$H^{\pm} = \sum_{i=1}^{n} B(c_i^\dagger c_i - \tfrac{1}{2}) - \tfrac{1}{2}\eta_i^{\pm}(J_+ c_i^\dagger c_{i+1} + J_- c_i^\dagger c_{i+1}^\dagger + h.c.)$$
$$= \sum_{k\in K_\pm} \lambda_k (a_k^\dagger a_k - \tfrac{1}{2}) \tag{A1}$$

where $J_\pm = \frac{1}{2}(J_x \pm J_y)$ and $n+1 \equiv 1$, $\eta_i^- = 1$, $\eta_i^+ = 1 - 2\delta_{in}$ [66]. In (A1), $K_+ = \{\frac{1}{2}, \ldots, n-\frac{1}{2}\}$, $K_- = \{0, \ldots, n-1\}$ and

$$\lambda_k = \sqrt{(B - J_+\cos\omega_k)^2 + J_-^2 \sin^2\omega_k}\,, \quad \omega_k = 2\pi k/n\,. \tag{A2}$$

The last form (A1) is obtained through a parity dependent discrete Fourier transform $c_j^\dagger = \frac{e^{i\pi/4}}{\sqrt{n}} \sum_{k\in K_\pm} e^{-i\omega_k j} c_k'^\dagger$, followed by a BCS-type Bogoliubov transformation $c_k'^\dagger = u_k a_k^\dagger + v_k a_{n-k}$, $c'_{n-k} = u_k a_{n-k} - v_k a_k^\dagger$ to quasiparticle fermionic operators a_k, $a_k^\dagger$, with $\binom{u_k^2}{v_k^2} = \frac{1}{2}[1 \pm (B - J_+\cos\omega_k)/\lambda_k]$.

For $B \geq 0$, we may set $\lambda_k \geq 0$ for $k \neq 0$ and $\lambda_0 = J_+ - B$, in which case the quasiparticle vacuum of $H^\pm$ has the right parity and the lowest energy is $E^\pm = -\frac{1}{2}\sum_{k\in K_\pm}\lambda_k$. At the factorizing field (57), $\lambda_k = J_+ - B_s\cos\omega_k$ and $E^\pm = -nJ_+/2$ [46].

The reduced state of a spin pair in the exact ground state can then be obtained from the basic contractions $\langle a_k^\dagger a_{k'}\rangle = 0$, $\langle a_k^\dagger a_{k'}^\dagger\rangle = 0$, leading to $\langle c'^\dagger_k c'_{k'}\rangle = v_k^2\delta_{kk'}$, $\langle c'^\dagger_k c'^\dagger_{k'}\rangle = u_k v_k \delta_{k,-k'}$ and $(L = i - j)$

$$\langle c_i^\dagger c_j\rangle_\pm = \frac{1}{n}\sum_{k\in K_\pm} e^{-i\omega_k L} v_k^2 = f_L + \tfrac{1}{2}\delta_{ij}\,,$$
$$\langle c_i^\dagger c_j^\dagger\rangle_\pm = \frac{1}{n}\sum_{k\in K_\pm} e^{-i\omega_k L} u_k v_k = g_L\,. \tag{A3}$$

Application of Wick's theorem then leads to [37, 66]

$$\langle s_{iz}\rangle = f_0,\ \langle s_{iz}s_{jz}\rangle = f_0^2 - f_L^2 + g_L^2\,,$$
$$\langle s_{i-}s_{j\mp}\rangle = \tfrac{1}{4}[\det(A_L^+) \mp \det(A_L^-)]\,,$$

where $(A_L^\pm)$ are $L\times L$ matrices of elements $(A_L^\pm)_{ij} = 2(f_{i-j\pm 1} + g_{i-j\pm 1})$. These results, valid for any finite n, were checked through direct diagonalization for small n.

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