Quantum correlations and coherence in spin-1 Heisenberg chains

A. L. Malvezzi,[1] G. Karpat,[1,2] B. Çakmak,[3,4] F. F. Fanchini,[1,*] T. Debarba,[5] and R. O. Vianna[6]

[1]*Faculdade de Ciências, UNESP - Universidade Estadual Paulista, Bauru, São Paulo 17033-360, Brazil*

[2]*Turku Center for Quantum Physics, Department of Physics and Astronomy, University of Turku, FI-20014 Turun yliopisto, Finland*

[3]*Department of Physics, Koç University, İstanbul, Sarıyer 34450, Turkey*

[4]*Instituto de Fisica Gleb Wataghin, Universidade Estadual de Campinas, P.O. Box 6165, Campinas, São Paulo 13083-970, Brazil*

[5]*Universidade Tecnológica Federal do Paraná (UTFPR), Campus Cornélio Procópio, Avenida Alberto Carazzai 1640, Cornélio Procópio, Paraná 86300-000, Brazil*

[6]*Departamento de Fisica, ICEx, Universidade Federal de Minas Gerais, Avenida Presidente Antônio Carlos 6627, Belo Horizonte 31270-901, Brazil*

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We explore quantum and classical correlations along with coherence in the ground states of spin-1 Heisenberg chains, namely the one-dimensional XXZ model and the one-dimensional bilinear biquadratic model, with the techniques of density matrix renormalization group theory. Exploiting the tools of quantum information theory, that is, by studying quantum discord, quantum mutual information, and three recently introduced coherence measures in the reduced density matrix of two nearest neighbor spins in the bulk, we investigate the quantum phase transitions and special symmetry points in these models. We point out the relative strengths and weaknesses of correlation and coherence measures as figures of merit to witness the quantum phase transitions and symmetry points in the considered spin-1 Heisenberg chains. In particular, we demonstrate that, as none of the studied measures can detect the infinite-order Kosterlitz-Thouless transition in the XXZ model, they appear to be able to signal the existence of the same type of transition in the biliear biquadratic model. However, we argue that what is actually detected by the measures here is the SU(3) symmetry point of the model rather than the infinite-order quantum phase transition. Moreover, we show in the XXZ model that examining even single site coherence can be sufficient to spotlight the second-order phase transition and the SU(2) symmetry point.

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I. INTRODUCTION

The investigations of many-body quantum systems have revealed very interesting and deep physical concepts such as quantum phase transitions (QPT). QPTs are abrupt changes in the ground state of a quantum many-body system as one or more parameters of the Hamiltonian is varied at absolute zero temperature [1]. In contrast to thermal phase transitions, which are driven by thermal fluctuations in the system, QPTs are driven by quantum fluctuations stemming from the uncertainty principle. However, it is also possible to see the effects of a QPT at sufficiently low but finite temperatures where the quantum fluctuations are not washed away by the thermal effects. Traditionally, phase transitions are classified based on the nonanalytic behavior in the derivatives of the ground state energy. In particular, a discontinuity in the first derivative of the ground state energy signals a first-order transition. On the other hand, a discontinuity or divergence in the second derivative of the ground state energy is recognized as a second-order transition in which case the transition is associated with a symmetry breaking. A more involved type of phase transition, which does not fit to the traditional classification scheme, is known as the Kosterlitz-Thouless (KT) transition. In this case, there is no divergence or discontinuity in the derivatives of the ground state energy and no symmetry breaking, thus KT transitions are said to be of infinite order [2].

Quantum many-body systems possess correlations of various different nature due to the interaction among their constituents. Therefore, in addition to the traditional ways of witnessing quantum phase transitions, it has been recently suggested that the tools of quantum information theory [3] can also be exploited to characterize the transition points (TPs) of quantum phase transitions. Especially, in quantum spin models, the behavior of entanglement [4], quantum discord [5], and many other correlation measures have been investigated, and their performance in detecting the TPs of the QPTs have been discussed [6,7]. Recently, a new line of research has emerged that concerns itself with the characterization and quantification of quantum coherence contained in a quantum state [8–12]. Based on these new quantum coherence measures, similar analysis have been done in the ground states of several spin chains [7]. However, many of these studies focusing on quantum correlations in spin chains have been done for spin-1/2 systems [6,7], where analytical solutions are available in many cases. On the other hand, spin-1 models have richer phase diagrams and show more complex physical phenomena, yet methods for obtaining the ground state of such systems are rather more involved [13–30]. For instance, a very important distinctive property of the integer-spin quantum systems as compared to the half-integer ones is the Haldane conjecture, which states that the system has a gapped ground state, giving rise to the so-called Haldane phase [31].

In this work, we will consider two very well known one-dimensional spin-1 Heisenberg models, namely, the spin-1 XXZ chain and the spin-1 bilinear biquadratic chain. Both of these models have been under extensive investigation in the literature from different perspectives due to the rich physics they exhibit. Here we obtain the ground state of these systems by making use of the methods of density

*fanchini@fc.unesp.br

matrix renormalization group theory (DMRG). Then, we extensively investigate the behavior of mutual information, quantum discord, and three recently introduced coherence measures—namely, relative entropy of coherence, l_1 norm of coherence [8], and Wigner-Yanase skew information [11,32]—for the reduced density matrix of two nearest-neighbor spins in the bulk. Our analysis lets us establish relations between the phase transitions and symmetry points in the considered spin-1 Heisenberg chains and the studied correlation and coherence measures.

This paper is organized as follows. In Sec. II, we introduce the spin-1 Heisenberg models used in this study along with the DMRG techniques required to obtain the numerical solution of these models. Section III presents the definitions of the considered correlation and coherence measures. We present our results in Sec. IV and conclude in Sec. V.

II. MODELS

In the section, we briefly discuss the different phases that the one-dimensional XXZ model and the one-dimensional bilinear biquadratic model favor with respect to their characteristic parameters, and the nature of phase transitions occurring among these phases. In order to calculate the ground state of the model Hamiltonians, we use the standard DMRG infinite system method [33]. In this version of DMRG, an open chain is grown iteratively by adding two sites at a time to the center of the chain. At each step the ground state for the whole chain is calculated and a renormalization procedure is performed. Typically, after a few hundred iterations the two central sites are embedded in a bulk. The reduced density matrix for these two central sites can then be obtained from the ground state. It is important to stress that, despite the renormalization, the spin interaction between the two central sites is always kept exact. As the model parameters vary, truncation errors in the renormalization procedure range from 10^{-10} to 10^{-6}, with the upper limit occurring around second-order phase transitions, where quantum fluctuations are stronger.

A. Spin-1 XXZ chain

The Hamiltonian describing the one-dimensional spin-1 XXZ model with nearest neighbor interaction reads

$$H = \sum_{i=1}^{N} \left[S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + \Delta S_i^z S_{i+1}^z \right], \tag{1}$$

where N is the total number of sites, $\mathbf{S}_i$ denotes the spin-1 operator at the site i, and Δ characterizes the anisotropy of the spin-exchange interaction in the model. It is well established that the model has four different phases depending on the value of the anisotropy parameter [13,16,21]. The system is in a ferromagnetic phase when $\Delta < -1$. There is a first-order phase transition at the TP $\Delta_{c1} = -1$, which separates the ferromagnetic phase from the XY phase. At the second TP Δ_{c2}, the system exhibits an infinite-order phase transition (that is believed to be of KT type), from the XY phase to the Haldane phase, which extends over the region $\Delta_{c2} < \Delta < \Delta_{c3}$. There is also a second-order phase transition taking place at the TP Δ_{c3} from the Haldane phase to the Néel phase, belonging to the two-dimensional Ising universality class. Even though the exact values of both TPs Δ_{c2} and Δ_{c3} have been the subject of various numerical studies, it is widely accepted that XY-Haldane and Haldane-Néel transitions respectively occur at the TPs $\Delta_{c2} \approx 0$ and $\Delta_{c3} \approx 1.185$ [16,21]. It should also be emphasized that, in addition to the phase transition points, the model also has a particular SU(2) symmetry point at $\Delta = 1$.

B. Spin-1 bilinear biquadratic chain

The Hamiltonian of the one-dimensional spin-1 bilinear biquadratic chain can be written as

$$H = \sum_{i=1}^{N} [\cos\theta(\mathbf{S}_i \cdot \mathbf{S}_{i+1}) + \sin\theta(\mathbf{S}_i \cdot \mathbf{S}_{i+1})^2], \tag{2}$$

where N is the total number of sites, $\mathbf{S}_i$ denotes the spin-1 operator at the site i, and $\theta \in [0,2\pi)$ is the angle quantifying the amount of coupling between nearest neighbor spins. The model system has an especially rich phase diagram. In the parameter region $-0.25\pi < \theta < 0.25\pi$, the system is in the Haldane phase. At the TP $\theta_{c1} = 0.25\pi$, there is a transition of the KT type, separating the Haldane phase from the gapless trimerized phase. A first-order transition from the trimerized phase to the ferromagnetic phase occurs at the TP $\theta_{c2} = 0.5\pi$. As the system favors the ferromagnetic phase throughout the parameter region $0.5\pi < \theta < 1.25\pi$, another first-order transition takes place at the TP $\theta_{c3} = 1.25\pi$ from the ferromagnetic phase to the gapped dimerized phase. Finally, there exists a second-order transition between the dimerized phase and the Haldane phase at the TP $\theta_{c4} = 1.75\pi$. Although it has been also suggested that the model might exhibit a nondimerized nematic phase in the region $5\pi/4 < \theta < 1.33\pi$ with a KT type transition at $\theta = 1.33\pi$ [30], it has been recently shown that no such nematic phase exists and the system remains in the dimerized phase all through this region [34]. It is also worthwhile to mention that at $\theta = 0.1024\pi$ the system corresponds to the Affeck-Kennedy-Lieb-Tasaki (AKLT) model [35] with an exact valence bond ground state, and at $\theta = 1.5\pi$ it can be solved exactly by the Bethe ansatz method [36]. Last but not least, we stress that, besides being a TP of the model, $\theta = 0.25\pi$ is also special in that the system has a SU(3) symmetry [37].

III. CORRELATIONS AND COHERENCE

This section serves as a brief introduction to description of the figures of merit that we will be using throughout this work, i.e., quantum mutual information, quantum discord, relative entropy of coherence, l_1 norm of coherence, and Wigner-Yanase skew information based measure of coherence.

The relevance of these measures to the study of quantum phase transition follows from different reasons. Quantum discord, for example, was broadly studied in the quantum critical systems and brought various new insights to the field when compared with entanglement measurements. Quantum discord can detect QPTs even when the entanglement measures fail to do so and it can be used even for thermal systems. However, to evaluate it for spin dimensions higher than two spin-1/2 particles is a highly demanding task. To overcome this difficulty, we have introduced a simple numerical procedure that will allow the analysis of quantum discord in high dimensional spin systems. Indeed, in our view, it will serve as an efficient new tool of the quantum information theory for the study of QPT. On the other hand, once again we would like to emphasize that, to the best of our knowledge, this is the first work which calculates the recently introduced coherence measures in a spin-1 model. The importance of the calculation of coherence measures stem from the facts that they can be used as a resource in quantum computing protocols [38], they can be calculated even for single spin density matrices, they are experimentally friendly quantities to calculate, and they are analytically (and easily) computable even for high spin dimensions.

A. Quantum discord

Let us commence by introducing the quantum mutual information. It quantifies the total amount of classical and quantum correlations in a bipartite quantum state ρ_{AB} as

$$\mathcal{I}(\rho_{AB}) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \tag{3}$$

where $\rho_{A(B)}$ is the reduced density matrix of subsystem A (B) and $S(\rho) = -\mathrm{Tr}\{\rho \log_2 \rho\}$ is the von Neumann entropy. On the other hand, the classical correlation, which is the maximum amount of classical information that can be obtained about the subsystem A by performing local measurements on the subsystem B, is given by

$$\mathcal{C}(\rho_{AB}) = \max_{\{\Pi_k^B\}} \left\{ S(\rho_A) - \sum_k p_k S(\rho_{A|k}) \right\}, \tag{4}$$

where the operators $\{\Pi_k^B\}$ constitute a positive operator valued measure (POVM) acting only on the subsystem B, and $\rho_{A|k} = \mathrm{Tr}_B(\Pi_k^B \rho_{AB} \Pi_k^B)/p_k$ is the remaining state of the subsystem A after obtaining the outcome k with probability $p_k = \mathrm{Tr}_{AB}(\Pi_k^B \rho_{AB} \Pi_k^B)$ in the subsystem B. Then, the amount of inaccessible information, by means of local measurements, defines the quantum discord as [5]

$$\mathcal{D}(\rho_{AB}) = \mathcal{I}(\rho_{AB}) - \mathcal{C}(\rho_{AB}). \tag{5}$$

In the following, we will describe a numerical recipe to efficiently calculate quantum discord. We should underline that, unlike most works in the literature, where quantum discord is evaluated for a pair of qubits and only using projective measurements, our method makes it possible to calculate quantum discord for the composite system of two spin-1 objects and using POVMs rather than projective measurements. Nonetheless, we restrict ourselves to the projective measurements in this work for the sake of simplicity.

Numerical evaluation of quantum discord

Although the calculation of quantum discord is an NP-complete problem [39], i.e., the necessary time to obtain the value for it grows exponentially with the Hilbert space dimension, we present a method to numerically compute quantum discord. In order to find the global minimum of quantum discord under projective measurements, we have to search all the Hilbert space to find the optimal orthonormal basis. One way of doing so is to generate a random unitary matrix, whose eigenvectors are used as a starting point for a global optimization technique, like steepest descent or variable metric methods as implemented in MATLAB, for instance. The minimization is repeated for different starting points.

The random unitary matrix is obtained by means of a circular unitary ensemble (CUE), which consists of all unitary matrices with Haar measure in the unitary group, following the technique proposed in [40,41]. The idea is to generate Euler angles (ϕ,ψ,χ), such that the arbitrary unitary matrix U be composed from unitary transformations $E^{(i,j)}(\phi,\psi,\chi)$ in two-dimensional subspaces [41]. The nonzero elements of the matrices $E^{(i,j)}$ are

$$\begin{aligned} &E_{kk}^{(m,n)} = 1, \quad k \neq m,n, \quad E_{mm}^{(m,n)} = \cos\phi_{mn} e^{i\psi_{mn}},\\ &E_{mn}^{(m,n)} = \sin\phi_{mn} e^{i\chi_{mn}}, \quad E_{nm}^{(m,n)} = -\sin\phi_{mn} e^{-i\chi_{mn}},\\ &E_{nn}^{(m,n)} = \cos\phi_{mn} e^{-i\psi_{mn}}. \end{aligned} \tag{6}$$

The matrices of Euler angles ψ and ϕ have dimension $(N-1)\times(N-1)$, and the matrix χ has dimension $(N-1)\times 1$, where N is the dimension of the Hilbert space. The angles in ψ and χ must be taken uniformly in the interval $[0,2\pi)$. The angles in ϕ are given by $\arcsin(\xi_{rs}^{1/(2r+2)})$, for $r = 0,1,\ldots,N-2$, with ξ_{rs} uniformly distributed in the interval $[0,1)$. The random unitary matrix U reads

$$U = e^{i\alpha} E_1 E_2 \cdots E_{N-1}, \tag{7}$$

where α is also taken uniformly in the interval $[0,2\pi)$, and the matrices E_k, for $k = 1,2,\ldots,N-1$, read

$$\begin{aligned} E_k = {} & E^{(N-k,N-k-1)}(\phi_{k-1,k},\psi_{k-1,k},0) \times \cdots \\ & \times E^{(N,N-1)}(\phi_{0,k},\psi_{0,k},\chi_k). \end{aligned} \tag{8}$$

In our numerical calculations, we generate the angles α, ϕ, ψ, and χ by means of a uniform random vector x_0, with $2(N-1)^2+N$ elements. The first element of x_0 is the angle α, the next $N-1$ elements correspond to the vector χ, and the last $2(N-1)^2$ elements generate the matrices ϕ and ψ. Therefore, following the technique presented above, we can create a random unitary matrix starting point, and search for the global minimum in the space of unitary matrices with Haar measure in the unitary group [42].

With the aid of the Naimark's theorem [43], the algorithm to optimize the quantum discord under projective measurements can also be used to perform the optimization under POVMs. Let us review the procedure. Consider a set of positive semidefinite operators P_a, acting on the Hilbert space $\mathcal{X}$, of dimension x. In order to form a POVM, the P_a must satisfy

$$\sum_a P_a = I_x, \tag{9}$$

where I_x is the identity operator acting on $\mathcal{X}$. To each P_a, we associate a projector $|a\rangle\langle a|$, acting on an extended Hilbert space $\mathcal{X}\otimes\mathcal{Y}$. We wish that a projective measurement in the extended Hilbert space $\mathcal{X}\otimes\mathcal{Y}$, of dimension $x\times y$, will reproduce the statistics of the POVM in the original space $\mathcal{X}$, namely,

$$\mathrm{Tr}(P_a\rho) = \mathrm{Tr}(A^\dagger|a\rangle\langle a|A\rho), \tag{10}$$

where A is an isometry that takes a vector in $\mathcal{X}$ to $\mathcal{Y}$,

$$A^\dagger A = I_x, \quad A^\dagger|a\rangle\langle a|A = P_a. \tag{11}$$

Let $|e_a\rangle$ be the canonical basis in $\mathcal{Y}$; then we choose

$$|a\rangle\langle a| = I_x \otimes |e_a\rangle\langle e_a|. \tag{12}$$

With this choice, the isometry A reads

$$A = \sum_a \sqrt{P_a} \otimes |e_a\rangle. \tag{13}$$

By choosing some arbitrary ancilla $|u\rangle$ in $\mathcal{Y}$, we can decompose the isometry as

$$A = UV, \quad V = (I_x \otimes |u\rangle), \tag{14}$$

where U is a unitary acting on $\mathcal{X} \otimes \mathcal{Y}$. Finally we have

$$\mathrm{Tr}(P_a \rho) = \mathrm{Tr}(Q_a \rho \otimes |u\rangle\langle u|), \tag{15}$$

where the projector Q_a reads

$$Q_a = U^{\dagger}(I_x \otimes |e_a\rangle\langle e_a|)U. \tag{16}$$

We conclude that the POVM $\{P_a\}$ in the original space is equivalent to the projective measurement $\{Q_a\}$ over the state $\rho \otimes |u\rangle\langle u|$ in the extended space. The unitary U is explicitly

$$U = AV^{+}, \tag{17}$$

where V^{+} is the pseudo-inverse of V.

B. Quantum coherence

Although quantum coherence plays a central role in quantum mechanics, being a manifestation of the quantum superposition principle, its quantification has been formalized only very recently. In particular, a set of conditions that is expected to be satisfied by any proper measure of coherence has been proposed in Ref. [8]. Two such measures that we study in this work are known as the relative entropy of coherence and the l_1 norm of coherence. While the former is defined as

$$C_{\mathrm{re}}(\rho) = S(\rho_{\mathrm{diag}}) - S(\rho), \tag{18}$$

where $S(\rho_{\mathrm{diag}})$ is obtained from the state ρ by deleting all of its off-diagonal elements, the latter is given by the sum of absolute values of all off-diagonal elements of ρ, that is,

$$C_{l_1}(\rho) = \sum_{i \neq j} |\rho_{i,j}|. \tag{19}$$

Naturally, it is only meaningful to talk about coherence measures once we set a specific basis for incoherent quantum states since coherence is clearly basis dependent.

On the other hand, there is a particular quantity which, despite not satisfying [44] the conditions proposed in Ref. [8], can still be considered as a measure of coherence in a conceptually different way [10,11]; i.e., as Wigner-Yanase skew information [32]:

$$C_{\mathrm{si}}(\rho, K) = -\tfrac{1}{2}\mathrm{Tr}[\sqrt{\rho}, K]^2, \tag{20}$$

where K is a nondegenerate Hermitian matrix, and $[.,.]$ denotes the commutator. We note that as the skew information reduces to the variance $V(\rho,K) = \mathrm{Tr}\,\rho K^2 - (\mathrm{Tr}\,\rho K)^2$ for pure states, it is upper bounded by the variance for mixed states. In fact, $C_{\mathrm{si}}(\rho,K)$ is a measure of asymmetry relative to the group of translations generated by the observable K, which in turn can be interpreted as a measure of coherence of the state ρ relative to the eigenbasis of the observable K [45]. From this point on, we will simply refer to $C_{\mathrm{si}}(\rho,K)$ as K coherence.

IV. RESULTS

In this section, we intend to investigate the behavior of the considered correlation and coherence measures in the ground state of the spin-1 XXZ chain for two nearest neighbor spins in the bulk. For our purposes, we consider the region where the anisotropy parameter lies in between $-1 < \Delta < 1.5$. Observing Fig. 1, at the TP $\Delta_{c2} \approx 0$, where the system has an infinite-order phase transition, we do not notice a nontrivial behavior in the quantum mutual information; i.e., it does not exhibit either a nonanalytical behavior or an extremum. In other words, the mutual information is not able to detect the existence of the KT type transition in the XXZ chain. On the other hand, at the point $\Delta_{c3} \approx 1.185$, we see a pronounced local minimum, which spotlights the second-order transition that the system has between the Haldane and Néel phases. Recalling that the XXZ chain also has a particular SU(2) symmetry point at $\Delta = 1$, we can observe that the mutual information shows a smooth local maximum at this special point.

Figure 2 displays the outcomes of our analysis for the quantum discord in the ground state of the XXZ chain. Similarly to the case of quantum mutual information, quantum discord is not capable of recognizing the location of the KT type transition. In fact, it is rather expected that neither mutual information nor quantum discord show a nonanalytic behavior at this point, since all derivatives of the ground state energy and thus the elements of the two-spin density matrix we study are continuous for an infinite-order transition. Moving to the second-order transition at the TP $\Delta_{c3} \approx 1.185$, we notice that quantum discord shows an inflection point; that is, the transition point might be easily captured looking at the derivative of Fig. 2 around this point, which would display a quite pronounced minimum. Finally, it is straightforward to observe that quantum discord has a sharp maximum at

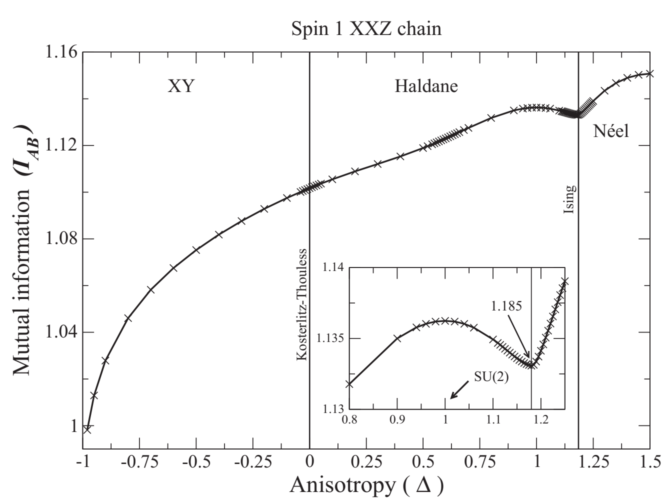

FIG. 1. Mutual information versus the anisotropy parameter Δ in the one-dimensional spin-1 XXZ model. Different phases, transition points, and the SU(2) symmetry point are shown.

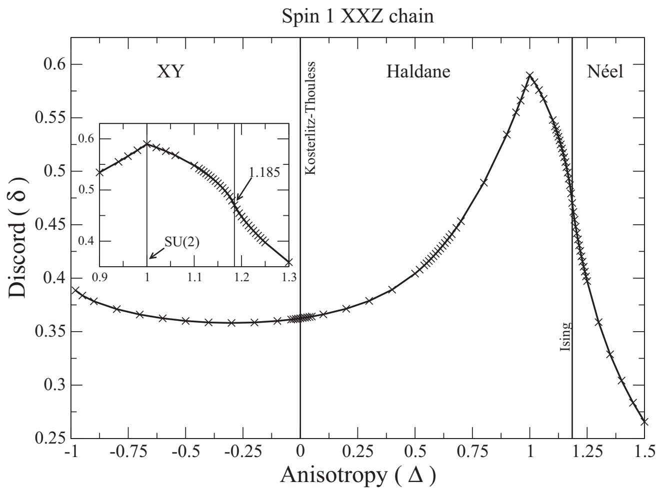

FIG. 2. Quantum discord versus the anisotropy parameter Δ in the one-dimensional spin-1 XXZ model. Different phases, transition points, and the SU(2) symmetry point are shown.

the SU(2) symmetry point $\Delta = 1$. Indeed, a closer inspection reveals that quantum discord has a sudden change at this value of the anisotropy parameter. That is to say that the optimal measurement basis for quantum discord suddenly changes at the SU(2) symmetry point, resulting in a clear identification of the symmetry point through quantum discord. We note that this is fundamentally different from the way mutual information detects the existence of the SU(2) symmetry point.

Next, we explore the quantum coherence using different measures in the ground state of the spin-1 XXZ chain for two nearest neighbor spins in the bulk. In Fig. 3, we plot the relative entropy of coherence, l_1 norm of coherence, the local S_x coherence, and the local S_z coherence versus the anisotropy parameter, where S_x and S_z are the usual spin-1 matrices. Local K-coherence means that the observable K in the definition of

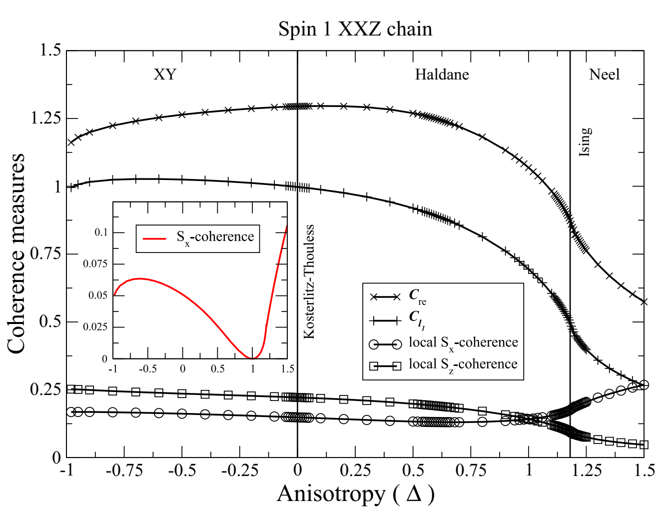

FIG. 3. Quantum coherence measures as quantified by l_1 norm of coherence, relative entropy of coherence, and K coherence versus the anisotropy parameter Δ in the one-dimensional spin-1 XXZ model. Different phases, transition points, and the SU(2) symmetry point are shown.

$C_{\mathrm{si}}(\rho, K)$ is simply $I \otimes K$. First of all, we immediately notice that none of the considered coherence measures can spotlight the infinite-order KT transition in the model since they do not exhibit a nontrivial behavior at the transition point. To put it differently, the KT transition in the spin-1 XXZ model escapes all of the correlation and coherence measures that we use in our investigation. On the other hand, all four coherence measures can detect the second-order transition occurring at the TP $\Delta_{c3} \approx 1.185$ via an inflection point. Turning our attention to the SU(2) symmetry point in the XXZ model, we observe that the relative entropy of coherence and l_1 norm of coherence are not able to detect the existence of this point at $\Delta = 1$. In addition, it is also not possible to detect the SU(2) symmetry point just by checking the local S_x coherence or the local S_z coherence individually. However, it is interesting that plotting the K coherence for two different observables reveals the SU(2) symmetry point through the intersection of these two curves. That is, the curves of the local S_x coherence or the local S_z coherence intersect at the SU(2) point $\Delta = 1$; i.e., the system has the same K coherence at the symmetry point, independently of the observable S_x and S_z.

Last, we study the S_x-coherence in the ground state of the spin-1 XXZ chain for a single spin in the bulk. The results of this investigation are shown in the inset of Fig. 3. Interestingly, an inflection point still appears even in the level of single-site coherence at the TP of the second-order phase transition at $\Delta_{c3} \approx 1.185$. Furthermore, the S_x coherence vanishes only at the SU(2) symmetry point $\Delta = 1$, pinpointing its location. The reason we do not display the relative entropy of coherence and l_1 norm of coherence here is that they are zero for all values of the anisotropy parameter due to the fact that the single spin density matrix is diagonal in S_z basis.

Having discussed the correlations and coherence in the spin-1 XXZ chain, we now examine the spin-1 bilinear biquadratic model from the perspective of bipartite correlations in the ground state of the chain. Here we report on the nature of correlations in the chain both for the nearest neighbor spins in the bulk and for a small chain of 12 spins under open boundary condition. We should also mention in passing that the reason we also considered a small chain of 12 spins in bilinear biquadratic model is to show the physical effects that can only be observed in the bulk in this case. Looking at Figs. 4 and 5, we can see that both first-order transitions taking place at TPs $\theta_{c2} = 0.5\pi$ and $\theta_{c3} = 1.25\pi$ are signaled by the discontinuous jumps in mutual information and quantum discord, respectively. Moreover, exploring the correlations just for a chain of 12 spins is sufficient to detect these transitions. The difference between the behaviors of quantum discord and mutual information at these points is that while mutual information first increases in a discontinuous fashion at the TP $\theta_{c2} = 0.5\pi$ and then again decreases at the TP $\theta_{c3} = 1.25\pi$, quantum discord behaves in the exact opposite way. When it comes to the second-order transition occurring at the TP $\theta_{c4} = 1.75\pi$ between the trimerized and Haldane phases, Figs. 4 and 5 show that it is not possible to pinpoint the TP in case of 12 spins since the curves of mutual information and quantum discord are smooth without any sign of the transition. However, performing the same analysis for two spins in the bulk, we see that a kink appears at $\theta = 1.78\pi$, which in turn lets the second derivatives of both mutual information and quantum

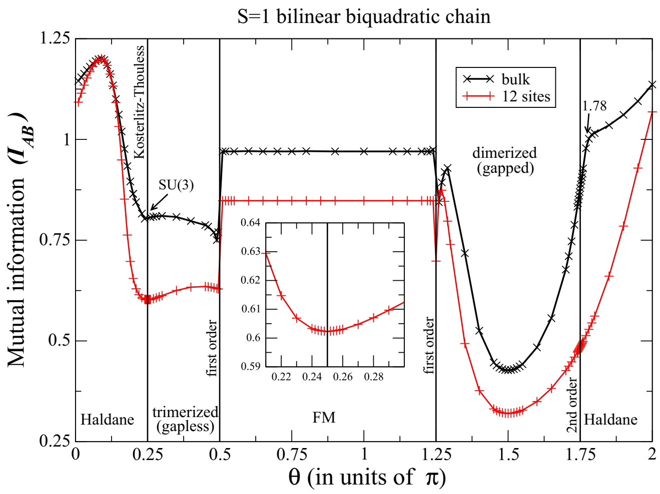

FIG. 4. Mutual information versus the parameter θ in the one-dimensional spin-1 bilinear biquadratic model. Different phases, transition points, and the SU(3) symmetry point are shown.

discord to display a sharp maximum at the TP $\theta_{c3} = 1.75\pi$. We emphasize that this is different from the case of first-order transitions, whose traces can be located regardless of the size of the chain.

We now recall that, in the spin-1 bilinear biquadratic model, the point $\theta_{c1} = 0.25\pi$ corresponds to both the TP of the infinite-order KT type transition and the SU(3) symmetry point. In Fig. 4, we clearly observe a local minimum at this point, which would let one conclude that the TP of the KT transition, despite being an infinite-order transition, can be detected through the behavior of mutual information both for bulk and 12 spins. Nonetheless, we argue that what is signaled here is actually the SU(3) symmetry point of the model rather than the TP of the KT transition. Our argument is based on what we have observed in case of the spin-1 XXZ model, that is, neither mutual information nor any other studied measure are able to capture the KT transition point due to the

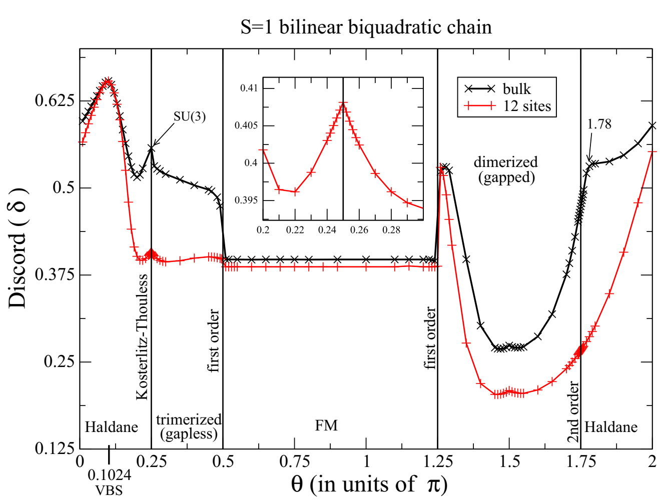

FIG. 5. Quantum discord versus the parameter θ in the one-dimensional spin-1 bilinear biquadratic model. Different phases, transition points, and the SU(3) symmetry point are shown.

analytical behavior of the ground state energy and all of its derivatives. On the other hand, Fig. 5 displays that a sharp peak in quantum discord can be seen at this point, which we believe again spotlights the SU(3) symmetry point rather than the TP of the KT transition. In particular, our numerical treatment also reveals that a sudden change emerges in the quantum discord at $\theta_{c1} = 0.25\pi$ which has its roots in the change of the optimizing basis in the definition of quantum discord. We stress that, in the spin-1 XXZ model, the SU(2) symmetry point has been also captured via discord through a sudden change, which supports our argument that what we in fact observe here in the bilinear biquadratic model is the effect of the SU(3) symmetry point and not the KT transition happening at the same point. Also, we recall that the measures for the 12 spins chain were unable to signal the second-order TP at $\theta_{c4} = 1.75\pi$, so it is quite unlikely they would detect a TP of infinite order. Finally, we point out that the special points of the spin-1 bilinear biquadratic model, namely $\theta = 0.1024\pi$ corresponding to the AKLT model and $\theta = 1.5\pi$, where the model has an exact solution with the Bethe ansatz method, can be seen to be shown respectively in Figs. 4 and 5 through the extrema of the mutual information and quantum discord.

As for the behavior of quantum coherence measures in case of the bilinear biquadratic model, even though we do not explicitly present our results here for the purposes of brevity and convenience, we have performed an analysis similarly to the case of the XXZ model. We have observed that all three coherence measures are able to capture the SU(3) symmetry point and the quantum phase transitions when two-spin coherence is studied. On the other hand, we have seen for a single spin that σ_x coherence can only detect the first-order phase transitions while the remaning two coherence measures vanish due to the fact that their density matrices are diagonal in S_z basis. This is in accord with the results of Ref. [17] where the single site entropy has been studied for the same model.

V. CONCLUSION

In summary, we have investigated the quantum mutual information, quantum discord, and quantum coherence in the ground states of spin-1 XXZ and bilinear biquadratic chains for two nearest neighbor spins in the bulk. On one hand, our study has enabled us to draw conclusions regarding the relation of the behavior of quantum correlations and coherence to the quantum phase transitions in these models. On the other hand, we have established a link between the particular symmetry points of the studied spin-1 Heisenberg chains and the considered correlation and coherence measures.

In particular, we have seen that neither the total and quantum correlations, as quantified by mutual information and quantum discord respectively, nor the coherence measures have been able to capture the TP of the infinite-order KT type transition occurring in the XXZ model. However, they were all able to locate the Ising type second-order transition. In case of the SU(2) symmetry point, whereas we have observed that both of the correlation measures can detect it, K coherence based on Wigner-Yanase skew information is the unique coherence measure in our study which is able to signal this symmetry point for a pair of nearest neighbor spins in the bulk. Furthermore, we have shown that even for a single spin in the bulk, K coherence can identify the SU(2) symmetry and the Ising transition in the spin-1 XXZ model.

Moreover, we have performed a similar analysis for the spin-1 bilinear biquadratic chain. Here, the mutual information and quantum discord have signaled the point $\theta = 0.25\pi$, which corresponds both to the TP of the infinite-order KT transition and the SU(3) symmetry point. Based on our findings regarding the KT transition and SU(2) symmetry point in the XXZ chain, we have argued that what might actually be observed through the measures is a consequence of the SU(3) symmetry rather than the effect of the KT transition occurring at the same point. Our argument is supported by the fact that quantum discord displays sudden changes due to the discontinuous change of the optimizing basis in its definition at the symmetry points in both models. Also, the density matrix elements of the nearest neighbor spins and all of their derivatives are analytical at the KT transition points, thus the sudden changes in quantum discord are likely to have their roots in the symmetries. We emphasize that the sudden change of quantum discord at the symmetry points is fundamentally different from the behavior of quantum mutual information, which shows a local extremum at these spots. Finally, we have pointed out the necessity of studying the correlations in the bulk, as opposed to just a small chain of 12 spins, to be able to spotlight the second-order transition in the chain.

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