Quantum discord and quantum phase transition in spin chains

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Quantum phase transitions of the transverse Ising and antiferromagnetic *XXZ* spin $S=1/2$ chains are studied using *quantum discord*. Quantum discord allows the measure of quantum correlations present in many-body quantum systems. It is shown that the *amount* of quantum correlations increases close to the critical points. The observations are in agreement with the information provided by the concurrence, which measures the entanglement of the many-body system.

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I. INTRODUCTION

Quantum phase transitions (QPTs) occur when the ground state of a many-body system at absolute zero temperature undergoes a qualitative change by variation in a coupling and/or an external parameter.[1] QPTs are present in spin systems as for example in the one-dimensional (1D) *XY* model[2,3] and in the antiferromagnetic *XXZ* model.[4–6] Quantum phase transitions in spin systems have been widely characterized considering the pairwise entanglement between two spin sites.[7] The concurrence, which is a good measure of entanglement,[8,9] is maximal close to the critical points, and its derivatives can signal more precisely the presence of a quantum phase transition at the critical points.[3]

In another register Ollivier and Zurek[10] introduced the *quantum discord* as a measure of quantum correlations between two separated subsystems of a many-body quantum system. In information theory the *mutual information* is defined as the measure of correlation between two random variables $\mathcal{A}$ and $\mathcal{B}$. For classical system the mutual information can be expressed in terms of two equivalent expressions $\mathcal{I}(\mathcal{A};\mathcal{B})$ and $\mathcal{J}(\mathcal{A};\mathcal{B})$ (explicit definitions of each expressions of the mutual information are provided later in the text). However for quantum systems the two expressions are not equal and their difference gives the quantum discord. In parallel to the concurrence, quantum discord measures the quantum correlations of a quantum system. In contrary to the concurrence, the quantum discord can be different to zero even if a quantum system is separable. The Werner state, $\rho_{\text{Werner}}=\frac{1-\lambda}{4}\mathbb{1}+\lambda|\Psi\rangle\langle\Psi|$, where λ is a parameter and $|\Psi\rangle=(|00\rangle+|11\rangle)/\sqrt{2}$, provides an example for which the concurrence is equal to zero (separable state) for $\lambda<1/3$ while the quantum discord is different to zero.[10] Hence quantum discord shows the existence of quantum correlations where concurrence shows that the system is separable. We point that the concurrence measures the *nonlocal quantumness* of correlations, while quantum discord measures the total *amount* of quantum correlations of a state ρ.

Quantum discord is used in several contexts[11,12] for its property to discernate quantum and classical correlations of quantum systems. The behavior of the quantum, as well as the classical correlations close to the critical points of QPTs, can be studied. We focus our attention here on the quantum phase transitions of the one-dimensional Ising model, which derives from the *XY* model and on the antiferromagnetic *XXZ* chain. Using the quantum discord we show that the *amount* of quantum correlations increases in the region close to the critical points. In opposite the *amount* of classical correlations close to the critical points decreases in the *XXZ* model while it is simply monotonous in the Ising model.

The outline of the paper is the following. In Sec. II we recall the elements of information theory which leads to the construction of quantum discord as demonstrated by Ollivier and Zurek.[10] In Secs. III and IV the quantum correlations close to the quantum phase transition of the Ising and *XXZ* models are studied. The Appendix provides the derivation of the quantum discord for spin $S=1/2$ chains.

II. QUANTUM DISCORD

Information on the correlations between two random variables $\mathcal{A}$ and $\mathcal{B}$ can be obtained by measure of the *mutual information*. In classical information theory the mutual information reads

$$\mathcal{I}(\mathcal{A};\mathcal{B}) = H(\mathcal{A}) + H(\mathcal{B}) - H(\mathcal{A},\mathcal{B}), \tag{1}$$

where the information entropy $H(\mathcal{A})=-\Sigma_a p_{\mathcal{A}=a}\log p_{\mathcal{A}=a}$ and $p_{\mathcal{A}=a}$ is the probability that a is the realization of the random variable $\mathcal{A}$. The joint entropy of $\mathcal{A}$ and $\mathcal{B}$ is defined by $H(\mathcal{A},\mathcal{B})=-\Sigma_{a,b}p_{\mathcal{A}=a,\mathcal{B}=b}\log p_{\mathcal{A}=a,\mathcal{B}=b}$, where $p_{\mathcal{A}=a,\mathcal{B}=b}$ is the joint probability of the variables $\mathcal{A}$ and $\mathcal{B}$ to take, respectively, the values a and b. Using the Bayes rule $p_{\mathcal{A},\mathcal{B}=b}=p_{\mathcal{B}=b}\times p_{\mathcal{A}|\mathcal{B}=b}$ the mutual information can be rewritten into the equivalent expression

$$\mathcal{J}(\mathcal{A};\mathcal{B}) = H(\mathcal{A}) - H(\mathcal{A}|\mathcal{B}), \tag{2}$$

where $H(\mathcal{A}|\mathcal{B})=-\Sigma_{a,b}p_{\mathcal{A}=a|\mathcal{B}=b}\log p_{\mathcal{A}=a|\mathcal{B}=b}$ is the conditional entropy of the random variables $\mathcal{A}$ and $\mathcal{B}$ and $p_{\mathcal{A}=a|\mathcal{B}=b}$ is the conditional probability of a being the realization of the random variable $\mathcal{A}$ knowing that b is the realization of the random variable $\mathcal{B}$. For classical random variables expressions (1) and (2) are strictly equivalent. However for quantum systems the two expressions of the mutual information are in general not equivalent and leads to define the quantum discord $\delta(\mathcal{A}:\mathcal{B})=\mathcal{I}(\mathcal{A};\mathcal{B})-\mathcal{J}(\mathcal{A};\mathcal{B})$ as demonstrated in Refs. 10 and 11. Quantum discord is the difference between the two classically equivalent expressions of the mutual information.

Mutual information expressions (1) and (2) for quantum systems are obtained by replacing the Shannon entropy by the von Neumann entropy. The von Neumann entropy for the joint state reads $H(\mathcal{A},\mathcal{B}) = -\mathrm{Tr}_{\mathcal{A},\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}} \ln \rho_{\mathcal{A},\mathcal{B}}$, where the trace runs over the Hilbert spaces of the subsystems $\mathcal{A}$ and $\mathcal{B}$, and $\rho_{\mathcal{A},\mathcal{B}}$ is the density matrix of the quantum system. In a similar way the entropy of the system $\mathcal{A}$ reads $H(\mathcal{A}) = -\mathrm{Tr}_{\mathcal{A}}\rho_{\mathcal{A}} \log \rho_{\mathcal{A}}$, where $\rho_{\mathcal{A}}$ is the reduced density matrix obtained by taking the trace over all states of the system $\mathcal{B}$, $\rho_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}}$. The quantum conditional entropy $H(\mathcal{A}|\mathcal{B})$ in Eq. (2) quantifies the ignorance of the state of $\mathcal{A}$ knowing the state of $\mathcal{B}$. It is worked out from the density matrix $\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}}$, which is related to the density matrix of the system $\rho_{\mathcal{A},\mathcal{B}}$ through[10]

$$\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}} = \Pi_j^{\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}}\Pi_j^{\mathcal{B}}/p_j,$$

where $\Pi_j^{\mathcal{B}}$ is the projector onto the state j of the subsystem $\mathcal{B}$ and the probability $p_j = \mathrm{Tr}_{\mathcal{A},\mathcal{B}}\Pi_j^{\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}}$. The quantum conditional entropy then reads $H(\mathcal{A}|\mathcal{B}) = H(\mathcal{A}|\{\Pi_j^{\mathcal{B}}\}) = \Sigma_j p_j H(\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}})$.

Finally the quantum discord measuring the quantum correlations between the two quantum subsystems $\mathcal{A}$ and $\mathcal{B}$ reads

$$\delta(\mathcal{A}:\mathcal{B}) = \min_{\{\Pi_j^{\mathcal{B}}\}}\{H(\mathcal{A}) - H(\mathcal{A},\mathcal{B}) + H(\mathcal{A}|\{\Pi_j^{\mathcal{B}}\})\}.$$

It must be noticed that the quantum discord is minimized over the set of state $\{\Pi_j^{\mathcal{B}}\}$. The information obtained on the subsystem $\mathcal{A}$ is affected by the measure on the state of the subsystem $\mathcal{B}$. In order to get the maximum information on the subsystem $\mathcal{A}$ we need to consider the projection onto the states of $\mathcal{B}$ that disturbs least the overall quantum system. Maximizing the information on the subsystem $\mathcal{A}$ corresponds to minimizing the quantum discord with respect to the set of projector $\{\Pi_j^{\mathcal{B}}\}$.

Quantum discord provides information on the quantum nature of the correlations between two systems. If two subsystems $\mathcal{A}$ and $\mathcal{B}$ are correlated *classically* the quantum discord is equal to zero. Moreover quantum discord shows that quantum correlations can be present for states that are not entangled. For example in Werner states the quantum correlations are still present while the system is separable.[10] To be more precise we can consider a quantum mixed state $\tilde{\rho} = |\psi\rangle\langle\psi|$ acting in an Hilbert space $\mathcal{H}_{\mathcal{A}} \otimes \mathcal{H}_{\mathcal{B}}$. The quantum mixed state is separable if its entanglement is equal to zero. In this case the quantum separable state can be written as a product of quantum states and reads $\tilde{\rho} = \Sigma_i p_i |\psi_{i,\mathcal{A}}\rangle\langle\psi_{i,\mathcal{A}}| \otimes \langle\psi_{i,\mathcal{B}}\rangle\langle\psi_{i,\mathcal{B}}|$, where $|\psi_{i,\mathcal{A}}\rangle \in \mathcal{H}_{\mathcal{A}}$, $|\psi_{i,\mathcal{B}}\rangle \in \mathcal{H}_{\mathcal{B}}$, and $\Sigma_i p_i = 1$. The two systems $\mathcal{A}$ and $\mathcal{B}$ can be correlated through the separable state $\tilde{\rho}$, and the quantum states $|\psi_{i,\mathcal{A}}\rangle$ and $|\psi_{i,\mathcal{B}}\rangle$ do not have in general any classical counterpart. A consequence of the quantumness of the states $|\psi_{\mathcal{A}}\rangle$ and $|\psi_{\mathcal{B}}\rangle$ is that the correlations between the two systems $\mathcal{A}$ and $\mathcal{B}$ have quantum as well as classical nature. The quantum discord is nonzero while the entanglement of the quantum separable state is equal to zero. A good example is furnished by the two-qubit separable mixed state[13]

$$\tilde{\rho} = \frac{1}{4}(|\psi_+\rangle\langle\psi_+|_{\mathcal{A}} \otimes |0\rangle\langle 0|_{\mathcal{B}} + |\psi_-\rangle\langle\psi_-|_{\mathcal{A}} \otimes |1\rangle\langle 1|_{\mathcal{B}} + |0\rangle\langle 0|_{\mathcal{A}} \otimes |\psi_-\rangle\langle\psi_-|_{\mathcal{B}} + |1\rangle\langle 1|_{\mathcal{A}} \otimes |\psi_+\rangle\langle\psi_+|_{\mathcal{B}}), \quad (3)$$

where $|\psi_\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle)$ and each qubit $\mathcal{A}$ and $\mathcal{B}$ have four nonorthogonal states. Two-qubit separable state (3) shows a product of quantum states that cannot have any equivalent classical system and also present quantum correlation. Quantum discord quantifies all quantum correlations including entanglement between $\mathcal{A}$ and $\mathcal{B}$.

Note that the mutual information $\mathcal{I}(\mathcal{A};\mathcal{B})$ is the sum of the quantum discord and the classical correlation $CC(\mathcal{A};\mathcal{B})$ defined in Ref. 14, $\mathcal{I}(\mathcal{A};\mathcal{B}) = \delta(\mathcal{A}:\mathcal{B}) + CC(\mathcal{A};\mathcal{B})$. In other words classical correlations $CC(\mathcal{A};\mathcal{B})$ are equal to the mutual information $\mathcal{J}(\mathcal{A};\mathcal{B})$.

Using quantum discord to discernate the quantum from the classical correlations we can study the behavior of such different correlations in quantum phase transitions. In Secs. III and IV we focus our attention on the quantum phase transitions of the Ising and the *XXZ* spin-1/2 chains and we study them using the quantum discord.

III. QUANTUM DISCORD AND QUANTUM PHASE TRANSITION IN THE ISING CHAIN

The Hamiltonian of the transverse one-dimensional Ising model reads

$$H_{\mathrm{Ising}} = -\sum_{i=1}^{N}(\lambda\sigma_i^x\sigma_{i+1}^x + \sigma_i^z),$$

with the boundary condition $\sigma_N^x = \sigma_1^x$ and σ^α with $\alpha = \{x,y,z\}$ as the Pauli matrices and $\sigma^0 = \mathbb{1}$. We denote by $|g\rangle = |\uparrow\rangle$ and $|e\rangle = |\downarrow\rangle$ the spin-up and spin-down states. For $\lambda = 0$ all spins are pointing in the z direction while for $\lambda \to \infty$ they point in the x direction. In the thermodynamic limit $N \to \infty$ the Ising spin chain undergoes a quantum phase transition at the critical point $\lambda_c = 1$. The correlation length diverges at this point.[6,7]

The quantum discord is worked out from the joint state of the two spins at the lattice sites i and j. The information on the joint state is contained in the two-site density matrix ρ_{ij}, which is derived from the following operator expansion:

$$\rho_{ij} = \mathrm{Tr}_{\overline{ij}}[\rho] = \frac{1}{4}\sum_{\alpha,\beta=0}^{3}\Theta_{\alpha\beta}\sigma_i^\alpha \otimes \sigma_j^\beta,$$

where the coefficients $\Theta_{\alpha\beta}$ of the expansion are related to the spin-spin correlation functions through the relation

$$\Theta_{\alpha\beta} = \mathrm{Tr}[\sigma_i^\alpha\sigma_j^\beta\rho_{ij}] = \langle\sigma_i^\alpha\sigma_j^\beta\rangle.$$

Owing to the symmetry of the Hamiltonian most of the coefficients $\Theta_{\alpha\beta}$ are equal to zero. Translation invariance requires that the density matrix verifies $\rho_{ij} = \rho_{i,i+r}$ and is independent of the position i. The reflection symmetry leads to $\rho_{ij} = \rho_{ji}$, the Hamiltonian being real, the density matrix verifies $\rho_{ij}^* = \rho_{ij}$, and the global rotation symmetry implies that the density matrix commutes with the operator $\sigma_i^z\sigma_j^z$. Combining

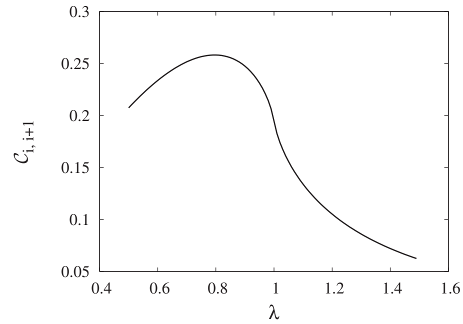

FIG. 1. Concurrence for nearest-neighbor spins in the Ising spin $S=1/2$ chain. The concurrence is maximal close to the critical coupling $\lambda_c=1$.

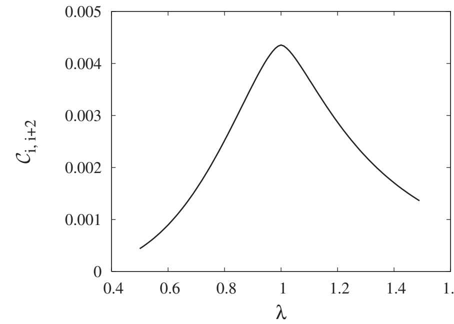

FIG. 2. Concurrence for next-nearest-neighbor spins in the Ising spin chain. The concurrence is maximal at the critical coupling $\lambda_c=1$.

all symmetry constraints the density matrix expressed in the natural basis $\{|gg\rangle,|ge\rangle,|eg\rangle,|ee\rangle\}$ reduces to[6]

$$\rho_{ij}=\begin{pmatrix} u_+ & 0 & 0 & y \\ 0 & w & x & 0 \\ 0 & x & w & 0 \\ y & 0 & 0 & u_- \end{pmatrix}, \tag{4}$$

with $u_\pm=\frac{1}{4}\pm\frac{\langle\sigma^z\rangle}{2}+\frac{\langle\sigma_i^z\sigma_j^z\rangle}{4}$, $w=\frac{1-\langle\sigma_i^z\sigma_j^z\rangle}{4}$, $x=\frac{\langle\sigma_i^x\sigma_j^x\rangle+\langle\sigma_i^y\sigma_j^y\rangle}{4}$, and $y=\frac{\langle\sigma_i^x\sigma_j^x\rangle-\langle\sigma_i^y\sigma_j^y\rangle}{4}$. The magnetization of the spin-1/2 Ising chain is given by[15]

$$\langle\sigma^z\rangle=-\frac{1}{\pi}\int_0^\pi d\phi\frac{(1+\lambda\cos\phi)}{\omega_\phi},$$

and $\omega_\phi=\sqrt{(\lambda\sin\phi)^2+(1+\lambda\cos\phi)^2}$ is the energy spectrum of the transverse Ising chain. The spin-spin correlations functions are related to the determinant of Toeplitz matrices[16]

$$\langle\sigma_i^x\sigma_{i+r}^x\rangle=\begin{vmatrix} G_{-1} & G_{-2} & \dots & G_{-r} \\ G_0 & G_{-1} & \dots & G_{-r+1} \\ \vdots & \vdots & \ddots & \vdots \\ G_{r-2} & G_{r-3} & \dots & G_{-1} \end{vmatrix},$$

$$\langle\sigma_i^y\sigma_{i+r}^y\rangle=\begin{vmatrix} G_1 & G_0 & \dots & G_{-r+2} \\ G_2 & G_1 & \dots & G_{-r+3} \\ \vdots & \vdots & \ddots & \vdots \\ G_r & G_{r-1} & \dots & G_1 \end{vmatrix},$$

and $\langle\sigma_i^z\sigma_{i+r}^z\rangle=\langle\sigma^z\rangle^2-G_rG_{-r}$, where

$$G_\kappa=\frac{1}{\pi}\int_0^\pi d\phi\cos(\phi\kappa)\frac{(1+\lambda\cos\phi)}{\omega_\phi}-\frac{\lambda}{\pi}\int_0^\pi d\phi\sin(\phi\kappa)\frac{\sin\phi}{\omega_\phi}.$$

The quantum phase transition can be signaled by measure of entanglement. Indeed the nearest- and next-nearest-neighbors entanglement reach their maximum at the critical point λ_c.[3,7] A good measure of the entanglement is provided by the concurrence $\mathcal{C}$. The concurrence of two spins may be computed from the joint state ρ_{ij} through the formula $\mathcal{C}=\max\{0,\gamma_1-\gamma_2-\gamma_3-\gamma_4\}$, where the γ_i are the eigenvalues in decreasing order of the matrix $R=\sqrt{\rho_{ij}\widetilde{\rho_{ij}}}$.[8,9] The matrix $\widetilde{\rho_{ij}}$ is related to the transpose of the two-site density matrix by $\widetilde{\rho_{ij}}=(\sigma^y\otimes\sigma^y)\rho_{ij}^*(\sigma^y\otimes\sigma^y)$. Hence the entanglement between two spins at site i and j is given by

$$\mathcal{C}_{ij}=2\max\{0,|x|-\sqrt{u_+u_-},|y|-w\}.$$

Figures 1 and 2 represent, respectively, the concurrence for the nearest-neighbor spins $\mathcal{C}_{i,i+1}$ and next-nearest-neighbor spins $\mathcal{C}_{i,i+2}$. It shows that the maximum of entanglement is reached close to $\lambda_c=1$. Only the derivatives of the concurrence show singularities at the critical points,[3] signaling the presence of the quantum phase transition.

Entanglement increases close to the quantum phase transition. However entanglement is only one kind of quantum correlation. It is then legitimate to ask: What is the behavior of the *total amount* of quantum correlations close to the critical point of the QPT? The answer is provided by the quantum discord. The details of the derivation of the quantum discord are given in the Appendix. Figure 3 represents the quantum discord for the Ising $S=1/2$ chain for nearest neighbor $\delta_{i,i+1}$ and next-nearest neighbor $\delta_{i,i+2}$. It shows that the quantum correlations increase and are maximal in a region close to the critical point λ_c.

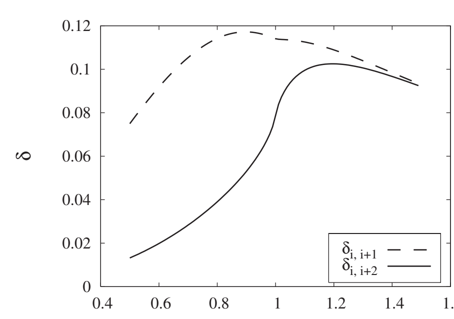

FIG. 3. Quantum discord δ for the nearest-neighbor (in dashed line) and next-nearest-neighbor (in full line) spin sites of the one-dimensional Ising model. The quantum discord is minimized for $\phi=0$ and θ varying progressively from zero for $\lambda<1$ to $\pi/4$ for $\lambda>1$ (see the Appendix for the details on the derivation).

More information on the location and the order of the quantum phase transition can be obtained by consideration of the derivatives of the quantum discord with respect to the coupling parameter λ. Indeed there is a relation between the nonanalyticity in energy and quantum discord that leads to the characterization of the quantum phase transition.[17] Considering the energy of the spin system in terms of the reduced density matrix of two spins at positions i and j, the energy reads

$$E(\rho_{ij}) = \sum_{ij} \mathrm{Tr}[\widetilde{H}_{ij}\rho_{ij}], \qquad (5)$$

where $\widetilde{H}_{ij}$ is the reduced Hamiltonian of the two spins at positions i and j. The sum of $\widetilde{H}_{ij}$ over the positions i,j is equal to the Hamiltonian of the spin system, $\Sigma_{ij}\widetilde{H}_{ij} \equiv H$. For the one-dimensional Ising model the reduced Hamiltonian reads $\widetilde{H}_{ij}^{\mathrm{Ising}} = -(\lambda\sigma_i^x\sigma_j^x\widetilde{\delta}_{i+1,j} + \sigma_i^z/N)$, where N is the number of spins and $\widetilde{\delta}_{ij}$ is the Kronecker delta. The order as well as the location of a quantum phase transition can be characterized by the nonanalyticity of the energy. If the first derivative of the ground-state energy presents a finite discontinuity then the quantum phase transition is of the first order. However if the first derivative is continuous while the second derivative shows discontinuity or divergence, then the quantum phase transition is of the second order. Moreover the derivatives of the energy are related to the derivatives of the reduced density matrix, and one can show that[17]

$$\frac{\partial E(\rho_{ij})}{\partial\lambda} = \sum_{ij} \mathrm{Tr}\left[\frac{\partial\widetilde{H}_{ij}}{\partial\lambda}\rho_{ij}\right],$$

$$\frac{\partial^2 E(\rho_{ij})}{\partial\lambda^2} = \sum_{ij}\left\{\mathrm{Tr}\left[\frac{\partial^2\widetilde{H}_{ij}}{\partial\lambda^2}\rho_{ij}\right] + \mathrm{Tr}\left[\frac{\partial\widetilde{H}_{ij}}{\partial\lambda}\frac{\partial\rho_{ij}}{\partial\lambda}\right]\right\}.$$

Note that the derivatives of the reduced Hamiltonian are continuous with respect to the coupling parameter λ. Hence a discontinuity in the first derivative $\frac{\partial E(\rho_{ij})}{\partial\lambda}$ of the energy at the critical point implies a discontinuity at least of one of the reduced density matrices ρ_{ij}. Similarly a discontinuity or a singularity in the second derivatives of the energy $\frac{\partial^2 E(\rho_{ij})}{\partial\lambda^2}$ requires the divergence of at least one of the derivatives $\frac{\partial\rho_{ij}}{\partial\lambda}$ at the critical points. It now becomes evident that the quantum phase transition can be characterized by an analysis of the derivatives of the quantum discord with respect to the coupling parameter λ. With the quantum discord being dependent on the reduced density matrix, one deduces that (i) a discontinuity in the quantum discord implies a discontinuity in ρ_{ij} (hence the first derivative of the energy is discontinuous) and a first-order QPT, and (ii) a singularity in the derivative of the quantum discord implies a discontinuity or a divergence of $\frac{\partial\rho_{ij}}{\partial\lambda}$ (the second derivative of the energy is discontinuous) and the QPT is of the second order.

Figure 4 shows that for nearest neighbors $\partial\delta_{i,i+1}/\partial\lambda$ presents a discontinuity at the critical point and for the next-nearest neighbors $\partial\delta_{i,i+2}/\partial\lambda$ shows a singularity. The fact that the quantum discord is continuous while its derivatives are discontinuous or singular at $\lambda=\lambda_c$ indicates that the precise location of the critical point is at $\lambda_c=1$ and that the QPT is of the second order.

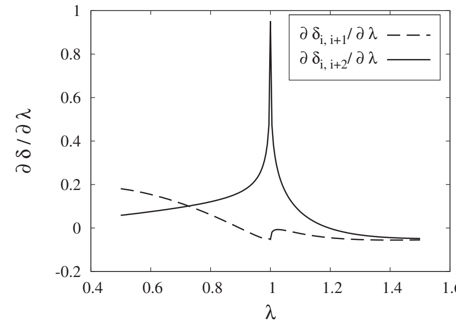

FIG. 4. First derivatives of the quantum discord with respect to the coupling parameter λ for the nearest-neighbor (in dashed line) and next-nearest-neighbor (in full line) spin sites of the one-dimensional Ising model.

For $\lambda > 1$ and approaching the critical point from the right, the classical correlations decrease in opposite to the quantum discord, which increases as depicted by Figs. 3 and 5. For $\lambda < 1$ both classical and quantum correlations are decreasing when the coupling parameter λ decreases. Classical correlations monotonically increase with respect to λ while quantum discord shows that the amplitude of the quantum correlations increases close to the critical point λ_c. From the mutual information we infer that the spins are uncorrelated for $\lambda \to 0$ as depicted in Fig. 6 and can be confirmed by the Hamiltonian which reduces to $H_{\mathrm{Ising},\lambda=0} = -\Sigma_{i=1}^N \sigma_j^z$. Close to the critical point the *amount* of quantum correlations is maximal as supported by the concurrence.

IV. QUANTUM DISCORD AND QUANTUM PHASE TRANSITION IN THE *XXZ* CHAIN

The Hamiltonian of the one-dimensional *XXZ* spin-1/2 chain reads

$$H_{XXZ} = \sum_{\langle ij\rangle} (S_i^x S_j^x + S_i^y S_j^y + \Delta S_i^z S_j^z),$$

where the sum runs over the nearest-neighbor bonds $\langle ij\rangle$. At the critical point $\Delta_c=1$ the *XXZ* spin chain undergoes a quan-

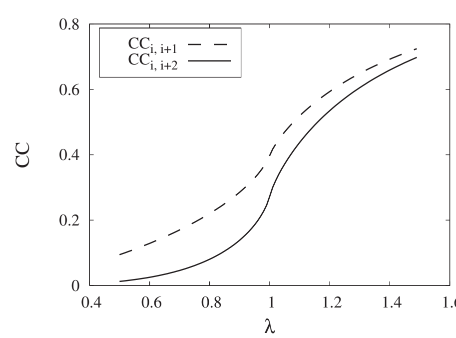

FIG. 5. Classical correlation *CC* for the nearest-neighbor (in dashed line) and next-nearest-neighbor (in full line) spin sites of the one-dimensional Ising model.

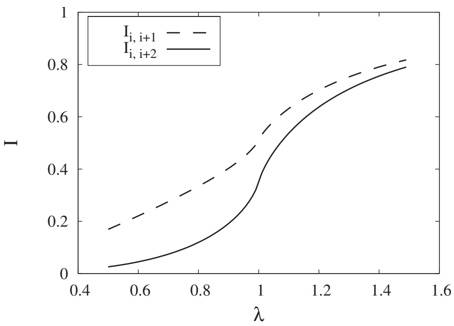

FIG. 6. Mutual information $\mathcal{I}(\mathcal{A};\mathcal{B})$ for the nearest-neighbor (in dashed line) and next-nearest-neighbor (in full line) spin sites of the one-dimensional Ising model.

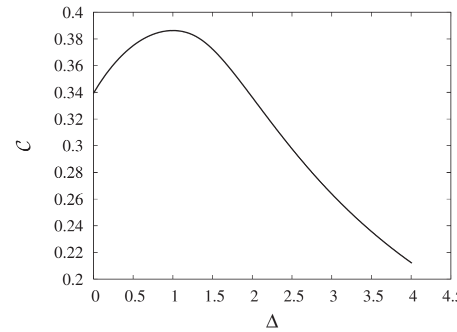

FIG. 7. Concurrence for nearest-neighbor spin sites in the *XXZ* spin $S=1/2$ one-dimensional model.

tum phase transition between an *XY* phase for $-1<\Delta<1$ and an Ising antiferromagnetic phase for $\Delta>1$.

The density matrix of two nearest-neighbor spin sites is given by Eq. (4). However owing to the spin-flip symmetry the magnetization is equal to zero, $\langle\sigma^z\rangle=0$, and the *XXZ* Hamiltonian is also symmetric with respect to the rotation in the *xy* plan, which leads to the equality between the spin-spin correlation function in the *xy* plan $\langle\sigma_i^x\sigma_j^x\rangle=\langle\sigma_i^y\sigma_j^y\rangle$. Gathering all the symmetry constraints of the *XXZ* Hamiltonian the joint density matrix ρ_{ij} reduces to

$$\rho_{ij}=\begin{pmatrix} u & 0 & 0 & 0\\ 0 & w & x & 0\\ 0 & x & w & 0\\ 0 & 0 & 0 & u\end{pmatrix},$$

with $u_\pm=u=\frac{1}{4}+\frac{\langle\sigma_i^z\sigma_j^z\rangle}{4}$, $w=\frac{1-\langle\sigma_i^z\sigma_j^z\rangle}{4}$, $x=\frac{\langle\sigma_i^x\sigma_j^x\rangle}{2}$, and $y=0$.

The spin-spin correlation functions between nearest-neighbor spin sites for $-1<\Delta<1$ are given by[18–20]

$$\langle\sigma_i^x\sigma_{i+1}^x\rangle=\frac{\cos\pi\Phi}{\pi^2}\int_{-\infty}^{\infty}\frac{dx}{\sinh x}\frac{x\cosh x}{\cosh^2(\Phi x)} - \frac{1}{\pi\sinh(\pi\Phi)}\int_{-\infty}^{\infty}\frac{dx}{\sinh x}\frac{\sinh[(1-\Phi)x]}{\cosh\Phi x},$$

where $\Delta=\cos(\pi\Phi)$, and

$$\langle\sigma_i^z\sigma_{i+1}^z\rangle=1-\frac{2}{\pi^2}\int_{-\infty}^{\infty}\frac{dx}{\sinh x}\frac{x\cosh x}{\cosh^2(\Phi x)} + \frac{2\cot(\pi\Phi)}{\pi}\int_{-\infty}^{\infty}\frac{dx}{\sinh x}\frac{\sinh[(1-\Phi)x]}{\cosh\Phi x}.$$

Also for $\Delta>1$ the correlation functions are given by[21–23]

$$\langle\sigma_i^x\sigma_{i+1}^x\rangle=\int_{-\infty+i/2}^{\infty+i/2}\frac{dx}{\sinh(\pi x)}\left(\frac{x}{\sin^2(\phi x)}\cosh\nu-\frac{\cot(\nu x)}{\sinh\nu}\right),$$

with $\Delta=\cosh\nu$, and

$$\langle\sigma_i^z\sigma_{i+1}^z\rangle=1+2\int_{-\infty+i/2}^{\infty+i/2}\frac{dx}{\sinh(\pi x)} \times\left(\cot(\nu x)\coth(\nu)-\frac{x}{\sin^2(\nu x)}\right).$$

The concurrence for the *XXZ* spin-1/2 chain is given by $\mathcal{C}=2\max\{0,|x|-|u|\}$. Figure 7 represents the dependence of the concurrence with respect to the control parameter Δ and shows that entanglement between the nearest-neighbor spin sites is maximal at the critical point $\Delta_c=1$.[6]

In parallel the quantum discord presents the maximum of the quantum correlations at the critical point. The derivation of the quantum discord for the *XXZ* model follows the same scheme as for the Ising model and the details of the derivation are provided in the Appendix. Figure 8 depicts the dependence of the quantum discord on the control parameter Δ. The quantum discord is minimized with respect to the angles ϕ and θ that control the axes of the projector $\Pi_j^{\mathcal{B}}$.

As depicted in Fig. 8 the quantum correlations are stronger close to the QPT. On the opposite the classical correlations are weaker close to the critical point Δ_c. Both classical and quantum correlations measured by quantum discord and the mutual information $\mathcal{J}(\mathcal{A};\mathcal{B})$ behave accordingly to the behavior of entanglement measured by the concurrence.

The cusps observed in Figs. 8 and 9 for both the classical correlation and the quantum discord arise from a level crossing between the ground-state energy and an excited-state en-

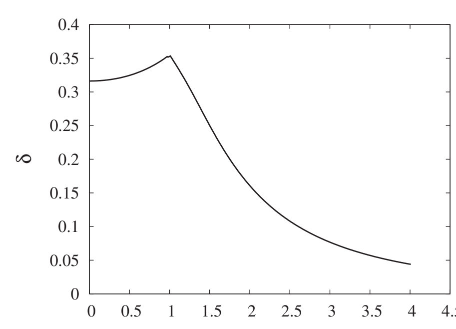

FIG. 8. Quantum discord for nearest-neighbor spins in the *XXZ* spin $S=1/2$ one-dimensional model. The quantum discord is minimized for $\phi=0$ and θ varying progressively from zero for $\lambda<1$ to $\pi/4$ for $\lambda>1$ (see the Appendix for the details on the derivation).

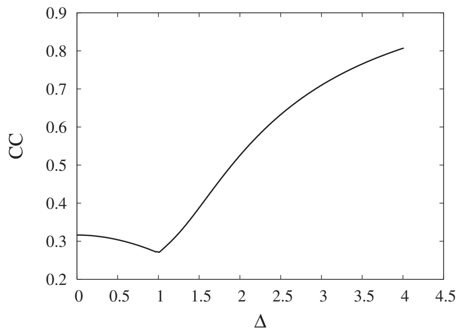

FIG. 9. Dependence of the classical correlation $CC(\mathcal{A};\mathcal{B})$ on the parameter Δ for the nearest-neighbor spin sites in the XXZ spin $S=1/2$ chain.

ergy. This scheme explains the cusp observed in the concurrence measuring the entanglement of nearest-neighbor spin in $(d \geq 2)$-dimensional XXZ model.[4] A similar mechanism explains also the fact that the concurrence is maximal at the critical points for the one-dimensional XXZ model.[24] Level crossing induces a qualitative change in the ground states at the critical point $\Delta_c=1$ and leads to the abrupt behavior of the quantum discord and classical correlation at the quantum phase transition. As depicted in Fig. 7 the concurrence is less sensitive to the level crossing than the quantum discord and the classical correlations since it does not present an abrupt cusp at Δ_c.

Remark that the quantum discord for the next-nearest-neighbor spins $\delta_{i,i+2}$ is not presented for the 1D XXZ model. The reason is that no more information can be gained by $\delta_{i,i+2}$ than already furnished by the quantum discord for nearest neighbors $\delta_{i,i+1}$. Indeed the quantum discord $\delta_{i,i+2}$ presents a similar dependence on the coupling parameter Δ as shown by $\delta_{i,i+1}$ and its amplitude verifies $\delta_{i,i+1} \sim 2\delta_{i,i+2}$.

V. CONCLUSION

Quantum phase transitions of the one-dimensional spin-1/2 Ising and antiferromagnetic XXZ models have been studied using the quantum discord.[10,11] Quantum discord is a measure of the quantum correlation given by the difference of two classically equivalent expressions of the mutual information. Using quantum discord and mutual information we showed that it is possible to discernate the quantum and the classical nature of the correlations between two elements of a quantum many-body system.

We demonstrated that the amount of quantum correlations is larger close to the critical points for the quantum phase transitions of the one-dimensional XXZ and Ising models. For the XXZ model the amount of classical correlations decreases at the critical point while for the Ising model they are simply monotonous with respect to the coupling parameter λ. The behaviors of the quantum and classical correlations measured by means of the quantum discord are in agreement with the behavior of the entanglement computed by the concurrence for both spin models.

Quantum discord is a good way to discernate the nature of the correlations between the components of a quantum system, and it is a good qualitative indicator of the existence of quantum phase transition. However depending on the model studied the maximum of the quantum discord is not necessarily located at the critical points as shown for the Ising model. The quantum discord can only be used for qualitative detection of quantum phase transitions. On the contrary the derivatives of the quantum discord provide precise information on the location and on the order of the quantum phase transitions. Quantum discord[10,11] and concurrence[4–7] are two useful tools to detect quantum phase transitions. Despite the fact that implementation of concurrence is more easy and/or rapid than for quantum discord, concurrence measures only the nonlocal quantumness of the correlations between two systems $\mathcal{A}$ and $\mathcal{B}$. Quantum discord measures the total amount of quantum correlations between $\mathcal{A}$ and $\mathcal{B}$ including entanglement.

We showed that quantum discord agrees with the predictions provided by the concurrence for the behavior of the quantum correlations close to quantum phase transitions for one-dimensional quantum systems. It would be interesting to confirm this observation in future investigation of quantum systems with higher dimensionality.

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APPENDIX: DERIVATION OF THE QUANTUM DISCORD FOR SPIN CHAINS

The quantum discord for two systems reads $\delta(\mathcal{A}:\mathcal{B}) = \min_{\{\Pi_j^{\mathcal{B}}\}}\{H(\mathcal{A}) - H(\mathcal{A},\mathcal{B}) + H(\mathcal{A}|\{\Pi_j^{\mathcal{B}}\})\}$ for which the three von Neumann entropies are computed over, respectively, the reduced density matrix $\rho_{\mathcal{A}}$, the joint state $\rho_{\mathcal{A},\mathcal{B}}$, and the conditional density matrix $\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}}$.

The reduced density matrix $\rho_{\mathcal{A}}$ is given by

$$\rho_{\mathcal{A}} = \mathrm{Tr}_{\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}} = (u_+ + w)|g\rangle\langle g|_{\mathcal{A}} + (u_- + w)|e\rangle\langle e|_{\mathcal{A}},$$

which leads to the von Neumann entropy of the reduced density matrix

$$\begin{aligned} H(\mathcal{A}) &= -\mathrm{Tr}_{\mathcal{A}}\rho_{\mathcal{A}} \log \rho_{\mathcal{A}} \\ &= -\frac{1}{2}(1+\langle\sigma^z\rangle)\log\left[\frac{1}{2}(1+\langle\sigma^z\rangle)\right] \\ &\quad -\frac{1}{2}(1-\langle\sigma^z\rangle)\log\left[\frac{1}{2}(1-\langle\sigma^z\rangle)\right]. \end{aligned} \tag{A1}$$

The joint density matrix is equal to the density matrix given in Eq. (4) $\rho_{\mathcal{A},\mathcal{B}} = \rho_{ij}$, and the von Neumann entropy is given by the sum of the Shannon entropy over the eigenvalues of the density matrix ρ_{ij} and reads

$$H(\mathcal{A},\mathcal{B}) = -\mathrm{Tr}_{\mathcal{A},\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}} \log \rho_{\mathcal{A},\mathcal{B}} = -(w+x)\log(w+x) - (w-x)\log(w-x) - \sum_{\epsilon=\pm} \Xi_\epsilon \log \Xi_\epsilon, \tag{A2}$$

where

$$\Xi_\pm = \frac{1}{2}\{(u_+ + u_-) \pm [(u_+ - u_-)^2 + 4y^2]^{1/2}\}.$$

The conditional density matrix $\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}}$ is given by projection on the arbitrary basis

$$|g\rangle_{\mathcal{B}} = \cos(\theta)|j_1\rangle_{\mathcal{B}} + e^{i\phi}\sin(\theta)|j_2\rangle_{\mathcal{B}},$$

$$|e\rangle_{\mathcal{B}} = e^{-i\phi}\sin(\theta)|j_1\rangle_{\mathcal{B}} - \cos(\theta)|j_2\rangle_{\mathcal{B}}.$$

The angles ϕ and θ control the projectors direction and the quantum discord is minimized with respect to these angles.

The conditional entropy is then given by

$$\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}} = \Pi_j^{\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}}\Pi_j^{\mathcal{B}}/p_j,$$

with $\Pi_{j_{\alpha=1,2}}^{\mathcal{B}} = \mathbb{1}_{\mathcal{A}} \otimes |j_\alpha\rangle\langle j_\alpha|_{\mathcal{B}}$ and $p_{j_\alpha} = \mathrm{Tr}_{\mathcal{A},\mathcal{B}}\mathbb{1}_{\mathcal{A}} \otimes |j_\alpha\rangle\langle j_\alpha|_{\mathcal{B}}\rho_{\mathcal{A},\mathcal{B}}$.

For the projection onto the state $|j_\alpha\rangle$ where $\alpha=1,2$, one gets

$$\rho_{\mathcal{A}|\Pi_{j_\alpha}^{\mathcal{B}}} = |j_\alpha\rangle\langle j_\alpha|_{\mathcal{B}} \otimes \{|g\rangle\langle g|_{\mathcal{A}}X_{j_\alpha,+} + |e\rangle\langle e|_{\mathcal{A}}X_{j_\alpha,-} + |g\rangle\langle e|_{\mathcal{A}}Y_{j_\alpha} + |e\rangle\langle g|_{\mathcal{A}}\bar{Y}_{j_\alpha}\}/p_{j_\alpha}, \tag{A3}$$

where for $\alpha=1$,

$$X_{j_1,+} = [u_+ \cos^2(\theta) + w\sin^2(\theta)],$$

$$X_{j_1,-} = [u_- \sin^2(\theta) + w\cos^2(\theta)],$$

$$Y_{j_1} = (e^{-i\phi}x + ye^{i\phi})\sin(\theta)\cos(\theta),$$

and with $p_{j_1} = \frac{1}{2}[1+\langle\sigma^z\rangle\cos(2\theta)]$. For the projection onto the state $|j_2\rangle$ the elements $X_{j_2,\pm}$ are given by

$$X_{j_2,+} = [u_+ \sin^2(\theta) + w\cos^2(\theta)],$$

$$X_{j_2,-} = [u_- \cos^2(\theta) + w\sin^2(\theta)],$$

$$Y_{j_2} = -(e^{-i\phi}x + ye^{i\phi})\sin(\theta)\cos(\theta),$$

and with $p_{j_2} = \frac{1}{2}[1-\langle\sigma^z\rangle\cos(2\theta)]$. The eigenvalues $\Psi_{j_\alpha,\pm}$ of conditional density matrix (A3) reads $\Psi_{j_\alpha,\pm} = \frac{1}{2p_{j_\alpha}}\{(X_{j_\alpha,+} + X_{j_\alpha,-}) \pm [(X_{j_\alpha,+} - X_{j_\alpha,-})^2 + 4Y_{j_\alpha}\bar{Y}_{j_\alpha}]^{1/2}\}$.

Finally the conditional von Neumann entropy reads

$$H(\mathcal{A}|\{\Pi_j^{\mathcal{B}}\}) = \sum_{j=1,2} -p_j\mathrm{Tr}_{\mathcal{A}}\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}}\log\rho_{\mathcal{A}|\Pi_j^{\mathcal{B}}} = -\sum_{\epsilon=\pm}\sum_{j=1,2} p_j\Psi_{j,\epsilon}(\phi,\theta)\log\Psi_{j,\epsilon}(\phi,\theta). \tag{A4}$$

The quantum discord is minimized with respect to the angles ϕ and θ that control the direction of the projector $\Pi_j^{\mathcal{B}}$ in the Hilbert space of the subsystem $\mathcal{B}$. The minimization must be achieved for each ensemble of values of the magnetization and the spin-spin correlations function which defines the joint density matrix. It can be shown numerically that for the one-dimensional Ising and antiferromagnetic *XXZ* models, the set of angles $\{\phi,\theta\}$ that minimize the quantum discord belong to the ranges $\phi=0$, $\theta\in[0,\pi/4]$.

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