Quantum and classical correlations in the one-dimensional *XY* model with Dzyaloshinskii-Moriya interaction

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(Received 11 December 2010; published 12 May 2011)

We study the effect of Dzyaloshinskii-Moriya (DM) interaction on pairwise quantum discord, entanglement, and classical correlation in the anisotropic *XY* spin-half chain. Analytical expressions for both quantum and classical correlations are obtained from the spin-spin correlation functions. These pairwise quantities exhibit interesting behaviors in relation to the relative strengths of the physical parameters. For the infinite chain, we show that the quantum discord can be useful to highlight the quantum phase transition, especially for the long-distance spins, where entanglement decays rapidly. We observe nonanalyticities of the derivatives of both quantum and classical correlations with respect to the magnetic intensity at the critical point; interestingly, the DM interaction weakens the critical behavior in the derivatives of these correlations. While the DM interaction suppresses the standard behaviors of the *XY* model, it enhances surprisingly the pairwise entanglement for the third nearest neighbor spins.

DOI: 10.1103/PhysRevA.83.052112 PACS number(s): 03.65.Ud, 03.65.Ta, 75.10.Jm, 03.67.Mn

I. INTRODUCTION

Entanglement, at the heart of quantum reality, has received great attention in various branches of quantum physics [1,2], mostly because of its promising features exhibited in quantum information processing. While interest remains strong, recent research has explored nonclassical correlations other than entanglement, which may be employed as alternative resources for quantum technology [3–6]. Among the quantum correlations, the quantum discord introduced by Ollivier and Zurek [4] has been studied relatively comprehensively and is supposed to characterize all of the nonclassical correlations in a bipartite state, including entanglement. While in pure states it coincides with the entanglement entropy, the quantum discord does not vanish in mixed separable states, even if entanglement is absent. This unique feature suggests that quantum correlations, in particular quantum discord, may have significant applications in revealing the advantage of certain quantum tasks and may be a more comprehensive resource than entanglement [7–21], as demonstrated, for example, by their behaviors in quantum critical phenomena. It was interesting to note that quantum discord, in contrast to entanglement, is able to signal the Kosterlitz-Thouless quantum phase transitions [22,23]. Moreover, study on pairwise quantum discord in the thermodynamic limit of the *XY* chain shows that quantum discord for spin pairs farther than second neighbors could still signal a quantum phase transition (QPT), while the corresponding pairwise entanglement vanishes [24].

This paper studies the behaviors of both quantum and classical correlations in the anisotropic *XY* spin-half chain with Dzyaloshinskii-Moriya (DM) interaction [25] $\sum_{\langle ij\rangle}\vec{D}_{ij}(\vec{S}_i\times\vec{S}_j)$, which arises from the spin-orbit coupling. Despite being small, this interaction can generate interesting effects [26,27] and is crucial to the description of many antiferromagnetic systems, such as $Cu(C_6D_5COO)_2\cdot 3D_2O$ [28], Yb_4As_3 [29], $BaCu_2Si_2O_7$ [30], and $K_2V_3O_8$ [31]. It also plays a significant role in quantum dots [32] and in performing universal quantum computation [33,34]. The behaviors of entanglement in spin chains [35,36] with DM interaction were studied extensively. The influence of DM interaction on quantum phase interference of spins was discussed [37]. The entanglement transfer in a spin chain with DM interaction was examined [38,39]. Now, we study the role of the important interaction in the behaviors of the quantum discord.

This paper is arranged as follows. Section II introduces the anisotropic *XY* spin chain with DM interaction and describes briefly the techniques of correlation functions used to obtain our results. We analyze the behaviors of quantum and classical correlations under the influence of the DM interaction in Sec. III. We conclude our work in Sec. IV.

II. QUANTUM AND CLASSICAL CORRELATIONS IN THE *XY* CHAIN WITH DM INTERACTION

Consider the anisotropic *XY* spin-half chain with DM interaction in the z direction,

$$H=\sum_{j=1}^{N}\{J[(1+\gamma)S_j^xS_{j+1}^x+(1-\gamma)S_j^yS_{j+1}^y + D(S_j^xS_{j+1}^y-S_j^yS_{j+1}^x)]-S_j^z\}, \tag{1}$$

where S_j^α ($\alpha=x,y,z$) are the spin-half operators at the jth lattice site, N is the total number of spins, and the periodic boundary conditions ($S_{N+1}^\alpha=S_1^\alpha$) are used. The parameter γ characterizes the degree of anisotropy, D denotes the intensity of the DM interaction along the z direction, and J is the strength of the inverse of the external transverse magnetic field.

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The two-spin density matrix ρ_{ij} for this system in the computational basis $(|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle)$ is given by [40]

$$\rho_{ij} = \begin{pmatrix} u_{ij}^{+} & 0 & 0 & y_{ij} \\ 0 & \omega_{ij}^{+} & x_{ij} & 0 \\ 0 & x_{ij} & \omega_{ij}^{-} & 0 \\ y_{ij} & 0 & 0 & u_{ij}^{-} \end{pmatrix}, \tag{2}$$

where matrix elements can be written in terms of one- and two-point correlation functions,

$$u_{ij}^{\pm} = \frac{1}{4} \pm \frac{\langle S_i^z \rangle}{2} \pm \frac{\langle S_j^z \rangle}{2} + \langle S_i^z S_j^z \rangle, \tag{3}$$

$$\omega_{ij}^{\pm} = \frac{1}{4} \mp \frac{\langle S_i^z \rangle}{2} \pm \frac{\langle S_j^z \rangle}{2} - \langle S_i^z S_j^z \rangle, \tag{4}$$

$$x_{ij} = \langle S_i^x S_j^x \rangle + \langle S_i^y S_j^y \rangle, \tag{5}$$

$$y_{ij} = \langle S_i^x S_j^x \rangle - \langle S_i^y S_j^y \rangle, \tag{6}$$

where for this model we calculate the concrete form of the magnetization density $\langle S_j^z \rangle$ at site j and obtain an analytical expression,

$$\langle S_j^z \rangle = -\frac{1}{N} \sum_{p>0}^{N/2} \frac{\tanh(\beta\Delta/2)}{\Delta} [J(\cos\phi_p - 2D\sin\phi_p) - 1], \tag{7}$$

where $\Delta = \sqrt{[J(\cos\phi_p - 2D\sin\phi_p) - 1]^2 + J^2\gamma^2 \sin^2\phi_p}$ with $\phi_p = 2\pi p/N$, $p = -N/2, \ldots, N/2$, and $\beta = 1/kT$ where k is the Boltzmann constant and T is the absolute temperature. When the system is translation invariant, we obtain $\langle S_i^z \rangle = \langle S_j^z \rangle$ $(\forall i,j)$ such that $\omega_{ij}^{+} = \omega_{ij}^{-}$. By using the method in Refs. [41] and [42], one can obtain analytical two-point correlation functions $\langle S_i^\alpha S_j^\beta \rangle$ $(\alpha,\beta = x,y,z)$ between sites i and j,

$$\langle S_i^x S_j^x \rangle = \frac{1}{4} \begin{vmatrix} G_{-1} & G_{-2} & \cdots & G_{i-j} \\ G_0 & G_{-1} & \cdots & G_{i-j+1} \\ \cdots & \cdots & \cdots & \cdots \\ G_{j-i-2} & G_{j-i-3} & \cdots & G_{-1} \end{vmatrix}, \tag{8}$$

$$\langle S_i^y S_j^y \rangle = \frac{1}{4} \begin{vmatrix} G_1 & G_0 & \cdots & G_{i-j+2} \\ G_2 & G_1 & \cdots & G_{i-j+3} \\ \cdots & \cdots & \cdots & \cdots \\ G_{j-i} & G_{j-i-1} & \cdots & G_1 \end{vmatrix}, \tag{9}$$

and

$$\langle S_i^z S_j^z \rangle = \langle S^z \rangle^2 - \frac{1}{4} G_{j-i} G_{i-j}. \tag{10}$$

For our model in Eq. (1), we derive the analytical forms of G_R,

$$G_R = -\frac{1}{N} \sum_{p>0}^{N/2} 2\cos(\phi_p R)[J(\cos\phi_p - 2D\sin\phi_p) - 1] \times \frac{\tanh(\beta\Delta/2)}{\Delta} + \frac{\gamma}{N} \sum_{p>0}^{N/2} 2J\sin(\phi_p R)\sin\phi_p \frac{\tanh(\beta\Delta/2)}{\Delta}, \tag{11}$$

where $R = j - i = 1,2,3,\ldots$ after tedious calculations. When $N \to \infty$, and $T = 0$, $\tanh(\beta\Delta/2) = 1$, and the limit values can be obtained by replacing ϕ_p with ϕ and the sum with the integral $\frac{1}{2\pi}\int_0^\pi d\phi$. On the basis of Eqs. (7) and (11) derived by us, we can give the eigenvalues of the density matrix ρ_{ij},

$$\lambda_1 = \tfrac{1}{4}\left(1 - 4\langle S_i^x S_j^x \rangle - 4\langle S_i^y S_j^y \rangle - 4\langle S_i^z S_j^z \rangle\right), \tag{12}$$

$$\lambda_2 = \tfrac{1}{4}\left(1 + 4\langle S_i^x S_j^x \rangle + 4\langle S_i^y S_j^y \rangle - 4\langle S_i^z S_j^z \rangle\right), \tag{13}$$

$$\lambda_3 = \tfrac{1}{4}\left[1 - 4\sqrt{\left(\langle S_i^x S_j^x \rangle - \langle S_i^y S_j^y \rangle\right)^2 + \langle S^z \rangle^2} + 4\langle S_i^z S_j^z \rangle\right], \tag{14}$$

$$\lambda_4 = \tfrac{1}{4}\left[1 + 4\sqrt{\left(\langle S_i^x S_j^x \rangle - \langle S_i^y S_j^y \rangle\right)^2 + \langle S^z \rangle^2} + 4\langle S_i^z S_j^z \rangle\right]. \tag{15}$$

We now briefly review the definition of the pairwise quantum discord. A bipartite quantum state ρ_{ij} contains both classical and quantum correlations, and the total correlations are measured jointly by quantum mutual information. The total correlations between subsystems i and j are

$$\mathcal{I}(\rho_{ij}) = S(\rho_i) + S(\rho_j) - S(\rho_{ij}), \tag{16}$$

where $\rho_{i(j)} = \mathrm{Tr}_{j(i)}(\rho_{ij})$ is the reduced density matrix of the subsystem $i(j)$ and $S(\rho) = \mathrm{Tr}\rho\log_2\rho$ is the von Neumann entropy. The quantum discord is defined as the difference between the total correlations and the classical correlation,

$$\mathcal{D}_Q(\rho_{ij}) = \mathcal{I}(\rho_{ij}) - \mathcal{C}_C(\rho_{ij}), \tag{17}$$

where the classical correlation $\mathcal{C}_C(\rho_{ij})$ between the subsystems is given by [43]

$$\mathcal{C}_C(\rho_{ij}) = S(\rho_i) - \min_{\{P_\kappa\}}\left[p_\kappa S(\rho_i^\kappa)\right], \tag{18}$$

where $\{P_\kappa\}$ is a set of projects performed locally on the subsystem j and $\rho_i^\kappa = \mathrm{Tr}_j[(I_i \otimes P_\kappa)\rho_{ij}(I_i \otimes P_\kappa)]/p_\kappa$ is the quantum state of the subsystem i conditioned on the measurement outcome labeled by κ, with probability $p_\kappa = \mathrm{Tr}[(I_i \otimes P_\kappa)\rho_{ij}(I_i \otimes P_\kappa)]$. Here, I_i is the identity operator for the subsystem i. The mutual information in Eq. (16) reads

$$\mathcal{I}(\rho_i : \rho_j) = 2(-\eta_1\log\eta_1 - \eta_2\log\eta_2) + \sum_{\upsilon=1}^{4}\lambda_\upsilon\log\lambda_\upsilon, \tag{19}$$

where $\eta_{1,2} = 1/2 \pm \langle S_i^z \rangle$ and λ_υ $(\upsilon = 1,2,3,4)$ correspond to eigenvalues of the reduced density matrices ρ_i and ρ_{ij}, respectively. The condition $S(\rho_i) = S(\rho_j)$ is satisfied such that the measurement of classical correlation assumes equal values, irrespective of whether the measurement is performed on site i or j. Here, we consider the complete set of orthogonal projectors $\{P_\kappa(\theta,\phi) = I \otimes |\kappa\rangle\langle\kappa|\}$ $(\kappa = 1,2)$ for a local measurement performed on site j, where the two projectors are defined by the spin states

$$|1\rangle = \cos\theta|\uparrow\rangle + e^{i\phi}\sin\theta|\uparrow\rangle, \tag{20}$$

$$|2\rangle = \sin\theta|\uparrow\rangle - e^{i\phi}\cos\theta|\downarrow\rangle. \tag{21}$$

It is straightforward to calculate the quantum discord [19]

$$\mathcal{D}_Q(\rho_{ij}) = \min\{\mathcal{D}_{Q1}, \mathcal{D}_{Q2}\}, \tag{22}$$

where

$$\mathcal{D}_{Q1} = S(\rho_i) - S(\rho_{ij}) - u_{ij}^{+} \log\left(\frac{u_{ij}^{+}}{u_{ij}^{+} + \omega_{ij}}\right) - \omega_{ij} \log\left(\frac{\omega_{ij}}{u_{ij}^{+} + \omega_{ij}}\right) - u_{ij}^{-} \log\left(\frac{u_{ij}^{-}}{u_{ij}^{-} + \omega_{ij}}\right) - \omega_{ij} \log\left(\frac{\omega_{ij}}{u_{ij}^{-} + \omega_{ij}}\right) \quad (23)$$

and

$$\mathcal{D}_{Q2} = S(\rho_i) - S(\rho_{ij}) - \frac{1+\Lambda}{2}\log\frac{1+\Lambda}{2} - \frac{1-\Lambda}{2}\log\frac{1-\Lambda}{2}, \quad (24)$$

with $\Lambda = \sqrt{(u_{ij}^{+} - u_{ij}^{-})^2 + 4(|x_{ij}| + |y_{ij}|)^2}$.

The quantum discord is a measure of nonclassical correlations. It may include but is independent of entanglement. For pure states and a mixture of Bell states, the quantum discord is equivalent to the entanglement entropy. However, for general

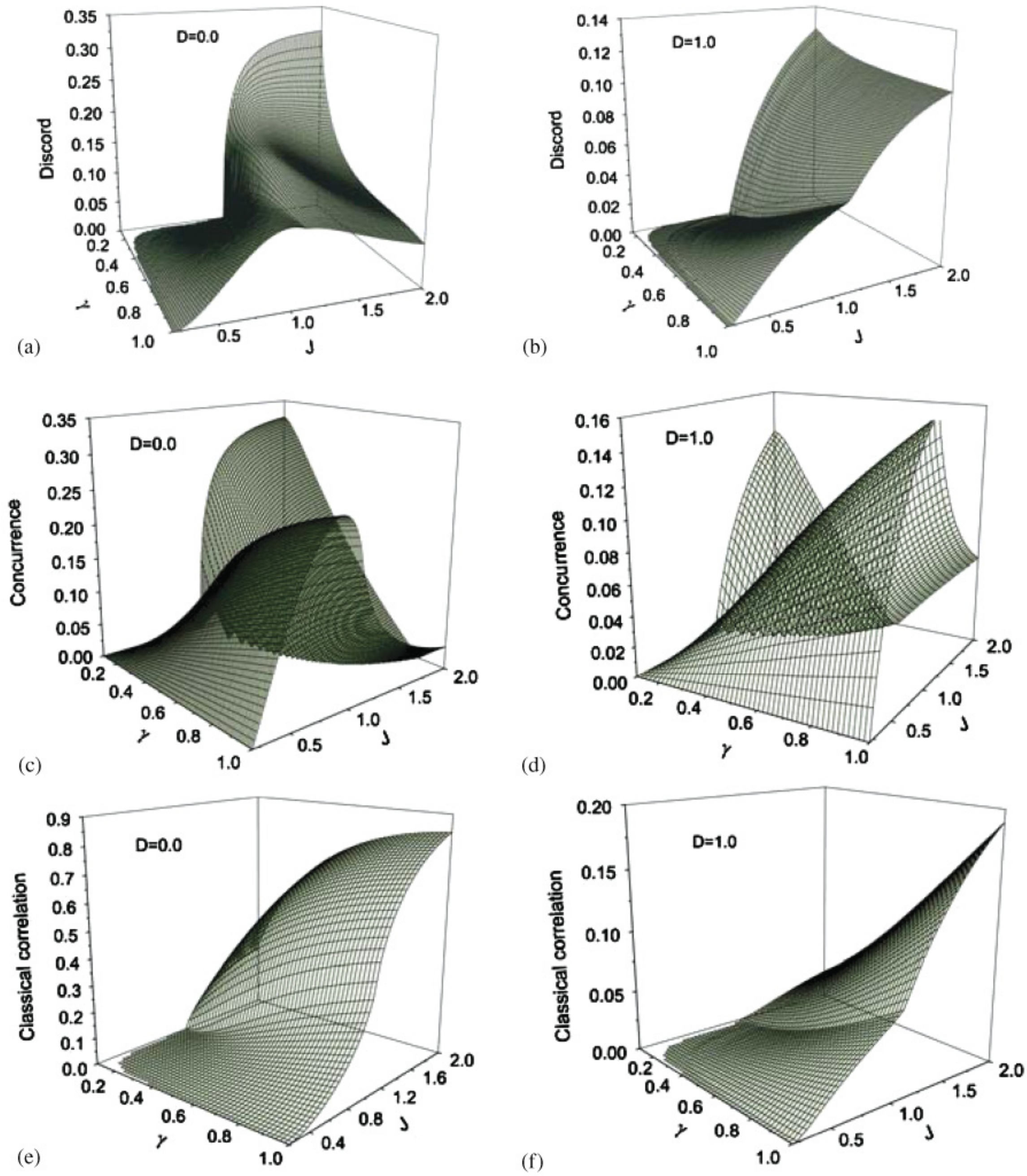

FIG. 1. (Color online) Quantum discord (a) and (b), entanglement (c) and (d), and classical correlation (e) and (f) for the nearest-neighbor spins in the XY spin chain as a function of anisotropy γ and magnetic intensity J at zero temperature for different values of DM interaction.

two-qubit mixed states, the correspondence between them is much more complicated. The following work will focus on the quantum discord, entanglement, and classical correlation in the anisotropic XY spin-half chain with DM interaction. We use concurrence as the measure of entanglement [44], defined by

$$C(\rho_{ij}) = \max\{\varsigma_1 - \varsigma_2 - \varsigma_3 - \varsigma_4, 0\}, \tag{25}$$

where ς_μ ($\mu = 1,2,3,4$) are the square roots of the eigenvalues in descending order of the operator $R_{ij} = \rho_{ij}\tilde{\rho}_{ij}$, $\tilde{\rho}_{ij} = (\sigma_i^y \otimes \sigma_j^y)\rho_{ij}^*(\sigma_i^y \otimes \sigma_j^y)$, with ρ_{ij}^* being the conjugate of ρ_{ij} and $\sigma_{i(j)}^y$ being the y component of the Pauli matrix for site i or j. The concurrence of the density matrix in Eq. (2) is

$$C(\rho_{ij}) = 2\max\{0, |x_{ij}| - \sqrt{u_{ij}^+ u_{ij}^-}, |y_{ij}| - \omega_{ij}\}. \tag{26}$$

In the thermodynamic limit, we plot the pairwise quantum discord, entanglement, and classical correlation in the XY chain for different values of DM interaction in Figs. 1(a)–1(f), respectively. Figures 1(a) and 1(b) show that there is a clear difference in quantum discord between the two regions $J \in [0,1]$ and $J \in [1,2]$. The quantum phase transition occurs at the critical point $J = 1$. When $J \leqslant 1$, the quantum discord increases with anisotropy and reaches its maximum at the point $\gamma = 1$. When $J > 1$, the quantum discord decays monotonously with anisotropy.

We now turn our attention to the effect of the DM interaction on quantum discord. It seems that the quantum discord is suppressed by the DM interaction. Furthermore, in the absence of anisotropy, quantum discord is insensitive to the DM interaction.

Before the numerical details are explored, it is interesting to note that there is a family of Hamiltonians containing the DM interaction, which leads to the same entanglement and discord [34]. In this family, the Hamiltonians are subject to single-spin unitary transformations,

$$W = \prod_{j=1}^{N} \exp\left[-i\left(\alpha_j S_j^x + \beta_j S_j^y + \delta_j S_j^z\right)\right], \tag{27}$$

such that $H' = WHW^\dagger$, where α_j, β_j, and δ_j are independent angles. For instance, if $W = \prod_{j=2,4,6,\ldots} \exp[-i\pi/2S_j^z]$ where j is even, the Hamiltonian in Eq. (1) can be rewritten as

$$H' = \sum_{j=1}^{N}\{J[-(1+\gamma)S_j^x S_{j+1}^y + (1-\gamma)S_j^y S_{j+1}^x + D(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y)] - S_j^z\}. \tag{28}$$

The DM interaction plays a special role in the isotropic XY model when $\gamma = 0$. On the basis of the following relations,

$$\exp\left(-i\vartheta S_j^z\right) S_j^x \exp\left(i\vartheta S_j^z\right) = S_j^x \cos\vartheta + S_j^y \sin\vartheta, \tag{29}$$

$$\exp\left(-i\vartheta S_j^z\right) S_j^y \exp\left(i\vartheta S_j^z\right) = -S_j^x \sin\vartheta + S_j^y \cos\vartheta, \tag{30}$$

the transformation $W = \prod_{j=2,4,6,\ldots} \exp[i\vartheta S_j^z]$ transfers the isotropic XY chain into

$$H' = \sum_{j=1}^{N}\{J'[S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + D'(S_j^x S_{j+1}^y - S_j^y S_{j+1}^x)] - S_j^z\}, \tag{31}$$

where $J' = J\cos\vartheta$ and $D' = \tan\vartheta$. It implies that the DM force in the isotropic case is given by single-spin transformation and does not make a significant contribution to the entanglement and quantum discord.

The pairwise entanglement for the general Hamiltonian in Eq. (1) is displayed in Figs. 1(c) and 1(d). As shown in the figures, the influence of the anisotropy γ on the entanglement is different between the $J < 1$ region and the $J > 1$ region. The DM interaction in the XY spin chain suppresses the pairwise entanglement and the pairwise quantum discord. In contrast to the quantum discord and entanglement, the classical correlation always increases with anisotropy as shown in the last subfigures of Fig. 1.

Figure 2 displays the quantum discord (dotted line), entanglement (dashed line), and classical correlation (solid line) as a function of J for the nearest-neighbor spins in the transverse Ising model ($\gamma = 1$) with different values of the DM interaction. It is clear that, in this particular case, both classical and quantum correlations are suppressed by the DM interaction. While the concurrence is initially larger than the quantum discord and classical correlation and then decreases, the quantum discord is always less than the classical

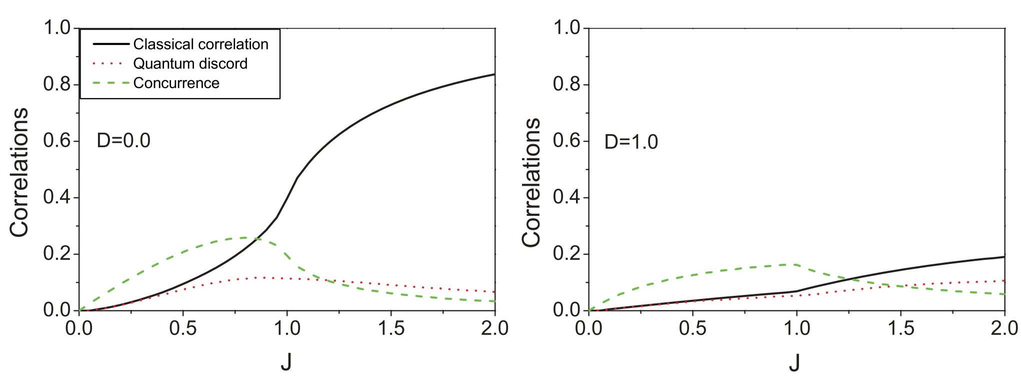

FIG. 2. (Color online) Quantum discord (dotted line), entanglement (dashed line), and classical correlation (solid line) as a function of J for the nearest-neighbor spins in the transverse Ising chain. (a) $D = 0.0$ and (b) $D = 1.0$ with $T = 0$.

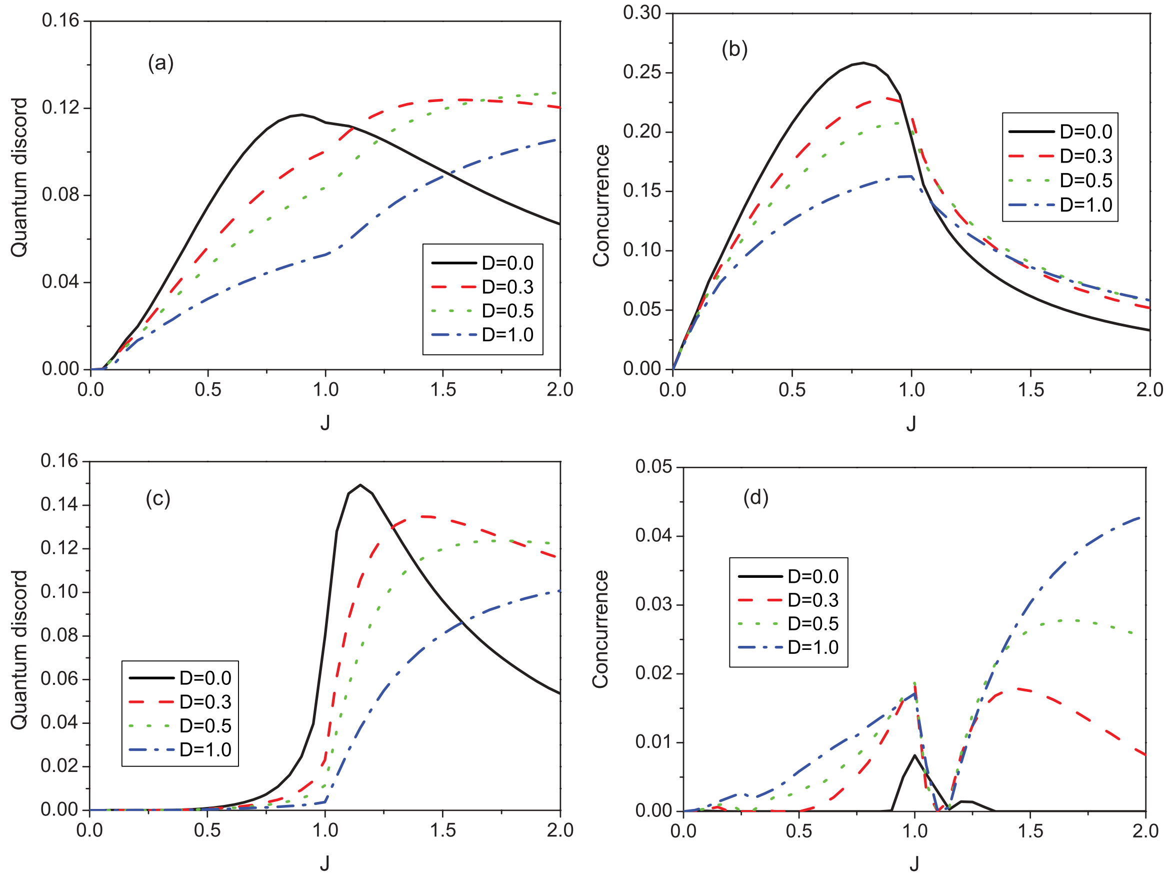

FIG. 3. (Color online) Quantum discord (a) and entanglement (b) for the nearest-neighbor spins as a function of J for different DM interaction, when $\gamma = 1.0$ and $T = 0$. (c) (d) Cases of the pairwise quantum correlations for the third nearest neighbor spins, when $\gamma = 0.5$.

correlation. Therefore, it is reasonable to conclude that the quantum discord is a measure independent of entanglement and the three correlations are substantially different qualitatively and quantitatively, as also noticed in a recent paper [12].

In order to better understand the DM interaction, we plot pairwise quantum discord and entanglement versus J, with different DM interaction in Fig. 3. The pairwise quantum discord shows distinct behaviors when the parameter D varies. In the region $J \in (0,1]$, the quantum discord can be suppressed by the DM interaction. As the DM interaction increases, quantum discord decreases. In the region $J \in [1,2]$, the pairwise quantum discord without the DM interaction decays monotonously. However, when the DM interaction is present, the situation becomes more complicated, as shown in this figure.

The entanglement for nearest-neighbor spins is presented in Fig. 3(b). The concurrence always has its maximum around the critical point $J = 1$, regardless of the DM interaction.

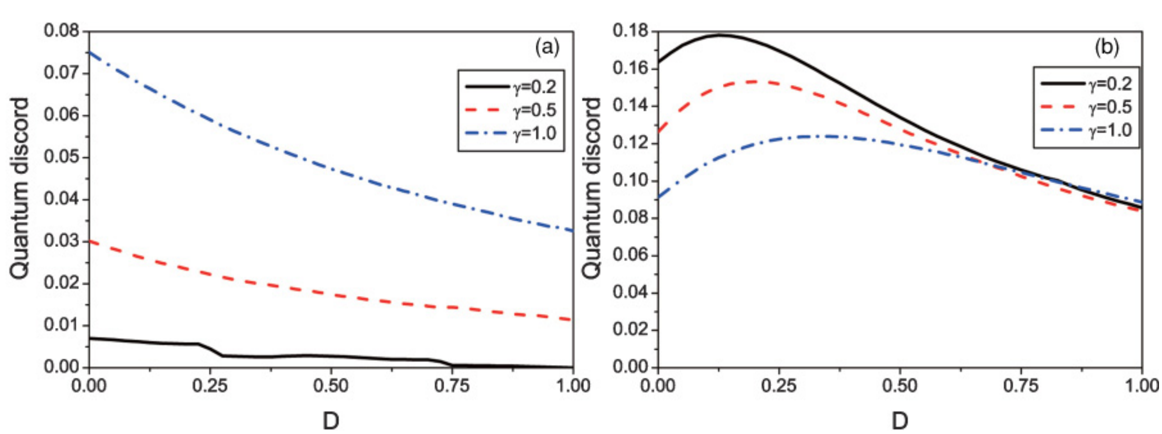

FIG. 4. (Color online) Quantum discord for the nearest-neighbor spins in the XY spin chain as a function of the DM interaction with different values of anisotropy, $T = 0$. (a) $J = 0.5$. (b) $J = 1.5$.

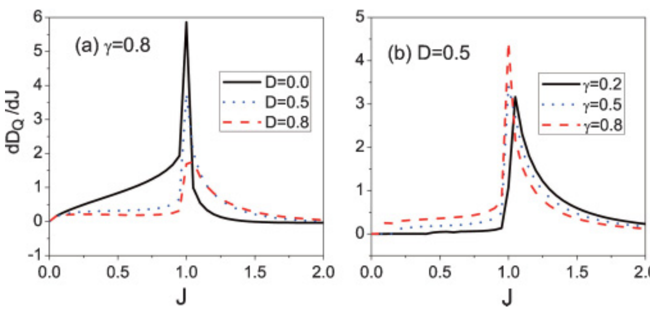

FIG. 5. (Color online) First derivative of the quantum discord for the nearest-neighbor spins with respect to J (a) for different values of DM interaction with $\gamma = 0.8$ and $T = 0$ and (b) for different values of anisotropy with $D = 0.5$.

When $J < 1$, the DM interaction restraints the growth of entanglement, while it rarely changes the decay rate of entanglement in the $J > 1$ region.

The quantum correlations decrease expectedly as the site distance increases. We plot the quantum discord and entanglement for third nearest neighbor spins with the anisotropy parameter $\gamma = 0.5$ in Figs. 3(c) and 3(d). The pairwise entanglement is tiny ($C_{\max} \approx 0.04$) or disappears completely for most of values of γ. In contrast, the quantum discord remains nonzero even for farther site distances. This may make quantum discord more promising in many aspects of quantum physics, such as being an indicator to a quantum phase transition [24]. Moreover, we observe that without the DM interaction the entanglement is zero, except in the vicinity of the critical point, as depicted in Fig. 3(d). It is interesting to note that the DM interaction enhances the concurrence greatly, which may imply that the DM interaction is able to promote long-distance entanglement.

Figure 4 shows the quantum discord versus the DM interaction for different values of $J$and anisotropy γ. When $J < 1$, the quantum discord as a function of D decays monotonously. When$J > 1$, curves of quantum discord have peaks at $D \approx 0.25$. This again supports the argument that

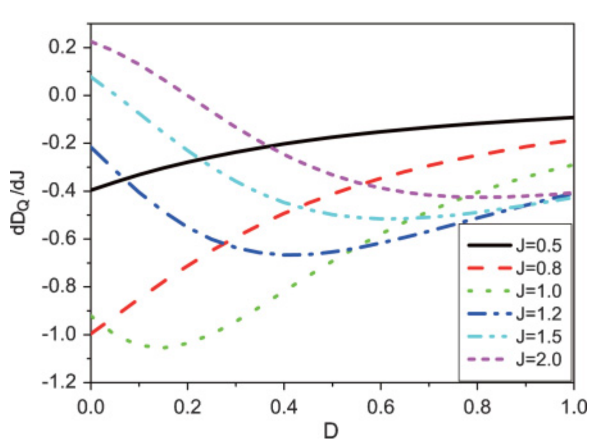

FIG. 6. (Color online) First derivative of the quantum discord with respect to the DM interaction for different values of J with $\gamma = 1$ and $T = 0$. Here, no singularity occurs.

the quantum discord is enhanced in the $J \in (0,1]$ region but reduced in the $J > 1$ region as anisotropy increases.

There exists a known second-order quantum phase transition at $J = 1$ in the model in Eq. (1). In Fig. 5, we plot the first derivative of the nearest-neighbor quantum discord with respect to J for different strengths of the DM interaction and anisotropy around the critical point. As expected, the nonanalyticities of dD_Q/dJ indicate a quantum phase transition at the critical point $J = 1$ for different values of both DM interaction and anisotropy. It is interesting to note that the DM interaction weakens the discontinuities in the derivative of quantum discord. However, the anisotropy may sharpen the singularities to some degree. As known in Ref. [35], the DM interaction does not change the universal class of the quantum phase transition of the present model.

Figure 6 plots dD_Q/dD as a function of the DM interaction. While no nonanalyticity is expected, as shown previously in Ref. [35], the derivative of quantum discord with respect to the DM interaction, dD_Q/dD, shows distinct behaviors for different regions of J. Specifically, it has minima when J is around the critical point, while it is monotonic elsewhere.

III. CONCLUSIONS

We have studied the pairwise quantum discord, entanglement, and classical correlation for the anisotropy XY spin-half chain with DM interaction. The quantum correlations increase monotonously with anisotropy in the $J < 1$ region, while in the $J > 1$ region the quantum correlations may decrease as anisotropy increases. In contrast, the pairwise classical correlation always increases with anisotropy. For the infinite chain, the quantum discord for the third nearest neighbor spins can still detect the QPT, whereas pairwise entanglement cannot achieve the same feat.

The DM interaction is the central topic of this paper. Our analysis shows that while the DM interaction suppresses the standard behaviors of the anisotropic XY model, it enhances the values of long-distance entanglement surprisingly. When the anisotropy parameter is very small, the quantum correlation is not significantly affected by the DM interaction, as shown generally in our family of Hamiltonians. The role of the DM interaction can also be understood by analyzing the derivative of quantum discord with respect to J and the DM interaction, respectively. While the singularities in dD_Q/dJ at the critical point $J = 1$ indicate the quantum phase transition, they are weakened and smoothened by the DM interaction. The derivatives of entanglement dC/dJ and the classical correlation $d\mathcal{C}_C/dJ$ have similar behaviors.

ACKNOWLEDGMENTS

We acknowledge financial support by the National Natural Science Foundation of China under Grant Nos. 11075013 and 10974016. L.-A. Wu has been supported by the Ikerbasque Foundation Start-up, the Basque Government (Grant IT472-10), and the Spanish Ministerio de Educación y Ciencia (MEC) (Project No. FIS2009-12773-C02-02). We thank Dr. Ping Lou and Dr. M. S. Sarandy for helpful suggestions.

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