Dzyaloshinskii-Moriya interaction and anisotropy effects on the entanglement of the Heisenberg model

M. Kargarian,[1] R. Jafari,[2,3] and A. Langari[1]
[1]*Department of Physics, Sharif University of Technology, Tehran 11155-9161, Iran*
[2]*Institute for Advanced Studies in Basic Sciences, Zanjan 45195-1159, Iran*
[3]*School of Physics, Institute for Studies in Theoretical Physics and Mathematics (IPM), 19395-5531, Tehran, Iran*
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In this paper the effect of Dzyaloshinskii-Moriya interaction and anisotropy on the entanglement of Heisenberg chain has been studied. While the anisotropy suppresses the entanglement due to favoring of the alignment of spins, the DM interaction restores the spoiled entanglement via creation of the quantum fluctuations. Thermodynamic limit of the model and emerging of nonanalytic behavior of the entanglement have also been probed. The singularities of the entanglement correspond to the critical boundary separating different phases of the model. The singularity of the entanglement derivative approaches the critical point from the gapped phase and will be symmetric if both phases on the boundary are gapped.

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I. INTRODUCTION

In recent years, the notion of entanglement has received much attention in quantum information theory due to its important features in developing the idea of quantum computers and other quantum information devices. Entanglement is a purely quantum correlation without classical counterpart [1] and has been realized as a crucial resource to process and send information in different ways such as quantum teleportation, supercoding, and algorithms for quantum computations [2]. Concerning the correlation content of the entanglement, the states of systems in condensed-matter physics may deserve the investigation of entanglement as a unique measure of quantum correlations. Interest will be intensified when we consider the relation between entanglement and quantum phase transition where a drastic change in the ground state of the system occurs [3]. This change will occur at zero temperature where all thermal fluctuations get frozen and only surviving quantum fluctuations drive the phase transition. In the past few years the subject of many activities was to investigate the role of entanglement in the vicinity of quantum critical point for different spin models [4–13].

Spin models provide not only a test ground for the mentioned issues but also a playground for implementation of many quantum information protocols [14,15]. Among them are Ising model in transverse field (ITF) and anisotropic Heisenberg (*XXZ*) models. Despite their simple Hamiltonian, low-energy behavior of many systems can be captured through them. Ising model in transverse field has the benefit of exact solvability by mapping to free fermions [3]. Such solvability provides the possibility to test the behavior of entanglement and its scaling close to the quantum critical point of the system and performs a finite-size scaling as has been done in the seminal work of Osterloh *et al.* [4]. The scenario is different in the *XXZ* model where the entanglement between the two nearest-neighbor sites develops a maximum at the isotropic point ($\Delta=1$) without any singularity in its first derivative [16] which vanishes at the critical point $\Delta=1$. However, the block-block entanglement [17] of the spin-1/2 *XX* model with three-spin and uniform long-range interactions shows a logarithmic and algebraic dependence on the size of block for different phases. Logarithmic divergences of the entanglement entropy is a general feature of all one-dimensional critical systems where the coefficient of the logarithm is just the central charge of the underlying critical theory [18].

The scaling of entanglement close to the phase transition and its connection to the universality class of the model can be further investigated through employing the renormalization group (RG). This method, as we will see in Secs. II and IV, provides a rather analytic framework for treating the phases of the model even for those that are beyond the exact solution. In this stream the scaling of the entanglement governs the critical exponents of the model [19,20]. However, the renormalization of quantum states has also been introduced in terms of matrix product states [21].

Both ITF and *XXZ* models can be supplemented with a magnetic term, the so-called Dzyaloshinskii-Moriya (DM) interaction, arising from the spin-orbit coupling. Based on the symmetry aspects [22], it can be derived microscopically as a linear correction to the standard superexchange mechanism [23]. The interaction has the form $\Sigma_{\langle ij\rangle}\vec{D}_{ij}\cdot(\vec{S_i}\times\vec{S_j})$ where the sum is over the pairs of spins. Some quantum antiferromagnetic (AF) systems are expected to be described by the DM interaction with the underlying helical magnetic structures. Ising model with DM interaction was extensively studied [24]. The DM interaction drives the quantum fluctuations resulting in a phase transition in the model. Quantum critical point separates the antiferromagnetic and chiral phases. The derivative of the entanglement diverges at the quantum critical point with the critical exponent of the model.

In this paper we address the behavior of the entanglement in the *XXZ* model with DM interaction. Including the DM interaction makes the phase diagram rich with a critical line instead of a single point [25]. First, we employ the quantum renormalization group to have a tractable problem. Afterward, the entanglement between degrees of freedom is treated through the renormalization of concurrence. We will see that the derivative of entanglement becomes singular at the phase boundary and its scaling correspond to the gapless and gapped phases of the model. The organization of the paper is as follows. In Sec. II we briefly introduce the renormalization-group approach. In Sec. III we exemplify the effect of anisotropy and DM interaction. Then, in Sec. IV we turn on to discuss the scaling of the entanglement, and finally Sec. V is devoted to conclusions.

II. QUANTUM RENORMALIZATION GROUP

The quantum renormalization group presents a tractable version of treating quantum systems at zero temperature. Implementing the renormalization the original model Hamiltonian is replaced by an effective one in the cost of renormalizing coupling constants. In this way the original Hilbert space is truncated to a reduced Hilbert space including the effective degrees of freedom. Getting rid of less important degrees of freedom gives rise to the flow of the coupling constants in the parameter space of the model. The version we employ to kill the degrees of freedom is Kadanoff's block approach since it is well suited to perform analytical calculations in the lattice models and they are conceptually easy to be extended to higher dimensions [26–29]. In Kadanoff's method, the lattice is divided into blocks in which the Hamiltonian is exactly diagonalized. By selecting a number of low-lying eigenstates of the blocks the full Hamiltonian is projected onto these eigenstates giving the effective (renormalized) Hamiltonian.

The Hamiltonian of the *XXZ* model with DM interaction in the z direction on a periodic chain of N sites is

$$H(J,\Delta) = \frac{J}{4}\sum_{i}^{N} [\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta\sigma_i^z\sigma_{i+1}^z + D(\sigma_i^x\sigma_{i+1}^y - \sigma_i^y\sigma_{i+1}^x)], \quad D,J,\Delta > 0. \tag{1}$$

We divide the chain into blocks each containing three sites. The block Hamiltonian ($H_B=\Sigma h_I^B$) of the three sites and its eigenstates and eigenvalues are given in Appendix A of Ref. [25]. However, we give only the degenerate ground states since we need them for the evaluation of entanglement and subsequent discussions as follows:

$$|\psi_0\rangle = \frac{1}{\sqrt{2q(q+\Delta)(1+D^2)}}\{2(D^2+1)|\downarrow\downarrow\uparrow\rangle - (1-iD)(\Delta+q)|\downarrow\uparrow\downarrow\rangle - 2[2iD+(D^2-1)]|\uparrow\downarrow\downarrow\rangle\}, \tag{2}$$

$$|\psi_0'\rangle = \frac{1}{\sqrt{2q(q+\Delta)(1+D^2)}}\{2(D^2+1)|\downarrow\uparrow\uparrow\rangle - (1-iD)(\Delta+q)|\uparrow\downarrow\uparrow\rangle - 2[2iD+(D^2-1)]|\uparrow\uparrow\downarrow\rangle\}, \tag{3}$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are eigenstates of the σ^z Pauli operator and $q=\sqrt{\Delta^2+8(1+D^2)}$. The projection operator of the ground-state subspace is defined by ($P_0=|\Uparrow\rangle\langle\psi_0|+|\Downarrow\rangle\langle\psi_0'|$), where $|\psi_0\rangle$ and $|\psi_0'\rangle$ are the doubly-degenerate ground states and $|\Uparrow\rangle$ and $|\Downarrow\rangle$ are the renamed base kets in the effective Hilbert space. We have kept two states ($|\psi_0\rangle$ and $|\psi_0'\rangle$) for each block to define the effective (new) site. Thus, the effective site can be considered as a spin $\frac{1}{2}$. The effective Hamiltonian is similar to the initial one, i.e.,

$$H^{\text{eff}} = \frac{J'}{4}\sum_{i}^{N} [\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y + \Delta'\sigma_i^z\sigma_{i+1}^z + D'(\sigma_i^x\sigma_{i+1}^y - \sigma_i^y\sigma_{i+1}^x)], \tag{4}$$

where J' and D' are the renormalized coupling constants. The renormalized coupling constants are functions of the original ones which are given by the following equations.

$$J' = J\left(\frac{2}{q}\right)^2(1+D^2), \quad \Delta' = \frac{\Delta}{1+D^2}\left(\frac{\Delta+q}{4}\right)^2, \quad D' = D. \tag{5}$$

The above RG equations show that there is a phase boundary $\Delta_c=\sqrt{1+D^2}$ that separates the spin-fluid phase, $\Delta<\sqrt{1+D^2}$, from the Néel phase, $\Delta>\sqrt{1+D^2}$ [25].

III. ENTANGLEMENT ANALYSIS

Many measures of entanglement have been introduced and analyzed [30–33], but the most relevant to this work is the "entanglement of formation." For a reduced density matrix ρ_{ij} of two qubits that arises after integrating out other degrees of freedom, the entanglement between two qubits is evaluated as $E=h(\frac{1}{2}+\frac{1}{2}\sqrt{1-C^2})$, where h is a binary entropy function $h(x)=-x\log_2 x-(1-x)\log_2(1-x)$ and C denotes the concurrence [31] defined as

$$C = \text{Max}\{\lambda_1-\lambda_2-\lambda_3-\lambda_4,0\}, \tag{6}$$

where λ_k ($k=1,2,3,4$) are the square roots of the eigenvalues in descending order of the operator R_{ij},

$$R_{ij} = \rho_{ij}\tilde{\rho}_{ij}, \quad \tilde{\rho}_{ij} = (\sigma_1^y\otimes\sigma_2^y)\rho_{ij}^*(\sigma_1^y\otimes\sigma_2^y).$$

In this section we consider only a three-site block and study the effect of the DM interaction and anisotropy parameter, i.e., D and Δ, respectively, on the entanglement between two spins located on the sides of the block. To this end, let $|\psi_0\rangle$ be the ground state of the block. By tracing the density matrix $\rho=|\psi_0\rangle\langle\psi_0|$ on the middle site of the block, the obtained reduced density matrix and Eq. (6) give an expression for the concurrence in terms of couplings D and Δ.

For different values of DM interaction and anisotropy parameters, the plots of concurrence between the first and third sites of block C_{13} have been depicted in Fig. 1. Consider first the case of $D=0$. In this case the model becomes the known *XXZ* model. Large value of Δ implies the Néel state. Naturally this state is a product state without any entanglement between its constituents. As the anisotropy parameter reduces the quantum fluctuations arising from the transverse interactions have dominant effect and destroy the Néel state. Indeed, the in-planar interactions drive the quantum correlations, i.e., the qubits in the presence of quantum fluctuations are quantum correlated. The main message of Fig. 1 is that the suppression of the entanglement can be compensated by

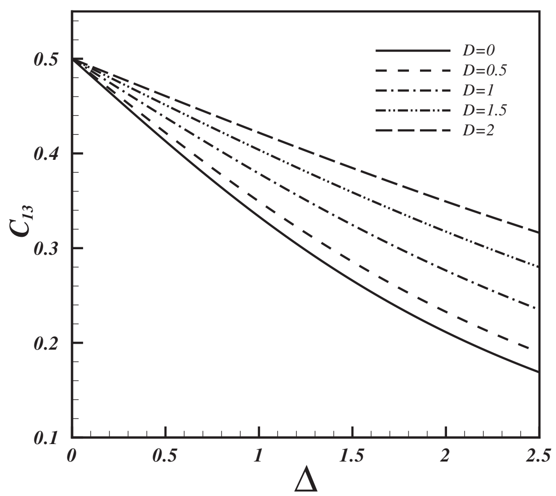

FIG. 1. Concurrence between the first and third sites of a three-site model in terms of anisotropy for different values of DM interactions.

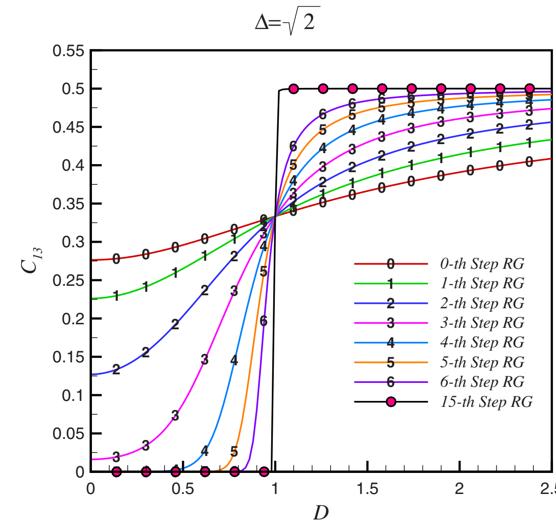

FIG. 2. (Color online) Representation of the evolution of entanglement entropy in terms of RG iterations at a fixed value of anisotropy $\Delta=\sqrt{2}$. Two different behaviors of the entanglement at the large iterations of RG correspond to the emerging phases of the model through the phase transition.

tuning the DM interaction. In the absence of the anisotropy, the entanglement is insensitive to the DM value since both transverse interaction and the DM term stimulate the quantum fluctuations of the same kind. It is clearly seen that for a nonzero value of anisotropy, turning on the DM interaction restores the spoiled entanglement. The emerging of the Néel state at a large value of anisotropy and dominant quantum fluctuations at small value tempts to conclude that in the thermodynamic limit of the model, there may occur quantum phase transition with the critical boundary based on the competition between the parameters in the Hamiltonian. We will address this issue in Sec. IV.

IV. THERMODYNAMIC LIMIT AND NONANALYTIC BEHAVIOR OF ENTANGLEMENT

In this section we would like to see how the quantum phase transition in the model, which can be signaled as an unstable fixed point of RG equations, can be realized by examining the behavior of the entanglement. Indeed, the nonanalytic behavior in some physical quantities is a feature of second-order quantum phase transition. It is also accompanied by a scaling behavior since the correlation length diverges and there is no characteristic length scale in the system at the critical point. As we already pointed out the renormalization group allows us to capture the thermodynamic properties of the model by considering a block of a few sites that is analytically tractable. In fact, the global properties of the model enter a few sites through the renormalizing of coupling constants. We exploit this advantage to study the scaling of the entanglement in the model. Notice that in the nth iteration of RG a system with size n_B^{n+1} (n_B is the number of sites in each block) describes effectively a model consisting of only n_B sites with the renormalized coupling constants. The case of the *XXZ* model has been extensively studied [20], where the critical point $\Delta=1$ separates spin-fluid and Néel phases. However, for the present model the contribution of the planar DM interaction tunes the critical point of the model due to involving the quantum fluctuations. Since the DM interaction does not flow, as is clear from the RG equations in Eq. (5), it can be treated as a fixed parameter. Now we put the next step forward to see the evolution of the entanglement as the size of the system becomes large through the RG iterations.

Zero iteration RG (or 0th step RG) represents a three-site model which has been studied in Sec. III. However, the first iteration RG stands for a nine-site model which effectively describes a three-site model in the cost of renormalized coupling constants. In that case the entanglement measures the correlation between effective degrees of freedom. In each RG iteration we can see the variation in the entanglement in terms of an anisotropy parameter with a fixed value of the DM interaction. All these data have been shown in Fig. 2. In this figure we have set $\Delta=\sqrt{2}$. It reveals that as the thermodynamic limit is touched via the increasing of RG iterations, the entanglement develops two rather different features. Indeed, there is a value for $D=1$ which separates the different features. This value is exactly the critical point of the model which is consistent with $\Delta_c=\sqrt{1+D^2}$ if we set $\Delta=\sqrt{2}$. Different features of the entanglement correspond to the emerging phases on both sides of the quantum critical point. For an anisotropy parameter larger than the values at the critical point the Néel ordering dominates the phase of the model, while for an anisotropy parameter less than the critical value the increasing of the planar quantum fluctuations spoil any magnetic ordering. This feature is not a specific character of the model arising at $\Delta=\sqrt{2}$. In fact, for any value of anisotropy larger than 1 ($\Delta>1$) such behavior emerges with the only difference that the critical point is tuned into a new one.

Further insight on the nonanalytic behavior can be probed by the divergence of the first derivative of entanglement at the critical point as long as the thermodynamic limit is approached. Plots related to the derivative of the entanglement at different RG iterations have been shown in Fig. 3. Each

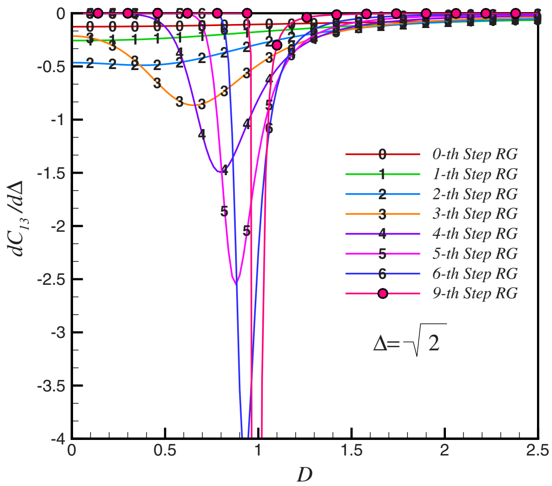

FIG. 3. (Color online) First derivative of entanglement entropy and its manifestation toward divergence as the number of RG iterations increases (Fig. 2).

plot reveals a minimum which becomes singular as the critical point is touched. At the limit of large sizes of the model the singular behavior of the entanglement becomes more pronounced. One may wonder how such emerging singularity connects to the critical exponents or universality class of the model. To this purpose, we shall see how the position of the minimum $D_{\min}$ and the minimum value itself $|\frac{dC}{d\Delta}|_{D_{\min}}$ scale by increasing the size (N) of the system. Such a computation determines the scaling law of entanglement in one-dimensional spin systems and explicitly uncovers an accurate correspondence with the critical properties of the model. The position of the minimum (D_m) of $\frac{dC}{d\Delta}$ tends toward the critical point as $D_m = D_c - N^{-0.46}$ which has been plotted in Fig. 4. Moreover, we have derived the scaling behavior of $y \equiv |\frac{dC}{d\Delta}|_{D_m}$ versus N. This has been plotted in Fig. 5 which shows a linear behavior of $\ln(y)$ versus $\ln(N)$. The exponent for this behavior is $|\frac{dC}{d\Delta}|_{D_m} \sim N^{0.46}$. It should be emphasized that this exponent is directly related to the correlation length

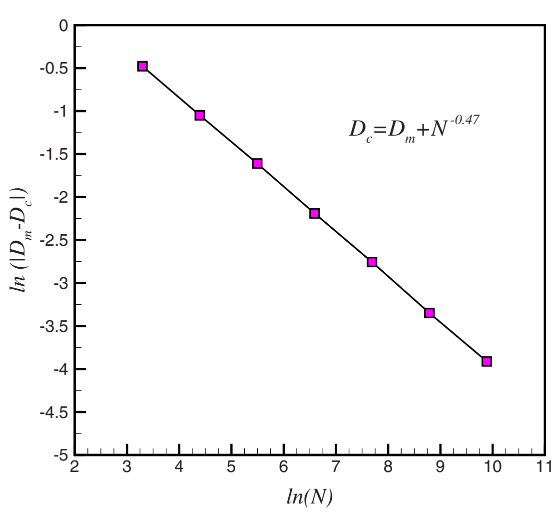

FIG. 4. (Color online) The scaling behavior of D_m in terms of system size (N) where D_m is the position of minimum in Fig. 3.

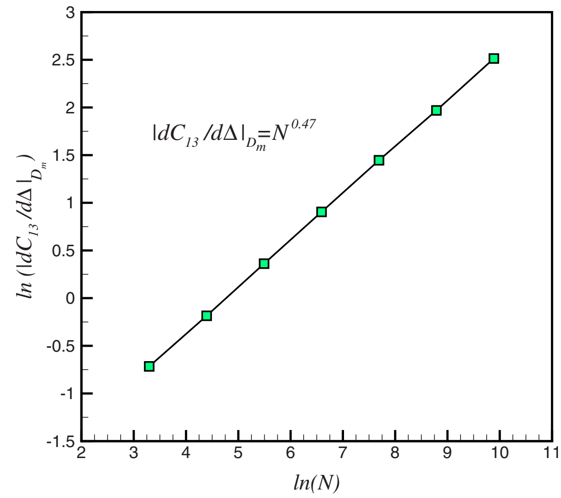

FIG. 5. (Color online) The logarithm of the absolute value of minimum, $\ln(|dC/d\Delta|_{\min})$ versus the logarithm of chain size, $\ln(N)$, which is linear and shows a scaling behavior. Each point corresponds to the minimum value of a single plot of Fig. 3.

exponent, ν, close to the critical point. It has been shown in Ref. [19] that $|\frac{dC}{d\Delta}|_{D_c} \sim N^{1/\nu}$ and $D_m = D_c - N^{-1/\nu}$.

The singular behavior of $\frac{dC}{d\Delta}$ corresponds to the phase transition for any value of the DM interaction. It exhibits a singular behavior at the transition points. The latter can be characterized by analyzing the derivative of entanglement for all values of the DM interaction. As an example, in Fig. 6 the derivative of entanglement in a three-dimensional view has been shown versus the D-Δ plane. Noticeably, the divergencies in the derivative are in perfect correspondence with the parameter value at which the phase transition occurs. The crack in the figure is just the critical line separating antiferromagnetic from the spin-fluid phases.

All the above scaling functions hold for any value of the anisotropy parameter as long as $\Delta > 1$, which is a direct result of the fact that the parameter D does not flow. This means that the emerging DM interaction term in the model does not change the universality class of the model. Thus far,

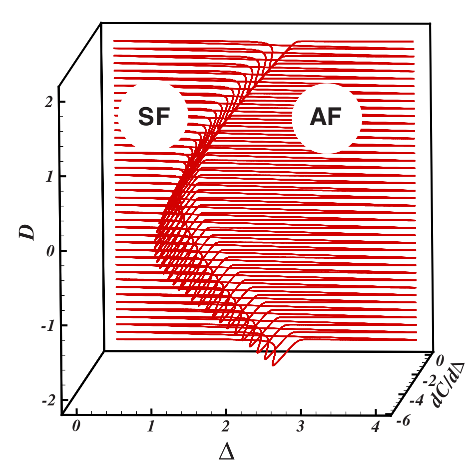

FIG. 6. (Color online) The crack appearing in the derivative of the entanglement corresponds to the critical line of the model that separates antiferromagnetic (right) and spin-fluid (left) phases.

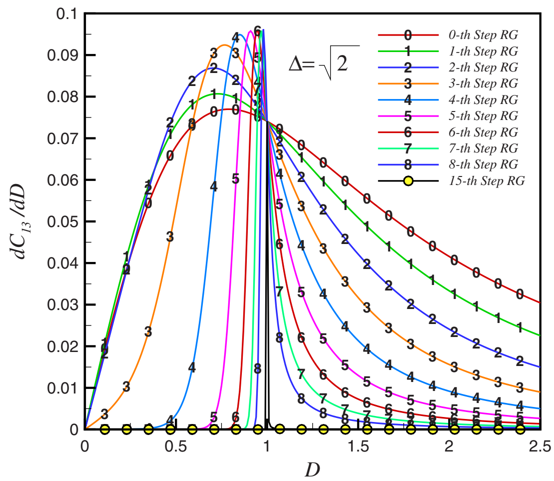

FIG. 7. (Color online) The derivative of entanglement $\frac{dC}{dD}$ versus DM interaction for a fixed value of anisotropy $\Delta=\sqrt{2}$. Even in the limit of high iterations of RG no singularity is observed.

taking the derivative of entanglement with respect to the anisotropy parameter, the singularity appears at the critical point. To get more insight on the role of the DM interaction in the singularity of the entanglement, it is convenient to plot $\frac{dC}{dD}$ versus the DM interaction which is presented in Fig. 7. Even at high RG iterations no singularity is detected. Note that the pair $(D=1, \Delta=\sqrt{2})$ stands for a point of singularity of the derivative of entanglement with respect to Δ as in Fig. 3. However, there is no signature of the divergence in the latter quantity at this point when the derivative is taken with respect to D. This, again, verifies that the DM interaction does not change the universality class of the model.

Indeed, for $\Delta > \sqrt{1+D^2}$ the long-range behavior of the model falls into the universality class of the Ising model that underlines the appearance of the antiferromagnetic long-range order [25]. We emphasize that here, the critical line is $\Delta_c=\sqrt{1+D^2}$ from the Ising phase, i.e., $D_m \to D_c^-$. This directly comes from the fact that the Ising phase is a gapped phase. Approaching the critical point, the gap is closed as $E_g \sim |D-D_c|^{\nu z}$, where z is the dynamical exponent. Since in the limit of large sizes of the system the critical point is touched as $D_c - D_m \sim N^{-1/\nu}$, we are left with the result that the gap of the Ising phase in the proximity of the critical point scales as $E_g \sim N^{-z}$.

Whenever $\Delta < \sqrt{1+D^2}$, the model is gapless. This can be realized through a simple canonical transformation to the well-known *XXZ* model [34,35] with the anisotropy $\tilde{\Delta} = \frac{\Delta}{\sqrt{1+D^2}}$. This implies that the model falls into a gapless spin-fluid phase when $\tilde{\Delta} < 1$.

Through this paper we have only considered the entanglement between two sites living on the sides of a three-site block, i.e., the middle site has been traced out through the reduced density matrix. We would like to emphasize that we have also considered the entanglement between the first two sites of the block. The entanglement between the first and second sites of the block is shown in Fig. 8. At the zero step of RG it represents a three-site model where increasing the DM interaction reduces the entanglement between sites. This

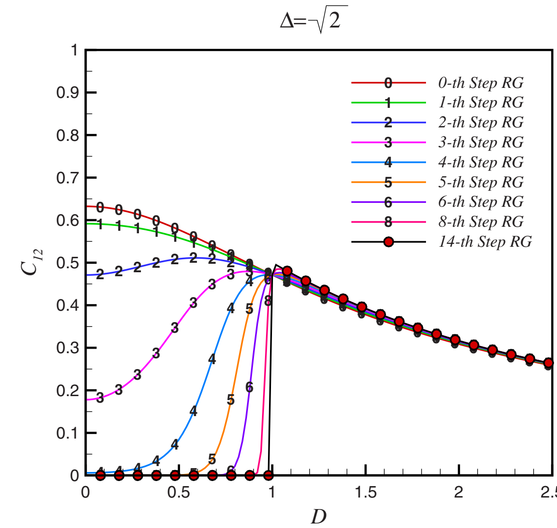

FIG. 8. (Color online) The entanglement between the first and second sites of the block in terms of the DM interaction at different RG iterations. As before the anisotropy parameter has been fixed at $\Delta=\sqrt{2}$.

is in agreement with the behavior in Fig. 2 where the entanglement between the first and third sites is increased by increasing the DM interaction. The reason is when two parties get more entangled, they restrict their entanglement with a third party and vice versa, that is, a reminiscence of the monogamy property [36] of entangled objects. In Fig. 8 for $D<1$ which corresponds to the Ising phase, the entanglement between two sites is shaved out. The anisotropy scales to infinity under the RG transformation, dictating the spins to align. On the contrary, for $D>1$ which corresponds to the gapless phase, all plots behave independently under RG transformations. Note that for $D<1$ neither first and second sites (C_{12}) nor first and third ones (C_{13}) in the large RG steps are entangled. This might not be surprising since in this limit the model is characterized by a polarized state. The situation is different for the gapless phase where the quantum fluctuations dominate the system, suppressing the alignment of spins.

If we were to take the derivative of plots, again the singularity reveals itself at the critical point. Although C_{13} and C_{12} present different behavior, they share in exhibiting the critical behavior of the model.

V. SUMMARY AND CONCLUSIONS

Condensed-matter systems have received impetus from the concepts developed in quantum information theory. Its central issue is that the entanglement is a unique measure of the quantum correlations. In this stream we studied the entanglement of a one-dimensional magnetic system in which many physical properties of realistic complex materials can be understood through it. This model is the well-known *XXZ* model supplemented by a magnetic term arising from the spin-orbit coupling. The phase diagram of the model is determined by the anisotropy and DM parameters. In a simple model consisting of only three qubits, the increasing of the anisotropy parameter favors the alignment of spins, antiferromagnetically yielding a product ground state without entanglement. However, tuning the DM interaction tends to build an entangled state and restores the spoiled entanglement. This reviving of entanglement can be understood via the fact that the DM interaction contributes the strong planar quantum fluctuations which pose the alignment ordering.

The thermodynamic limit of the model is realized by implementing the RG approach. This method not only allows us to derive the critical points as well as the phase diagram of the model but also allows us to keep track the variation in the entanglement as the size of the system becomes large. RG equations imply that the DM interaction tunes the critical point, i.e., there is a quantum critical line instead of a single critical point. However, the universality class of the model is not affected in the presence of the DM interaction, which can be clearly seen from both the RG equations and the scaling we obtained for the entanglement. The role of the DM interaction can be well understood by analyzing and comparing the derivative of entanglement with respect to the DM interaction and anisotropy parameter. In the former case, even for large RG steps, no singularity is observed. This can also be justified by mapping the model into the well-known *XXZ* model using a canonical transformation. In this way, if we change the coordinates of the phase diagram from (Δ, D) to $(\Delta, \frac{\Delta}{\sqrt{1+D^2}})$, any critical lines defined by $\Delta_c = \sqrt{1+D^2}$ will fall on a single-quantum critical point. The derivative of entanglement diverges at all points on the quantum critical line. The singularity line corresponds to the phase boundary separating the antiferromagnetic from the spin-fluid phases. The singularity is accompanied by some scaling functions with an emerging exponent that is related to the correlation length exponent close to the quantum phase transition. We have also verified that the gapped or gapless nature of a phase is relevant to the crossing behavior close to quantum phase transition. Via enlarging the size of system, the singularity becomes more pronounced and touches the critical line from the gapped phase (antiferromagnetic). In other words, the singularity touches the quantum critical point symmetrically if both phases on the phase boundary are gapped, otherwise it approaches the quantum critical point from the gapped phase asymmetrically. This phenomenon gives the scaling of the Ising phase with the size of the system which is governed by the dynamical exponent.

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