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Global Entanglement Measures and Quantum Phase Transitions in the 1D $J_1 - J_2$ Model

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Abstract We have analyzed the behavior of multipartite global entanglement and average bipartite concurrence for the sign of quantum phase transitions in the frustrated $J_1 - J_2$ model by using exact diagonalization technique for a chain of 12 qubits. It is found that although the magnitude of two classes of the measures show opposite trends the absolute value of their derivatives show similar structure near critical points.

Keywords $J_1 - J_2$ model · Global entanglement · Quantum phase transitions

1 Introduction

Entanglement which refers to quantum correlations has emerged as one of the important tools to investigate the critical behavior of various many-body quantum mechanical systems in the last decade (for a review, see [1]). These systems show quantum phase transition (QPT) as some characteristic parameter of the related Hamiltonian is varied at zero temperature; the transition is driven by quantum fluctuations in contrast to classical phase transitions which are driven by thermal effects. It is expected that quantum nature of entanglement might provide explanatory and predictive power for the investigation of quantum phase transitions in model condensed matter systems [2, 3]. Osterloh et al. and Osborne and Nielsen have used one-dimensional Ising model in an external magnetic field as an example system and showed that the bipartite entanglement displays scaling at the critical magnetic field strength [2, 3]. There has been a large number of studies on similar systems [1, 4–9] soon after [2] and [3]. A critical scaling of the derivative of concurrence was found for 1D chains with Heisenberg and Ising type interactions. Although the initial investigations of the entanglement-QPT connection was promising, a number of counter examples and arguments raised the question of universality of the aforementioned connection. It is obvious that for the most of the transitions there is some structure in the entanglement at the phase transition point. However, as shown by Yang [10], the discontinuity in the first derivative

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of entanglement might be due to the definition of the entanglement measure itself instead of being related to any QPT. Wei et al. [11, 12] have found a set of requirements for the entanglement-QPT relations for the systems with only two-body interactions. One important question that arises within this context is related to the type of entanglement which is expected to be maximum at the critical point.

The subject of computable entanglement measures itself has been a very active area of research. Among the proposed measures concurrence, pairwise entanglement between any two qubits of a chain, and the entanglement between any qubit and the rest of the chain are the most widely used measures in QPT related entanglement studies. Both of these measures are for bipartite states and due to monogamous nature of entanglement they are expected to actually decrease at the critical point, if entanglement is shared by the whole system. Entanglement of multipartite states is more difficult to quantify, partly because of the possibility of many different types of entanglement they can contain. Among the proposed multipartite entanglement measures, global entanglement defined by Meyer and Wallach [13] has been investigated in detail by a number of groups and found to be effective in detecting the QPT for Ising model in a transverse magnetic field [14–16]. Along these lines, Roscilde et al. [17, 18] showed that the multipartite entanglement is enhanced in an external magnetic field driven QPT by investigating the ratio of the one-tangle, an average global entanglement measure, to concurrence. Similarly, Wei et al. [12] used a global entanglement measure [11] to investigate the entanglement of XY spin system in an external magnetic field and found a diverging field derivative for the entanglement measure along the critical line.

Frustration in low-dimensional spin systems is expected to lead to new exotic phases and has been studied very intensely in recent years. In the one-dimensional case, key features of frustration can be analyzed in depth and in this respect, the phase diagram of one-dimensional spin-1/2 $J_1 - J_2$ model has been studied extensively over the years [19–23]. The model is displayed schematically in Fig. 1. The system can be considered as a linear chain with nearest neighbor (NN) and next nearest neighbor (NNN) interactions J_1 and J_2, respectively. Same system can also be considered as a coupled chain with zigzag inter-chain interaction (Fig. 1b). The ratio of next nearest to nearest neighbor interaction coefficients $\alpha = J_2/J_1$ is called the frustration parameter. For $\alpha < 0$, the *NNN* coupling strengthens the correlations produced by the *NN* coupling reinforcing the antiferromagnetic order. However, for $\alpha > 0$, the *NN* and *NNN* couplings compete with each other because the latter interaction frustrates the ordering tendency of the former. Since this model exhibits a rich phase structure (as detailed in the body of the paper), it provides a good testing ground for the investigation of entanglement-quantum phase transition relations. The entanglement properties of this model has been investigated by using bipartite entanglement measures concurrence [24–26] as well as entanglement entropy [27]. We extend those studies to the behavior of multipartite entanglement measures for the same model.

In this paper, we report the behavior of bipartite and extended global entanglement at critical points for the frustrated $J_1 - J_2$ model in an external magnetic field. Our aim is to compare and contrast the information available from these two classes of entanglement measures as it relates to the quantum phase transitions. The outline of this paper is as follows: In Sect. 2 we review the model and the formulation of bipartite and extended global entanglement measures. In the following sections results of calculations for the extended global entanglement as function of frustration parameter α (Sect. 3.1), external magnetic field (Sect. 3.2) are presented and discussed as they relate to the phase transitions of the $J_1 - J_2$ model. The paper concludes with a brief review of the main findings reported in the paper.

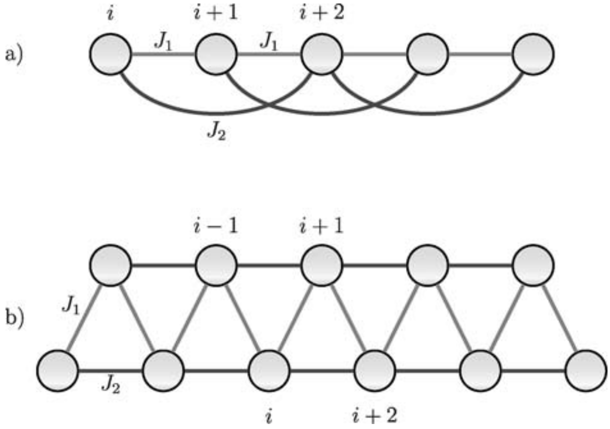

Fig. 1 Diagram of the $J_1 - J_2$ model which can be considered either as a linear chain (**a**) or a zigzag chain (**b**). The nearest neighbor interaction is J_1 while the next nearest neighbor interaction is parametrized by J_2

2 Model and the Global Entanglement

The antiferromagnetic one-dimensional $J_1 - J_2$ model generalizes the one dimensional Heisenberg model by taking into account the exchange interaction between the next-next nearest neighbour spins. Model is displayed in Fig. 1 and can be considered as localized spin-$\frac{1}{2}$ particles coupled to the nearest neighbors through exchange interaction J_1 and to second nearest neighbors through J_2.

For an N qubit system which is in a uniform external magnetic field B in z-direction, the one-dimensional Hamiltonian is given by

$$H = J_1 \sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta_1 \sigma_i^z \sigma_{i+1}^z\right) + J_2 \sum_{i=1}^{N} \left(\sigma_i^x \sigma_{i+2}^x + \sigma_i^y \sigma_{i+2}^y + \Delta_2 \sigma_i^z \sigma_{i+2}^z\right) + B \sum_{i=1}^{N} \sigma_i^z \tag{1}$$

where σ_i^α are the Pauli matrices ($\alpha = x, y, z$) for the qubit at position i, Δ_1 and Δ_2 are the anisotropy parameters for the *NN* and *NNN* interactions in z-direction. Periodic boundary conditions are assumed, i.e. $\sigma_{N+i}^\alpha = \sigma_i^\alpha$. For $J_2 = 0$, (1) reduces to XXZ model, while $J_2 = 0$ and $\Delta_1 = 0$ it reduces to the XX model.

We will investigate the entanglement in the frustrated Heisenberg model by calculating bipartite measures, namely mean concurrence and negativity and several multipartite measures which are known as extended global entanglement. The concurrence and negativity are widely known measures and we will not repeat their formulation here, the interested reader can consult [28] and [29]. We define $\bar{C}$ and $\bar{N}$ as the average of the bipartite concurrence and negativity in the system, respectively. Averaging is carried out by summing the concurrence or negativity between any one spin with all its neighbors and dividing the sum by the total number of neighbors. As the bipartite entanglement in $J_1 - J_2$ model does not extend beyond third neighbor [24], as a result $\bar{C}$ and $\bar{N}$ are small, as will be presented in the results section.

The global entanglement (GE) of an N-partite qubit system was defined by Meyer and Wallach [13]. Let $H = \bigotimes_{i=1}^{N} H_i$ be the Hilbert space of a system whose density matrix is given as $\rho = |\Psi\rangle\langle\Psi|$ where $|\Psi\rangle \in H$. Then the GE of the state is

$$E_G^{(1)} = 2 - \frac{2}{N}\sum_{j=1}^{N}\mathrm{Tr}(\rho_j^2) = \frac{1}{N}\sum_{j=1}^{N} S_L(\rho_j) \tag{2}$$

which was shown to be related to N single qubit purities [30–32]. de Oliveira et al. have generalized this definition to arbitrary number of partitions and called the measure extended global entanglement (EGE) which is defined as [14]

$$E_G^{(n)}(\rho) = \frac{1}{C_n^N}\sum_{i_1=1}^{N-1}\sum_{i_2=i_1+1}^{N-1}\cdots\sum_{i_{n-1}=i_{n-2}+1}^{N-1}(N-i_{n-1})\,G(n,i_1,i_2,\ldots,i_{n-1}), \tag{3}$$

where

$$G(n,i_1,i_2,\ldots,i_{n-1}) = \frac{d}{d-1}\left[1 - \frac{1}{N-i_{n-1}}\sum_{j=1}^{N-i_{n-1}}\mathrm{Tr}\left(\rho^2_{j,j+i_1,\ldots,j+i_{n-1}}\right)\right], \tag{4}$$

and

$$C_n^N = \frac{N!}{(N-n)!n!}$$

In (4), $\rho^2_{j,j+i_1,\ldots,j+i_{n-1}}$ is the reduced density matrix obtained by tracing out all the degrees of freedom of the system except $j, j+i_1, \ldots, j+i_{n-1}$. The index n represents the number of qubits involved in the measure, which implies that $0 < n < N-1$. The fraction $d/(d-1)$ is a normalization constant which assures that $G(n,i_1,i_2,\ldots,i_{n-1}) \le 1$ and it depends on the dimension of the Hilbert space associated with the reduced state [14]. Among all the possible EGEs defined by (3) we are interested in the four lowest order ones; namely $E_G^{(n)}$ where $n = 1$ until 4; as $E_G^{(n)}$ is related to the different multipartite entanglement (ME) classes labeled by index n, we want to investigate whether different ME classes would provide any extra information about the QPTs in the system. Let us remind that $E_G^{(1)}$ is the mean linear entropy or Meyer-Walach global entanglement for qubits while $E_G^{(2)}$ is the mean linear entropy of two qubits with rest of the chain irrespective of the distance between them. Similar descriptions hold for $E_G^{(3)}$ and $E_G^{(4)}$. EGE, also, is related to block entanglement [5].

3 Results and Discussion

In this section, we present the results of the numerical calculations of $\bar{C}$, $\bar{N}$ and $E_G^{(n)}$ where $n = 1, 2, 3, 4$ for the Hamiltonian of (1) for a chain of ten qubits. A comparison of the results for an 12 qubit chain with the reported results suggest that the gross features of the calculated quantities are similar. The state structure of the model as function of the frustration parameter and external field magnitude were presented in [24, 26] and will not be repeated here. The results reported in this Section are obtained for the isotropic case $\Delta_1 = \Delta_2 = 1$.

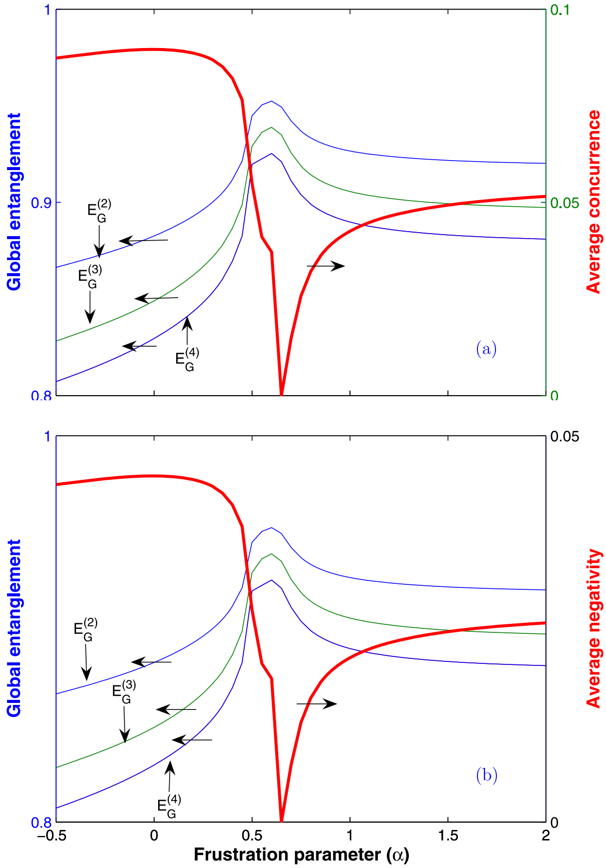

Fig. 2 Frustration parameter, α, dependence of extended global entanglement measures $E_G^{(2)}$, $E_G^{(3)}$ and $E_G^{(4)}$ along with average concurrence $\bar{C}$ (a) and average negativity ($\bar{N}$)

3.1 Frustration Dependence of Global Entanglement

There is one QPT as a function of frustration parameter α in the isotropic one-dimensional $J_1 - J_2$ model [21]. Below $\alpha = 0.241$ the system is in spin-fluid phase which is characterized by a power-law decay of spin correlations. This transition involves the change in the first excited state's symmetry and is not expected to be captured by entanglement measures that are functions of only the ground state wave-function. In Figs. 2(a) and (b), we display the extended global entanglement $E_G^{(2)}$, $E_G^{(3)}$ and $E_G^{(4)}$ along with the mean concurrence and negativity as function of α, respectively. The measure $E_G^{(1)}$ is found to have no structure as function of α and is not displayed in Fig. 2. As it can be seen clearly from this figure, neither the EGE measures nor the average bipartite measures show any structure at or around $\alpha = 0.241$.

A special point of the isotropic $J_1 - J_2$ model as a function of α is at the $\alpha = 0.5$ which is called Majumar-Ghosh point. At this value of frustration, the model has exact solution in terms of singlets which can be formed by neighboring sites [33]. All the extended global entanglement measures as well as $\bar{C}$ and $\bar{N}$ seem to detect this special point quite well as displayed in Fig. 2. The maximum of $E_G^{(n)}$ is located near $\alpha = 1/2$ while the mean value of bipartite measures approaches zero around the same point. This finding seem to support the idea that at the special points where multipartite entanglement goes to a maximum the

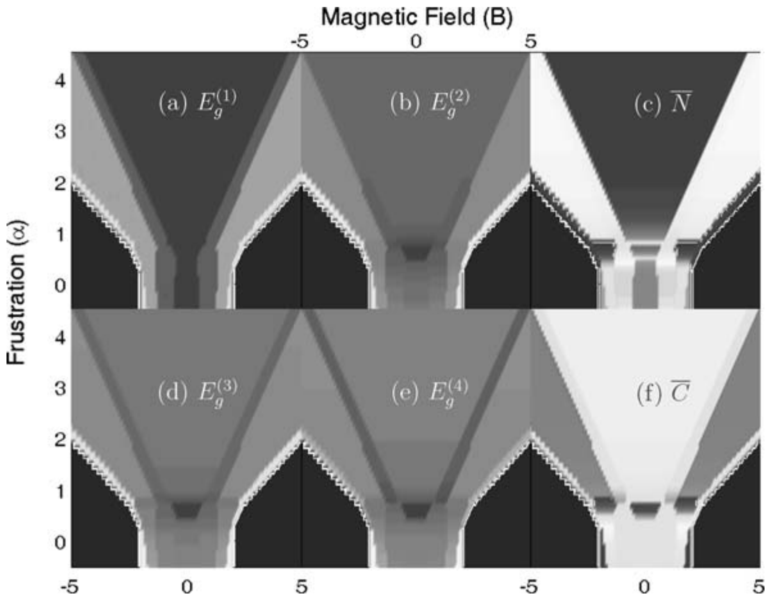

Fig. 3 External magnetic field and frustration dependence of extended global entanglement measures (**a**) $E_G^{(1)}$, (**b**) $E_G^{(2)}$, (**d**) $E_G^{(3)}$ and (**e**) $E_G^{(4)}$ along with average concurrence (**f**) $\bar{C}$ and average negativity (**c**) ($\bar{N}$)

bipartite entanglement should be a minimum because of the entanglement monogamy principle [3] which was also observed for XY model by de Oliveira et al. [16].

The main conclusions from the frustration dependent global entanglement study are: (a) neither bipartite (concurrence) nor multipartite entanglement measures are able to detect the spin-fluid to dimer phase transition at $\alpha = 0.241$ [24]. Since, all the measures considered in the present study use the ground-state wavefunction of the system, they are not expected to show any structure at $\alpha = 0.241$ at which point the model has level-crossing at the first excited state [24]. (b) Concurrence between the nearest neighbors goes to zero [24] while $E_G^{(n)}$ approaches its maximum value around the Majumdar-Ghosh point. The value of $E_G^{(n)}$s tend to a constant value as α is further increased in the frustrated phase.

3.2 Magnetic Field Dependence of Global Entanglement

An applied magnetic field in z-direction would try to break the antiferromagnetic ordering of the system and align all the spins along its own direction after a critical value of B_c. In 1-D spin models with only nearest-neighbor interaction this transition would be at one critical B_c value. However, in $J_1 - J_2$ model magnetic field acts against the combination of first and second neighbor interactions and aligning of the spins along B-direction goes in a step by step process. Magnetic field dependence of the ground state was reported in [26] and will not be repeated here.

Calculated frustration and magnetic field dependent average negativity, concurrence, and $E_G^{(n)}$ ($n = 1, 2, 3, 4$) are displayed in Fig. 3. The most important observation from these figures is that all the considered measures show almost identical behavior: For $\alpha < 0.25$ the system is in spin-fluid phase and as the strength of the external field is increased beyond its saturation value ($B_c = 2$ for $\alpha < 1/4$), all the spins are aligned with the field and the state of the system becomes ferromagnetic which is a product state with zero entanglement.

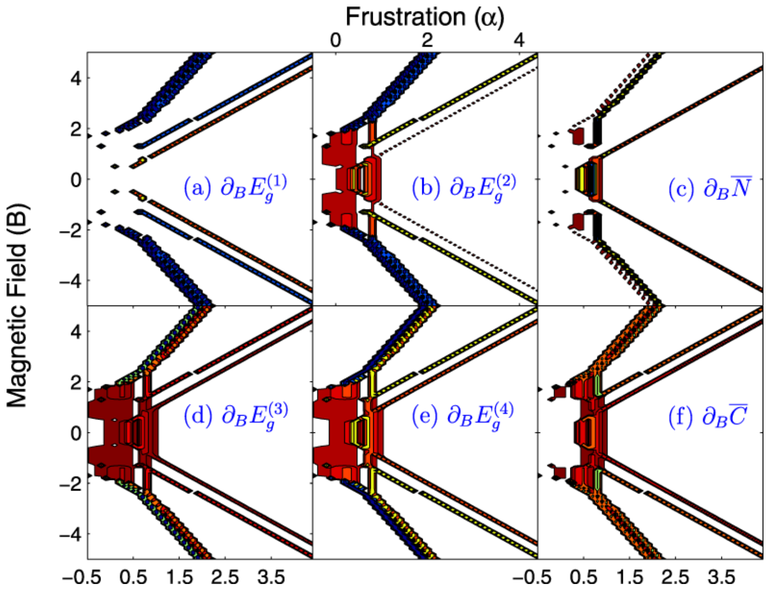

Fig. 4 Partial derivative with respect to the external field strength B for the six entanglement measures considered in this study as function of the external magnetic field and the frustration parameter. *White sections* of the plots indicate a zero derivative

The saturating magnetic field B_c depends linearly on the α for $\alpha > 1/4$ [21] which is reflected in the graphs of the considered measures in Fig. 3 as the straight lines that separates the zero entanglement region from the nonzero one for the $\alpha > 1/4$ region. Also, all six of the calculated measures show a linearly frustration dependent entanglement-magnetic field structure (V-shaped features in Fig. 3) which might be related to the fact that in the frustrated regime, as the external field strength is increased, the alignment of the spins might be happening in clusters. The main difference among the measures can be observed around $\alpha = 1/2$ Majumdar-Ghosh point. In all, except $E_G^{(1)}$, there is a prominent kink around $\alpha = 1/2$ for the small values of the external field.

We have also calculated the field and frustration derivatives of the extended global entanglement and the mean concurrence and negativity and display the results as contour plots in Figs. 4 and 5. As it is more obvious from these figures there are three main concentric V-shaped transition regions in all but the mean negativity measure (which has only two). At the parameter space around $\alpha \approx 0.5$ and small field magnitude the field derivatives of $E_G^{(2)}$, $E_G^{(3)}$ and $E_G^{(4)}$ are almost indistinguishable and quite similar to that of average concurrence and negativity. α derivatives of all the extended global entanglement measures are very similar while the $\partial_\alpha \bar{N}$ and $\partial_\alpha \bar{C}$ show small differences compared to $\partial_\alpha E_G^{(n)}$.

4 Conclusions

We have investigated the behavior of extended global and average bipartite entanglement measures around the quantum phase transition points of the $J_1 - J_2$ model by exact diagonalization of a system consisting of 12 spin 1/2 particles. Multipartite character of extended global entanglement comes from the fact that $E_G^{(n)}$ is a measure of mean linear entropy of

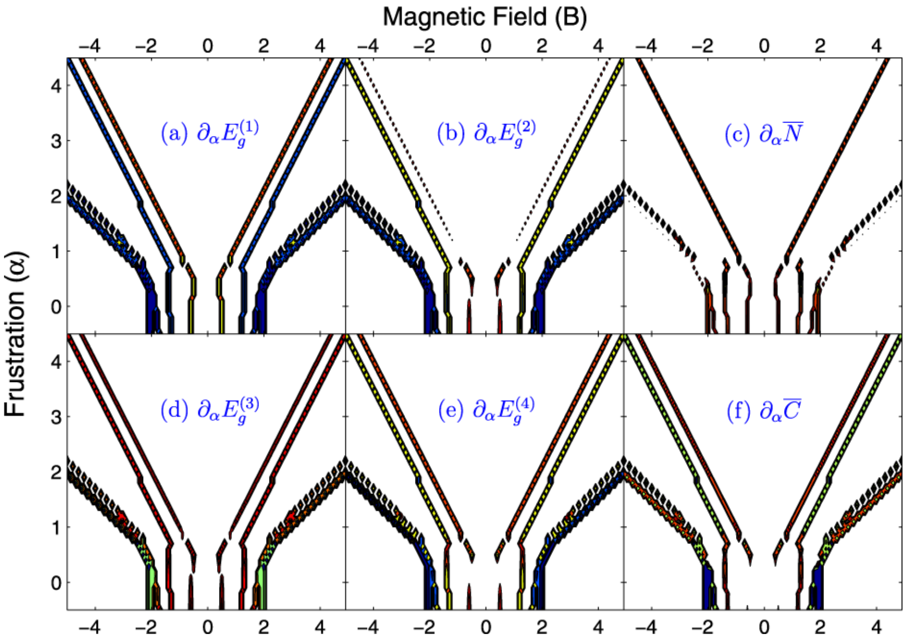

Fig. 5 Partial derivative with respect to the frustration parameter α for the six entanglement measure considered in this study as function of the external magnetic field and the frustration parameter. *White sections* of the plots indicate a zero derivative

the subsystem with n elements with the remaining $N - n$ elements. Although none of the entanglement measures considered in the present study was able to detect the spin fluid-dimer QPT at $\alpha = 0.241$, the conjecture that the multipartite entanglement measures should approach its maximum value in the neighborhood of the QPT is found to be valid for all but $n = 1$ variants of $E_G^{(n)}$ at the Majumdar-Ghosh special point. Increasing n beyond three does not provide any new information on the entanglement-QPT relation, at least for the $J_1 - J_2$ model for the parameter range considered in the current study.

Our aim at the start was to compare and contrast the features in multipartite and bipartite entanglement measures at and near the quantum phase transition points. We have found that qualitative information content of both class of measures are similar, especially when one looks at the parameter derivatives of the measures. Of course, the quantitative differences, such as bipartite measures approaching zero while $E_G^{(n)}$ approaching its maximum at $\alpha = 1/2$, exists. But as it is displayed in Figs. 4 and 5 the field derivatives of both class of measures show similar overall structure. The source of this similarity might partly come from the averaging procedure; for example the bipartite concurrence and negativity between the first, second and the third neighbor spins of the present model were found to be quite different than each other [24]. For example, it was found that the nearest neighbor entanglement is zero for $\alpha \gtrsim 1/2$ while the next nearest neighbor entanglement is zero for $\alpha \lesssim 1/2$ and nonzero for $\alpha \gtrsim 1/2$ [25, 26]. Averaging over these quantities would give nonzero mean bipartite entanglement for all the frustration range, similar to the extended global entanglement. Comparing $G(n, i_1, i_2, \ldots, i_{n-1})$ of (4) with individual bipartite measures might shed more light on the relation between the $E_G^{(n)}$s and the concurrence and the negativity.

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