

# Quantum Critical Point and Entanglement in a Matrix Product Ground State

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## Abstract

In this paper, we study the entanglement properties of a spin-1 model the exact ground state of which is given by a Matrix Product state. The model exhibits a critical point transition at a parameter value  $a = 0$ . The longitudinal and transverse correlation lengths are known to diverge as  $a \rightarrow 0$ . We use three different entanglement measures  $S(i)$  (the one-site von Neumann entropy),  $S(i, j)$  (the two-body entanglement) and  $G(2, n)$  (the generalized global entanglement) to determine the entanglement content of the MP ground state as the parameter  $a$  is varied. The entanglement length, associated with  $S(i, j)$ , is found to diverge in the vicinity of the quantum critical point  $a = 0$ . The first derivative of the entanglement measure  $E$  ( $= S(i), S(i, j)$ ) w.r.t. the parameter  $a$  also diverges. The first derivative of  $G(2, n)$  w.r.t.  $a$  does not diverge as  $a \rightarrow 0$  but attains a maximum value at  $a = 0$ . At the QCP itself all the three entanglement measures become zero. We further show that multipartite correlations are involved in the QPT at  $a = 0$ .

## I. INTRODUCTION

The entanglement characteristics of the ground states of many body Hamiltonians describing condensed matter systems constitute an important area of study

in quantum information theory. Entanglement is an essential resource in quantum computation and communication protocols. Condensed matter, specially, spin systems have been proposed as candidate systems for the realization of some of the protocols. Entanglement provides a measure of non-local quantum correlations in the system and it is of significant interest to determine how the correlations associated with the ground state of the system change as one or more than one parameter of the system is changed. The focus on ground state characteristics arises from the possibility of quantum phase transitions (QPTs) which occur at temperature  $T = 0$  (when the system is in its ground state) and are driven solely by quantum fluctuations [1]. A QPT is brought about by tuning a parameter, either external or intrinsic to the Hamiltonian, to a special value termed the transition point. In thermodynamic critical phenomena, the thermal correlation length diverges and the thermodynamic quantities become singular as the critical point is approached. In the quantum case, the correlation length diverges in the vicinity of the QCP and the ground state properties develop non-analytic features. An issue of considerable interest is whether the quantum correlations, like the usual correlation functions, become long-ranged near the QCP. In a wider perspective, the major goal is to acquire a clear understanding of the variation in entanglement characteristics as a tuning parameter is changed. QPTs have been extensively studied in spin systems both theoretically and experimentally. In recent years, several theoretical studies have been undertaken to elucidate the relationship between QPTs and entanglement in spin systems [2, 3, 4, 5, 6, 7]. In particular, a number of entanglement measures have been identified which develop special features close to the transition point. One such measure is concurrence which quantifies the entanglement between two spins ( $S = \frac{1}{2}$ ). At a QCP, as illustrated by a class of exactly-solvable spin models ( $S = \frac{1}{2}$ ), the derivative of the ground state concurrence has a logarithmic singularity though the concurrence itself is non-vanishing upto only next-nearest-neighbour-distances between two spins [2, 3]. Discontinuities in the ground state concurrence have been shown to characterize first order QPTs [8, 9, 10]. Later, Wu et al. [5] showed that under some general assumptions a first order QPT, associated with a discontinuity in the first derivative of the ground state energy, gives rise to a discontinuity in a bipartite entanglement measure like concurrence and negativity. Similarly, a discontinuity or a divergence in the first derivative of the same entanglement measure is the signature of a second order phase transition with a discontinuity or a divergence in the second derivative of the ground state energy. Another measure of entanglement, studied in the context of QPTs, is the entropy of entanglement between a block of  $L$  adjacent spins in a chain with the rest of the system [4]. At the QCP, the entropy of entanglement diverges logarithmically with the length of the block. There is, however, no direct relation with the long range correlations in the system.

A number of entanglement measures have recently been proposed which are characterized by a diverging length scale, the entanglement length, close to a QCP. The localizable entanglement (LE) between two spins is defined as the maximum average entanglement that can be localized between them by performing local measurements on the rest of the spins [11]. The entanglement length sets the scale over which the LE decays. The two-body entanglement  $S(i, j)$  is a measure of the entanglement between two separated spins, at sites  $i$  and  $j$ , and the rest of the spins [7]. Let  $\rho(i, j)$  be the reduced density matrix for the two spins, obtained from the full density matrix by tracing out the spins other than the ones at sites  $i$  and  $j$ . The two body entanglement  $S(i, j)$  is given by the von Neumann entropy

$$S(i, j) = -Tr \rho(i, j) \log_2 \rho(i, j) \quad (1)$$

In a translationally invariant system,  $S$  depends only on the distance  $n = |j - i|$ . As pointed out in [7], the spins that are entangled with one or both the spins at sites  $i$  and  $j$  contribute to  $S$ . The following results have been obtained in the case of the  $S = \frac{1}{2}$  exactly solvable anisotropic XY model in a transverse magnetic field. The model, away from the isotropic limit, belongs to the universality class of the transverse Ising model. The two-body entanglement  $S(i, j)$  has a simple dependence on the spin correlation functions in the large  $n$  limit. Away from the critical point,  $S(i, j)$  is found to saturate over a length scale  $\xi_E$  as  $n$  increases. Near the QCP, one obtains

$$S(i, j) - S(\infty) \sim n^{-1} e^{-\frac{n}{\xi_E}} \quad (2)$$

The entanglement length (EL),  $\xi_E$ , has an interpretation similar to that in the case of LE. The EL diverges with the same critical exponent as the correlation length at the QCP.  $S(i, j)$  thus captures the long range correlations associated with a QPT. At the critical point itself,  $S(i, j) - S(\infty)$  has a power-law decay, i.e.,  $S(i, j) - S(\infty) \sim n^{-\frac{1}{2}}$ . In the limit of large  $n$ , the first derivative of  $S(i, j)$  w.r.t. a Hamiltonian parameter develops a  $\lambda$ -like cusp at the critical point. The universality and a finite-size scaling of the entanglement have also been demonstrated. The one-site von Neumann entropy

$$S(i) = -Tr \rho(i) \log_2 \rho(i) \quad (3)$$

is also known to be a good indicator of a QPT [3]. It provides a measure of how a single spin at the site  $i$  is entangled with the rest of the system. The reduced density matrix  $\rho(i)$  is obtained from the full density matrix by tracing out all the spins except the one at the site  $i$ . Oliveira et al. [6] have proposed a generalized global entanglement (GGE) measure  $G(2, n)$  which quantifies multipartite entanglement (ME).  $G(2, n)$  for a translationally symmetric system is given by

$$G(2, n) = \frac{d}{d-1} \left[ 1 - \sum_{l,m=1}^{d^2} |[\rho(j, j+n)]_{lm}|^2 \right] \quad (4)$$

where  $\rho(j, j+n)$  is the reduced density matrix of dimension  $d$ . The factor 2 in  $G(2, n)$  indicates that the reduced density matrix is that for a pair of particles. Wu et al. [5] considered QPTs characterized by non-analyticities in the derivatives of the ground state energy. These arise from the non-analyticities in one or more of the elements of the reduced density matrix. In terms of the GGE, a discontinuity in  $G(2, n)$  signals a first order QPT, brought about by a discontinuity in one or more of the elements,  $[\rho_{j,j+n}]_{lm}$  of the reduced density matrix [6]. A discontinuity or divergence in the first derivative of  $G(2, n)$  w.r.t. the tuning parameter occurs due to a discontinuity or divergence in the first derivatives of one or more of the elements of the reduced density matrix. The associated QPT is of second order. Non-analyticities in  $G(2, n)$  and its derivatives thus serve as indicators of QPTs. In the case of the XY  $S = \frac{1}{2}$  spin chain, the GGE measure shows a diverging EL as the QCP is approached. The EL  $\xi_E = \frac{\xi_C}{2}$  where  $\xi_C$  is the usual correlation length. Thus, both the length scales diverge with the same critical exponent near the QCP.

The relationship between entanglement and QPTs has mostly been explored for spin- $\frac{1}{2}$  systems. The entanglement properties of the ground states of certain spin-1 Hamiltonians have been studied using different measures [11, 12, 13]. Numerical studies show that the LE has the maximal value for the ground state of the spin-1 Heisenberg antiferromagnet with open boundary conditions (OBC) [13]. In the case of the spin-1 Affleck-Kennedy-Lieb-Tasaki (AKLT) model [14], the result can be proved exactly. A class of spin-1 models, the  $\phi$ -deformed AKLT models, is characterized by an exponentially decaying LE with a finite EL  $\xi_E$ . The length  $\xi_E$  diverges at the point  $\phi = 0$  though the conventional correlation length remains finite [13]. A recent study [15] shows that in the case of spin-1 systems, the use of LE for the detection of QPTs is not feasible. An example is given by the  $S = 1$  XXZ Heisenberg antiferromagnet with single-ion anisotropy. The model has a rich phase diagram with six different phases. The LE is found to be always 1 in the entire parameter region and hence is insensitive to QPTs. The ground states of certain spin-1 models have an exact representation in terms of matrix product states (MPS) [16, 17, 18]. The ground state of the spin-1 AKLT model, termed a valence bond solid (VBS) state, is an example of an MPS. The ground state is characterized by short-ranged spin-spin correlations and a hidden topological order known as the string order. The excitation spectrum of the model is further gapped. In the MPS formalism, ground state expectation values like the correlation functions are easy to calculate. This has made it particularly convenient to study phase transitions in spin models with MP states as exact ground states [17]. The

transitions identified so far include both first and second order transitions and are brought about by the tuning of the Hamiltonian parameters. The second order transition in the class of finitely correlated MP states, however, differs from the conventional QPT in one important respect. The spin correlation function is always of the form  $A_C e^{-\frac{n}{\xi_C}}$  for large  $n$ . The correlation length  $\xi_C$  diverges as the transition point is approached. The pre-factor  $A_C$ , however, vanishes at the transition point [17]. This is in contrast to the power-law decay of the correlation function at a conventional QCP. Some distinct features of QPTs in MP states have recently been identified [19]. One of these relates to the analyticity of the ground state energy density for all values of the tuning parameter. In a conventional QPT, the energy density becomes non-analytic at the QCP. The MP states appear to provide an ideal playground for exploring novel types of QPTs. In this paper, we consider a spin-1 model, the exact ground state of which is given by an MP state [20]. The model has a rich phase diagram with a number of first order phase transitions and a critical point transition. We study the entanglement properties of the ground state with a view to pinpoint the special features which appear close to the critical point. This is done by using three different entanglement measures, namely, the single-site, two-body and generalized global entanglement defined earlier.

## II. REDUCED DENSITY MATRIX OF MP GROUND STATE

We consider a spin-1 chain Hamiltonian proposed by Klümper et al. [20] which describes a large class of antiferromagnetic (AFM) spin-1 chains with MP states as exact ground states. The Hamiltonian satisfies the symmetries : (i) rotational invariance in the  $x - y$  plane, (ii) invariance under  $S^z \rightarrow -S^z$  and (iii) translation and parity invariance. The Hamiltonian has the general form

$$H = \sum_{j=1}^L h_{j,j+1}$$

$$h_{j,j+1} = \alpha_0 A_j^2 + \alpha_1 (A_j B_j + B_j A_j) + \alpha_2 B_j^2 + \alpha_3 A_j + \alpha_4 B_j (1 + B_j) + \alpha_5 ((S_j^z)^2 + (S_{j+1}^z)^2) + C \quad (5)$$

where  $L$  is the number of sites in the chain and periodic boundary conditions (PBC) hold true. The parameters  $\alpha_j$  are real and  $C$  is a constant. The nearest-neighbour (n.n.) interactions are

$$\begin{aligned} A_j &= S_j^x S_{j+1}^x + S_j^y S_{j+1}^y \\ B_j &= S_j^z S_{j+1}^z \end{aligned} \quad (6)$$

The constant  $C$  in Eq. (5) may be adjusted so that the ground state eigenvalue of  $h_{j,j+1} = 0$ . Hence

$$h_{j,j+1} \geq 0 \quad \Rightarrow \quad H \geq 0 \quad (7)$$

i.e.,  $H$  has only non-negative eigenvalues. In the AFM case, the  $z$ -component of the total spin of the ground state  $S_{tot}^z = 0$ . Klümper et al. showed that in a certain subspace of the  $\alpha_j$ -parameter space, the AFM ground state has the MP form. Let  $|0\rangle$  and  $|\pm\rangle$  be the eigenstates of  $S^z$  with eigenvalues 0, +1 and -1 respectively. Define a  $2 \times 2$  matrix at each site  $j$  by

$$g_j = \begin{pmatrix} |0\rangle & -\sqrt{a}|+\rangle \\ \sqrt{a}|-\rangle & -\sigma|0\rangle \end{pmatrix} \quad (8)$$

with non-vanishing parameters  $a, \sigma \neq 0$ .

The global AFM state is written as

$$|\psi_0(a, \sigma)\rangle = Tr(g_1 \otimes g_2 \otimes \dots \otimes g_L) \quad (9)$$

where ' $\otimes$ ' denotes a tensor product. One can easily check that  $S_{tot}^z |\psi_0\rangle = 0$ , i.e., the state is AFM. One now demands that the state  $|\psi_0(a, \sigma)\rangle$  is the exact ground state of the Hamiltonian  $H$  with eigenvalues 0. For this, it is sufficient to show that

$$h_{j,j+1}(g_j \otimes g_{j+1}) = 0 \quad (10)$$

Eq. (3) and (10) are satisfied provided the following equalities

$$\begin{aligned} 1) \sigma &= sign(\alpha_3), & 2) a \alpha_0 &= \alpha_3 - \alpha_1, \\ 3) \alpha_5 &= |\alpha_3| + \alpha_0(1 - a^2), & 4) \alpha_2 &= \alpha_0 a^2 - 2|\alpha| \end{aligned} \quad (11)$$

and inequalities

$$a \neq 0, \alpha_3 \neq 0, \alpha_4 > 0, \alpha_0 > 0 \quad (12)$$

hold true. The state  $|\psi_0(a, \sigma)\rangle$  is the ground state of the Hamiltonian (5) with ground state energy zero provided the equalities in (8) are satisfied. The inequalities constrain the other eigenvalues of  $h_{j,j+1}$  to be positive. If the inequalities are satisfied, the ground state can be shown to be unique for any chain length  $L$ . Also, in the thermodynamic limit  $L \rightarrow \infty$ , the excitation spectrum has a gap  $\Delta$ . With equality signs in the inequalities (12), the state  $|\psi_0(a, \sigma)\rangle$  is still the

ground state but is no longer unique. The spin-1 model has the typical feature of a Haldane-gap (HG) antiferromagnet. In fact, the AKLT model is recovered as a special case with  $a = 2$ ,  $\sigma = 1$ ,  $\alpha_3 = 3\alpha_0 > 0$ ,  $\alpha_2 = -2\alpha_0$  and  $\alpha_4 = 3\alpha_0$ . The state (9) now represents the VBS state.

Using the transfer matrix method [16], the ground state correlation functions can be calculated in a straightforward manner. The results are ( $L \rightarrow \infty$ ,  $r \geq 2$ ): Longitudinal correlation function

$$\langle S_1^z S_r^z \rangle = -\frac{a^2}{(1 - |a|)^2} \left( \frac{1 - |a|}{1 + |a|} \right)^r \quad (13)$$

Transverse correlation function

$$\langle S_1^x S_r^x \rangle = -|a| [\sigma + \text{sign } a] \left( \frac{-\sigma}{1 + |a|} \right)^r \quad (14)$$

The correlations (13) and (14) decay exponentially with the longitudinal and transverse correlation lengths given by

$$\xi_l^{-1} = \ln \left| \frac{1 + |a|}{1 - |a|} \right|, \quad \xi_t^{-1} = \ln(1 + |a|) \quad (15)$$

Furthermore, the string order parameter has a non-zero expectation value in the ground state. One finds that the correlation lengths diverge as  $a \rightarrow 0$ . At the point  $a = 0$ , the correlation functions given by Eq. (13) and (14) are zero. At a conventional QCP, the correlation functions have a power-law decay. We will, however, refer to the point as a QCP since the correlation lengths diverge as the point is approached. A consequence of the diverging correlation length is that the excitation spectrum of the spin-1 model, which is gapped (the Haldane phase) for  $a > 0$ , becomes gapless at the critical point  $a = 0$  [20]. The presence or absence of a gap in the excitation spectrum of a system is reflected in the low temperature thermodynamic properties of the system. Furthermore, the string order parameter has a non-zero expectation value in the ground state for  $a > 0$  and becomes zero at  $a = 0$  indicating the appearance of a new phase. Refs. [16, 17] provide several other examples of spin-1 models with finitely correlated MP states as exact ground states. All these models exhibit critical point transitions with features similar to those in the case of the spin-1 model described by the Hamiltonian in Eq. (5). We now focus on the entanglement properties of the MP ground state (Eq. (9)). We consider  $a$  to be  $\geq 0$  and  $\sigma = +1$  in Eq. (8). The one-site reduced density matrix  $\rho(i)$  (Eq. (3)) obtained by tracing out all the spins except the  $i$ -th spin from the ground state density matrix  $\rho = |\psi_0\rangle\langle\psi_0|$ , can be calculated using the transfer matrix method [16]. The density matrix, from Eq. (9), is

$$\rho = |\psi_0\rangle\langle\psi_0| = \sum_{\{n_\alpha, m_\alpha\}} g_{n_1 n_2} g_{n_2 n_3} \cdots g_{n_L n_1} g_{m_1 m_2}^\dagger g_{m_2 m_3}^\dagger \cdots g_{m_L m_1}^\dagger \quad (16)$$

The summation is over all the indices,  $n_i, m_i, i = 1, 2, \dots, L$ .

We define a  $4 \times 4$  matrix  $f$  (the elements of which are operators) at any lattice site as

$$f_{\mu_1 \mu_2} \Rightarrow f_{(n_1, m_1)(n_2, m_2)} \equiv g_{n_1 n_2} g_{m_1 m_2}^\dagger \quad (17)$$

The convention of the ordering of the multi-indices is  $\mu = 1, 2, 3, 4 \leftrightarrow (11), (12), (21), (22)$ . Thus,  $f$  can be written as

$$f = \begin{pmatrix} |0\rangle\langle 0| & -\sqrt{a}|0\rangle\langle 1| & -\sqrt{a}|1\rangle\langle 0| & a|1\rangle\langle 1| \\ \sqrt{2}|0\rangle\langle -1| & -|0\rangle\langle 0| & -a|1\rangle\langle -1| & \sqrt{a}|1\rangle\langle 0| \\ \sqrt{a}|-1\rangle\langle 0| & -a|-1\rangle\langle 1| & -|0\rangle\langle 0| & \sqrt{a}|0\rangle\langle 1| \\ a|-1\rangle\langle -1| & -\sqrt{a}|-1\rangle\langle 0| & -\sqrt{a}|0\rangle\langle -1| & |0\rangle\langle 0| \end{pmatrix} \quad (18)$$

Also,

$$\rho(i) = \text{Tr}_{1, \dots, L}^i |\psi_0\rangle\langle\psi_0| \quad (19)$$

where the trace is over all the spins except the  $i$ -th one. The transfer matrix  $F$  at a site  $m$  is obtained by taking the trace over  $f$  at the same site, i.e.,

$$F_m = \sum_k \langle k| f_m |k\rangle \quad (20)$$

where the states  $|k\rangle$  are the states  $|0\rangle, |\pm 1\rangle$ . The transfer matrix  $F$  is obtained as

$$F = \begin{pmatrix} 1 & 0 & 0 & a \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ a & 0 & 0 & 1 \end{pmatrix} \quad (21)$$

The eigenvalues are

$$\varepsilon_1 = 1 + a, \varepsilon_2 = 1 - a, \varepsilon_3 = -1, \varepsilon_4 = -1 \quad (22)$$

The corresponding eigenvectors are

$$\begin{aligned} |e_1\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, & |e_2\rangle &= \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 0 \\ 1 \end{pmatrix} \\ |e_3\rangle &= \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, & |e_4\rangle &= \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix} \end{aligned} \quad (23)$$

From Eq. (20),

$$\rho(i) = \frac{\sum_{\alpha=1}^4 \langle e_\alpha| F^{L-1} f |e_\alpha\rangle}{\sum_{\alpha=1}^4 \langle e_\alpha| F^L |e_\alpha\rangle} \quad (24)$$



The factor in the denominator takes care of the condition  $Tr \rho = 1$ . On taking the thermodynamic limit  $L \rightarrow \infty$ , we get

$$\rho(i) = \varepsilon_1^{-1} \langle e_1 | f | e_1 \rangle \quad (25)$$

In the  $|0, \pm 1\rangle$  basis, the reduced density matrix becomes

$$\rho(i) = \begin{pmatrix} \frac{1}{1+a} & 0 & 0 \\ 0 & \frac{a}{2(1+a)} & 0 \\ 0 & 0 & \frac{a}{2(1+a)} \end{pmatrix} \quad (26)$$

The calculation of the two-site reduced density matrix  $\rho(i, j)$  follows in the same manner.  $\rho(i, j)$  is given by

$$\rho(i, j) = Tr_{1, \dots, L}^{i, j} |\psi_0\rangle \langle \psi_0| \quad (27)$$

where the trace is taken over all the spins except the  $i$ -th and  $j$ -th ones.

$$\rho(i, j) = \frac{\sum_{\alpha=1}^4 \langle e_\alpha | F^{i-1} f F^{j-i-1} f F^{L-j} | e_\alpha \rangle}{\sum_{\alpha=1}^4 \langle e_\alpha | F^L | e_\alpha \rangle} \quad (28)$$

In the thermodynamic limit  $L \rightarrow \infty$ ,  $\rho(i, j)$  reduces to

$$\rho(i, j) = \sum_{\alpha=1}^4 \varepsilon_\alpha^{-2} \left( \frac{\varepsilon_\alpha}{\varepsilon_1} \right)^{n+1} \langle e_1 | f | e_\alpha \rangle \langle e_\alpha | f | e_1 \rangle \quad (29)$$

where  $n = |j - i|$ .

The matrix  $\rho(i, j)$  is a  $9 \times 9$  matrix and defined in the two-spin basis states  $|lm\rangle$  with the ordering

$$|lm\rangle \equiv |11\rangle, |10\rangle, |01\rangle, |1-1\rangle, |-11\rangle, |00\rangle, |0-1\rangle, |-10\rangle, |-1-1\rangle \quad (30)$$

The non-zero matrix elements,  $b_{pq}$  ( $p = 1, \dots, 9$ ,  $q = 1, \dots, 9$ ), of  $\rho(i, j)$  are :

$$\begin{aligned} b_{11} &= b_{99} = \frac{a^2}{4(1+a)^2} - \frac{a^2}{4(1-a^2)} \left( \frac{1-a}{1+a} \right)^n \\ b_{22} &= b_{33} = b_{77} = b_{88} = \frac{a}{2(1+a)^2} \\ b_{44} &= b_{55} = \frac{a^2}{4(1+a)^2} + \frac{a^2}{4(1-a^2)} \left( \frac{1-a}{1+a} \right)^n \\ b_{23} &= b_{32} = b_{46} = b_{64} = b_{56} = b_{65} = b_{78} = b_{87} = \frac{a}{2(1+a)} \left( -\frac{1}{1+a} \right)^n \\ b_{66} &= \frac{1}{(1+a)^2} \end{aligned} \quad (31)$$

It is easy to check that  $\rho(i, j)$  has a block-diagonal form.

### III. ENTANGLEMENT MEASURES $S(i)$ , $S(i, j)$ , $G(2, n)$

We now determine the entanglement content of the ground state  $|\psi_0\rangle$  (Eq. (9)) of the Hamiltonian (Eq. (5)) using the entanglement measures  $S(i)$ ,  $S(i, j)$ , and  $G(2, n)$ . The calculations are carried out for different values of the parameter  $a$  in Eq. (8). The ultimate aim is to probe the special features, if any, of entanglement in the vicinity of the QCP at  $a = 0$ . From Eq. (3) and (26), the one-site entanglement

$$S(i) = \frac{1}{1+a} [(1+a)\log_2(1+a) - a\log_2 a + a] \quad (32)$$

Figure 1 (top) shows the variation of  $S(i)$  w.r.t.  $a$ . The one-site entanglement has the maximum possible value  $\log_2 3$ . This is attained at the AKLT point  $a = 2$ . The VBS state is in this case the exact ground state. In the VBS state, each spin-1 at a specific lattice site can be considered as a symmetric combination of two spin- $\frac{1}{2}$ 's [14]. In the VBS state, each spin- $\frac{1}{2}$  at a particular lattice site forms a spin singlet with a spin- $\frac{1}{2}$  at a neighbouring lattice site.  $S(i)$  has the value zero at the QCP  $a = 0$ . Figure 1 (bottom) shows the variation of  $\frac{\partial S(i)}{\partial a}$  with the parameter  $a$ . The derivative diverges as the QCP is approached. This is the expected behaviour at the QCP of a conventional QPT. In the latter case, however,  $S(i)$  has the maximum value at the QCP [3].

From Eq. (1) and (31), the two-body entanglement  $S(i, j)$  is

$$S(i, j) = - \sum_{i=1}^9 \lambda_i \log_2 \lambda_i \quad (33)$$

Where  $\lambda_i$ 's are the eigenvalues of the reduced density matrix  $\rho(i, j)$ . These are given by

$$\begin{aligned} \lambda_1 &= \lambda_2 = \frac{a}{2(1+a)^2} - \frac{a}{2(1+a)} \left( -\frac{1}{1+a} \right)^n \\ \lambda_3 &= \lambda_4 = \frac{a}{2(1+a)^2} + \frac{a}{2(1+a)} \left( -\frac{1}{1+a} \right)^n \\ \lambda_5 &= \frac{a^2}{4(1+a)^2} + \frac{a^2}{4(1-a^2)} \left( \frac{1-a}{1+a} \right)^n \\ \lambda_6 &= \lambda_7 = \frac{a^2}{4(1+a)^2} - \frac{a^2}{4(1-a^2)} \left( \frac{1-a}{1+a} \right)^n \\ \lambda_8 &= \frac{1}{2} \left( \frac{a^2}{4(1+a)^2} + \frac{a^2}{4(1-a^2)} \left( \frac{1-a}{1+a} \right)^n + \frac{1}{1+a^2} \right) - \frac{1}{2(1+a)} \\ \lambda_9 &= \frac{1}{2} \left( \frac{a^2}{4(1+a)^2} + \frac{a^2}{4(1-a^2)} \left( \frac{1-a}{1+a} \right)^n + \frac{1}{1+a^2} \right) + \frac{1}{2(1+a)} \\ &\left( \frac{(a^2-4)^2}{16(1+a)^2} + 2a^2 \left( -\frac{1}{1+a} \right)^{2n} + \frac{a^4}{16(1-a)^2} \left( \frac{1-a}{1+a} \right)^{2n} + \frac{a^2(a^2-4)}{8(1-a^2)} \left( \frac{1-a}{1+a} \right)^{2n} \right)^{\frac{1}{2}} \\ &\left( \frac{(a^2-4)^2}{16(1+a)^2} + 2a^2 \left( -\frac{1}{1+a} \right)^{2n} + \frac{a^4}{16(1-a)^2} \left( \frac{1-a}{1+a} \right)^{2n} + \frac{a^2(a^2-4)}{8(1-a^2)} \left( \frac{1-a}{1+a} \right)^{2n} \right)^{\frac{1}{2}} \end{aligned} \quad (34)$$

Knowing the reduced density matrix  $\rho(i, j)$ , the correlation functions  $\langle S_i^\alpha S_j^\alpha \rangle$  ( $\alpha = x, y, z$ ) can be calculated in the usual manner. One then recovers the expressions in Eq. (13) and (14) ( $r = n + 1$ , where  $n = |j - i|$ ). Figure 2 (top) shows the variation of  $S(i, j)$  as a function of  $a$  for  $n = 1000$ . Figure 2 (bottom) shows the variation of the derivative  $\frac{\partial S(i, j)}{\partial a}$  w.r.t.  $a$  for the same value of  $n$ . The maximum of  $S(i, j)$  is at the AKLT point  $a = 2$  and has the value zero at  $a = 0$ . For large  $n$ , the derivative  $\frac{\partial S(i, j)}{\partial a}$  diverges near the QCP at  $a = 0$ . The last feature is characteristic of a conventional QPT [7].

We next calculate the GGE  $G(2, n)$  (Eq. (4)). This is easily done as the matrix elements of the reduced density matrix (Eq. (3)) are known. Figure 3 (top) shows the variation of  $G(2, n)$  versus  $a$  for  $n = 1000$ . Figure 3 (bottom) shows the plot of  $\frac{\partial G(2, n)}{\partial a}$  against  $a$ . Again  $G(2, n)$  has the maximum value at the AKLT point and is zero at  $a = 0$ . The derivative  $\frac{\partial G(2, n)}{\partial a}$  does not diverge as  $a \rightarrow 0$  in contrast to the case of a conventional QPT [6]. The derivative, however, attains the maximum value at the QCP  $a = 0$ . Figure 4 (top) shows the plots of  $S(i)$ ,  $S(i, j)$ , and  $G(2, n)$  versus  $a$  for  $n = 1000$ . Figure 4 (bottom) shows the plots of the first derivatives of the same quantities w.r.t.  $a$  for  $n = 1000$ . The plots are shown for comparing the different entanglement measures.

We next determine the EL  $\xi_E$  and its variation w.r.t. the parameter  $a$ . We consider the entanglement measure  $S(i, j)$  for this purpose. Close to the QCP  $a = 0$  and in the limit of large  $n$ , one can write

$$S(n = |j - i|) - S(\infty) \sim A_e e^{-\frac{n}{\xi_E}} \quad (35)$$

The longitudinal and transverse correlation functions,  $p_n^z = \langle S_1^z S_{n+1}^z \rangle$  and  $p_n^x = \langle S_1^x S_{n+1}^x \rangle$  are given by Eq. (13) and (14) with  $r = n + 1$ . For  $a < 1$ ,  $p_n^z$  decays faster than  $p_n^x$  with  $n$ . The eigenvalues  $\lambda_i$ 's,  $i = 1, \dots, 9$ , can be expressed in terms of the correlation functions  $p_n^z$  and  $p_n^x$ . For large  $n$ , the contributions from  $p_n^z$  can be ignored. The eigenvalues now reduce to the expressions

$$\begin{aligned} \lambda_1 = \lambda_2 &= \frac{a}{2(1+a)^2} - 4p_n^x \\ \lambda_3 = \lambda_4 &= \frac{a}{2(1+a)^2} + 4p_n^x \\ \lambda_5 &= \frac{a^2}{4(1+a)^2} \\ \lambda_6 = \lambda_7 &= \frac{a^2}{4(1+a)^2} \\ \lambda_8 &= \frac{1}{2} \left( \frac{a^2}{4(1+a)^2} + \frac{1}{1+a^2} \right) - \frac{1}{2} \left( \frac{(a^2-4)^2}{16(1+a)^2} + 2(p_n^x)^2 \right)^{\frac{1}{2}} \\ \lambda_9 &= \frac{1}{2} \left( \frac{a^2}{4(1+a)^2} + \frac{1}{1+a^2} \right) + \frac{1}{2} \left( \frac{(a^2-4)^2}{16(1+a)^2} + 2(p_n^x)^2 \right)^{\frac{1}{2}} \end{aligned} \quad (36)$$

From Eq. (1) and (36), one ultimately arrives at the expressions

$$S(n = |j - i|) - S(\infty) \sim A'_e (p_n^x)^2 \sim A_e e^{-\frac{n}{\xi_E}} \quad (37)$$

The pre-factor  $A_e = 0$  at the QCP  $a = 0$ . The EL  $\xi_E$  is given by

$$\xi_E = \frac{\xi_t}{2} = \frac{1}{2 \ln(1+a)} \quad (38)$$

where  $\xi_t$  is the transverse correlation length (Eq. (15)). In the case of the  $S = \frac{1}{2}$  anisotropic XY model in a transverse field, an expression similar to that in Eq. (37) is obtained close to the QCP in the limit of large  $n$  [7]. The pre-factor in this case, however, does not vanish at the QCP but has a power-law dependence on  $n$ . Figure 5 shows the variation of  $\xi_E$  w.r.t.  $a$  based on the entanglement measure  $S(i, j)$ .

The total correlations, with both classical and quantum components, between two sites  $i$  and  $j$  are quantified in terms of the quantum mutual information [21, 22]

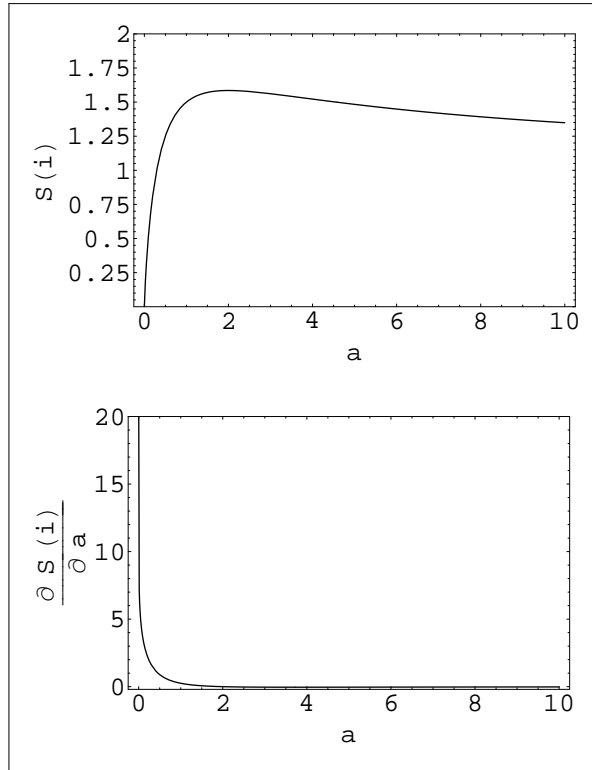
$$I_{ij} = S(i) + S(j) - S(i, j) \quad (39)$$

As explained in [21], a comparison of the singular behaviour of  $S(i)$  with that of  $I_{ij}$  allows one to determine whether two-point ( $Q2$ ) or multipartite ( $QS$ ) quantum correlations are important in a QPT. Figure 6 (top) shows a plot of  $I_{ij}$  versus  $a$  for  $n = 1000$ . Figure 6 (bottom) shows the variation of  $\frac{\partial I_{ij}}{\partial a}$  versus  $a$  for  $n = 1000$ . The derivative does not diverge as  $a \rightarrow 0$ , a behaviour distinct from that of  $\frac{\partial S(i)}{\partial a}$  close to  $a = 0$ . The difference in the singular behaviour of quantities associated with  $S(i)$  and  $I_{ij}$  indicates that multipartite quantum correlations are involved in the QPT.

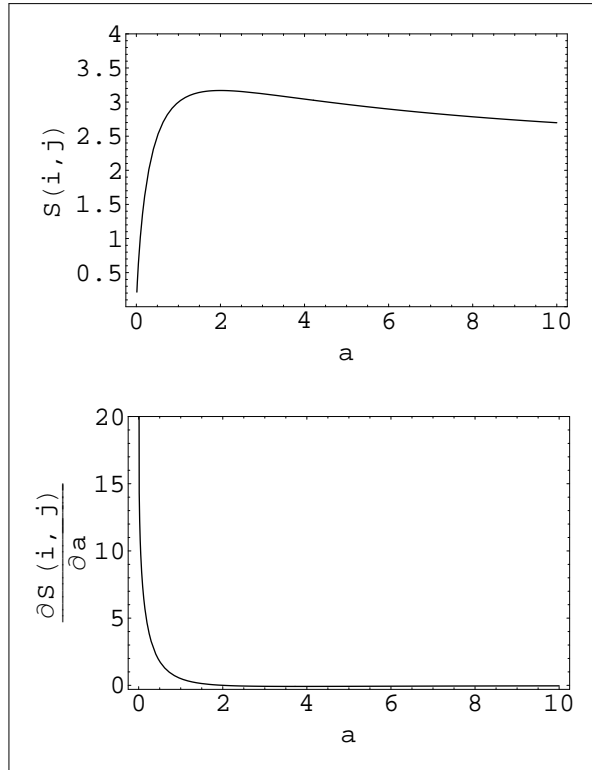
## IV. DISCUSSIONS

The MP states provide exact representations of the ground states of several spin models in low dimensions [17]. The remarkable features of such states arises from the fact that complicated many body states have a simple factorized form. The simplicity in structure makes the calculation of the ground state expectation values particularly easy to perform. The spin-1 AKLT model is a well-known example of a spin model in 1d the exact ground state of which (a VBS state) has an MP representation. The AKLT model and the spin-1 Heisenberg AFM chain belong to the same universality class [23]. The insight gained from the study of models in the MP formalism is expected to be of relevance in understanding the properties of more physical systems. The MP states also serve as good trial wave functions for standard spin models. The MP representation lies at the heart of the powerful density matrix renormalization group (DMRG) method and provides the basis for several interesting developments in quantum information [24].

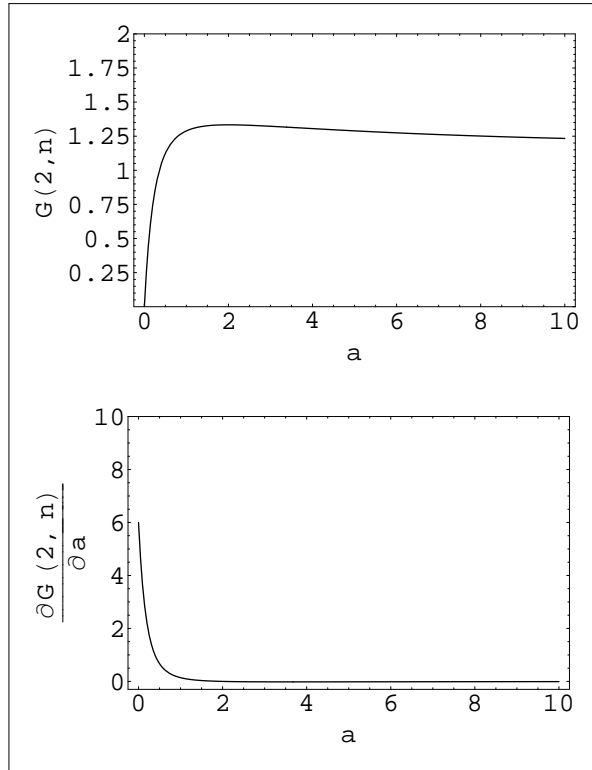
Studies of the entanglement characteristics of the MP states have begun only recently. The QPTs which occur in such states have characteristics different from



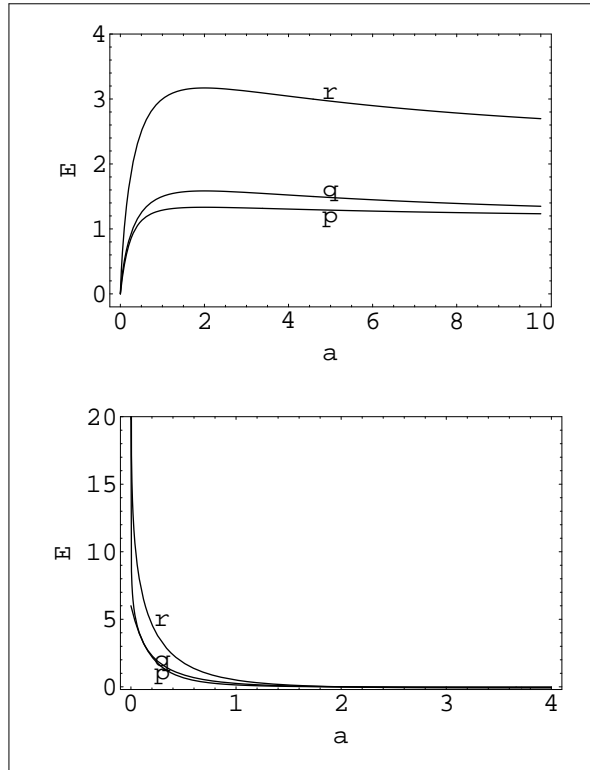
**FIG. 1:** Plot of  $S(i)$  (top) and  $\frac{\partial S(i)}{\partial a}$  (bottom) vs.  $a$  .



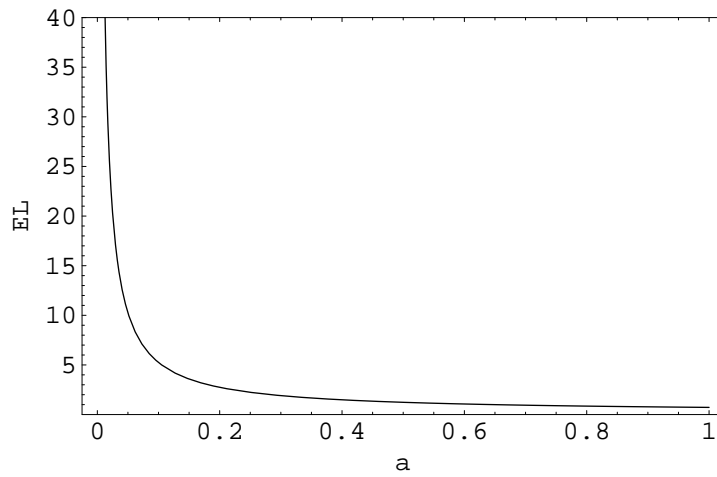
**FIG. 2:** Plot of  $S(i, j)$  (top) and  $\frac{\partial S(i, j)}{\partial a}$  (bottom) as a function of  $a$ .



**FIG. 3:** Plot of  $G(2, n)$  (top) and  $\frac{\partial G(2, n)}{\partial a}$  (bottom) as a function of  $a$ .

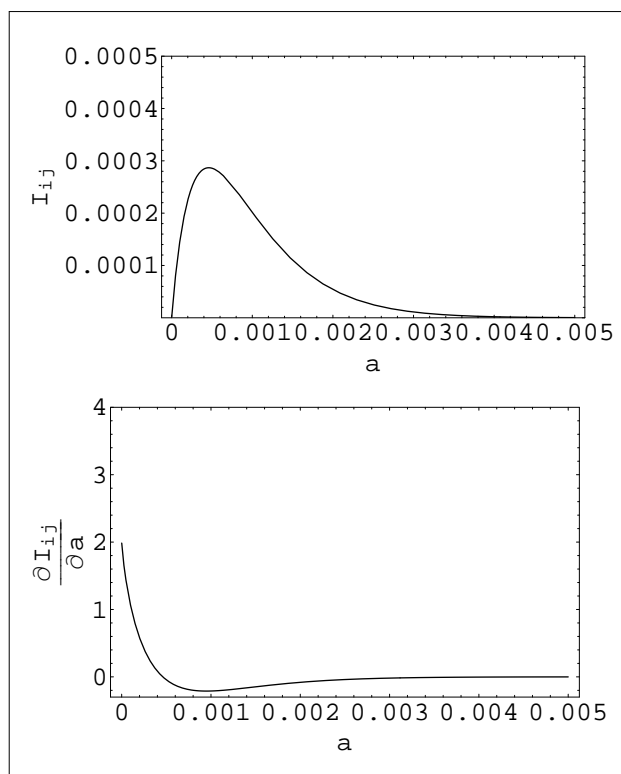


**FIG. 4:** Plots of  $S(i)$  ( $q$ ),  $S(i, j)$  ( $r$ ), and  $G(2, n)$  ( $p$ ) (top) and the corresponding first derivatives w.r.t.  $a$  (bottom) as a function of  $a$ .  $E$  represents the entanglement measure.



**FIG. 5:** Plot of  $EL$  as a function of  $a$ .





**FIG. 6:** Plots of  $I_{ij}$  (top) and  $\frac{\partial I_{ij}}{\partial a}$  (bottom) as a function of  $a$ .

those of conventional QPTs. It is thus of considerable interest to determine whether the entanglement content of MP states develops special features close to a QCP. In this paper, we consider a spin-1 model the exact ground state of which is of the MP form over a wide range of parameter values. The model exhibits a novel QPT in that the longitudinal and transverse correlation lengths diverge as the QCP is approached but the correlation functions vanish at the QCP. In a conventional QPT, the correlation functions have a power-law decay at the QCP. In the spin-1 model, the divergence of correlation lengths is accompanied by the excitation gap going to zero. The string order parameter, which has a non-zero expectation value in the MP state for  $a > 0$ , vanishes at the QCP  $a = 0$ . The distinctive signatures indicate the appearance of a new phase. We study the entanglement properties of the MP state for different values of the parameter  $a$ . The measures used are  $S(i)$  (one-site von Neumann entropy),  $S(i, j)$  (two-body entanglement) and  $G(2, n)$  (GGE). All the entanglement measures have zero value at the QCP so that the ground state is disentangled at that point. As seen from the different plots, figures (1), (2), (3), and (4), the entanglement content, as measured by  $E = S(i)$ ,  $S(i, j)$  and  $G(2, n)$ , has a slow variation w.r.t.  $a$  for  $a > 2$ . At the AKLT point  $a = 2$ ,  $E$  reaches its maximum value and as  $a$  is reduced further, the magnitude of  $E$  falls rapidly to approach zero value at  $a = 0$ . The study of conventional QPTs shows that  $E$  is maximum at a QCP [3, 6, 7]. Also,  $\frac{\partial E}{\partial a}$  diverges as the QCP is approached. The EL,  $\xi_E$ , as calculated from  $S(i, j)$  and  $G(2, n)$  for large  $n$ , also diverges with  $\xi_E = \frac{\xi_C}{2}$  where  $\xi_C$  is the usual correlation length. In the case of the spin-1 model under consideration,  $\frac{\partial E}{\partial a}$  diverges as  $a \rightarrow 0$  when  $E = S(i)$  and  $S(i, j)$ . The EL,  $\xi_E$ , as calculated from  $S(i, j)$  in the large  $n$  limit, also diverges with  $\xi_E = \frac{\xi_C}{2}$ . One now has the interesting situation that the entanglement content of the MP state decreases as  $a \rightarrow 0$  but the entanglement is spread over larger distances. The derivative  $\frac{\partial G(2, n)}{\partial a}$ , however, does not diverge as  $a \rightarrow 0$  but attains a maximum value at the QCP. The results can be understood by noting that in all the three cases,  $E = S(i)$ ,  $S(i, j)$  and  $G(2, n)$ , the reduced density matrices  $\rho(i)$  and  $\rho(i, j)$  smoothly approach the forms associated with pure states as the parameter  $a$  tends to zero. The matrix elements of the reduced density matrices do not develop non-analyticities in the parameter region of interest. Thus, the energy density, calculated from the reduced density matrix  $\rho(i, j)$ , does not develop a non-analyticity at the QCP. The derivative  $\frac{\partial G(2, n)}{\partial a}$  depends upon the first derivatives of the matrix elements of  $\rho(i, j)$ . Since the latter is analytic for  $a \geq 0$ ,  $\frac{\partial G(2, n)}{\partial a}$  does not diverge in the whole parameter regime including the point  $a = 0$ . In the cases of the entanglement measures  $E = S(i)$  and  $S(i, j)$ , the derivative  $\frac{\partial E}{\partial a}$  diverges as  $a \rightarrow 0$  due to the divergence of  $\log_2 a$  in the same limit. The divergence is thus due to the special form of the von Neumann entropy and occurs for  $n \geq 1$ . A recent work [25] provides another example of such a singularity. Though  $\frac{\partial G(2, n)}{\partial a}$  does

not diverge or become discontinuous at the QCP  $a = 0$ , it attains its maximum value at the point. The first derivative of the string order parameter w.r.t.  $a$  also attains its maximum value at  $a = 0$  though the order parameter itself vanishes at the point. Figure (4) shows that amongst the three entanglement measures  $E = S(i)$ ,  $S(i, j)$  and  $G(2, n)$ , used in this study to obtain a quantitative estimate of the entanglement content of the MP ground state, the measure  $S(i, j)$  yields the largest value of the entanglement at different values of  $a$ . The difference in the singular behaviour of the measures  $S(i)$  and the mutual information entropy  $I_{ij}$  as  $a \rightarrow 0$  indicates that multipartite quantum correlations are involved in the QPT. In summary, the present study identifies the entanglement characteristics of the MP ground state of a spin-1 model close to the critical point  $a = 0$ . The features are distinct from those associated with conventional QPTs. Several spin models are known for which the MP states are the exact ground states [17]. Some of these models have interesting phase diagrams exhibiting both first and second order phase transitions. It will be of interest to extend the present study to other spin models (both  $S = \frac{1}{2}$  and 1) in order to identify the universal characteristics of QPTs in MP states.

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