Entanglement in first excited states of some many-body quantum spin systems: indication of quantum phase transition

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(Dated: September 22, 2020)

We compute concurrence, a measure of bipartite entanglement, of the first excited state of the 1-D Heisenberg frustrated $J_1$-$J_2$ spin-chain and observe a sudden change in the entanglement of the eigenstate near the coupling strength $\alpha = J_2/J_1 \approx 0.241$, where a quantum phase transition from spin-fluid phase to dimer phase has been previously reported. We numerically observe this phenomena for spin-chain with 8 sites to 16 sites, and the value of $\alpha$ at which the change in entanglement is observed asymptotically tends to a value $\alpha_c \approx 0.24116$. We have calculated the finite-size scaling exponents for spin chains with even and odd spins. It may be noted that bipartite as well as multipartite entanglement measures applied on the ground state of the system, fail to detect any quantum phase transition from the gapless to the gapped phase in the 1-D Heisenberg frustrated $J_1$-$J_2$ spin-chain. Furthermore, we measure bipartite entanglement of first excited states for other spin models like 2-D Heisenberg $J_1$-$J_2$ model and Shastry-Sutherland model and detect quantum phase transitions.

I. INTRODUCTION

Advances in technology in the field of low temperature experiments have made it possible to engineer some quantum many-body Hamiltonians using ultracold atoms and ions [1]. Such quantum spin systems may be important as substrates for quantum computation. Quantum entanglement is a resource for quantum computational tasks. Therefore, it is important to study and understand entanglement in such systems. Bipartite and multipartite entanglement [2-7] in ground states of quantum spin systems have been studied and critical quantum phenomena [8-14] have been detected. However, entanglement of low lying excited states of quantum spin systems have not been exhaustively studied [15-17]. In this paper, we compute a nearest neighbor bipartite entanglement measure namely concurrence [18] of qubits in first excited states of some non-integrable quantum spin systems.

The systems that we have studied are the one dimensional Heisenberg frustrated $J_1 - J_2$ spin-chain, the two dimensional Heisenberg $J_1 - J_2$ spin system and the Shastry-Sutherland model. The ground states of these systems have been investigated and bipartite and multipartite quantum entanglement have been measured [8]. Quantum phase transitions (QPT), a zero temperature phase transition driven by system parameters [19], have been detected in some of the cases. However, the quantum phase transition from the spin fluid phase to dimer phase has not been detected using any quantum entanglement measure for the one dimensional Heisenberg frustrated $J_1 - J_2$ spin-chain. The quantum phase transition from the gapless phase to the gapped phase in the one dimensional Heisenberg frustrated $J_1 - J_2$ spin chain was investigated by Haldane [20], Tonegawa and Harada [21], Okamoto and Nomura [22] using exact diagonalization and field theory methods. It was reported that the ground state is in the gapless or gapped phase depending on the value of the coupling strength $\alpha$. The quantum phase transition point was estimated by investigating the singlet-triplet energy gap of finite size systems [21] followed by extrapolation to infinite system. In Ref. [22], the phase transition point was determined by investigating the difference between the singlet-triplet gap and the singlet-singlet gap for finite size systems. In Ref. [21, 22], the singlet-triplet energy gap was defined as

$$G_{\alpha l}(N,\alpha) \equiv E_{1}^{(0)}(N,\alpha) - E_{0}^{(0)}(N,\alpha)$$

while the singlet-singlet energy gap was defined as

$$G_{\alpha s}(N,\alpha) \equiv E_{0}^{(1)}(N,\alpha) - E_{0}^{(0)}(N,\alpha)$$

where $E_{0}^{(0)}(N,\alpha)$ and $E_{0}^{(l)}(N,\alpha)$ are the ground state energy and the $l$th excited state energy in the $S_{total} = m$ subspace, respectively.

The first excited states of the systems, considered in this paper, are degenerate. Let $| E_1 \rangle$ denote the $i$-th degenerate eigenstate corresponding to the eigenenergy $E_1$. Then the density matrix corresponding to the first excited $d$-fold degenerate eigenstate is given by

$$\rho_{1} = \frac{1}{d} \sum_{i=1}^{d} | E_{1,i} \rangle \langle E_{1,i} |$$

Note that in this paper we do not consider different total spin subspaces explicitly.

We measure the nearest neighbor concurrence of the first excited state $\rho_1$ of the spin chain, and notice a sudden change in the value of concurrence near the quantum phase transition point [22, 23]. The computation along with the appropriate scaling analysis is done for spin chains consisting of 8 to 16 qubits. The scaling analysis and the corresponding finite size scaling exponents are different for even and odd spin chains. The quantum critical point $\alpha_c \approx 0.24116$ is estimated from the scaling analysis of spin chains with even number of qubits.
The finite size scaling exponent $\beta = -1.962$. The concurrence versus driving parameter plot Fig. 1 for spin chains with odd number of qubits shows two discontinuities with both of them converging to the quantum phase transition point in the asymptotic limit. The scaling exponent of the right shifting and left shifting discontinuities are $\beta_R = -1.92$ and $\beta_L = -2.082$ respectively. The nearest neighbor concurrence of first excited states of the two dimensional Heisenberg $J_1-J_2$ spin system and the Shastry-Sutherland model for 16 qubits in a $(4 \times 4)$ sites square lattice have also been calculated. We get indications of quantum phase transition in both the systems.

In Section III we discuss the results for the one dimensional Heisenberg $J_1-J_2$ model in details and highlight the importance of investigating the low lying excited states in quantum spin systems. In Sections III and IV we discuss the results obtained for the two dimensional Heisenbergs $J_1-J_2$ model and Shastry-Sutherland spin model respectively. Finally, we discuss our method and results and conclude in Section V.

II. THE ONE DIMENSIONAL HEISENBERG $J_1-J_2$ SPIN CHAIN

We consider the Heisenberg frustrated one dimensional $J_1-J_2$ model in which the nearest neighbor couplings $J_1$ and the next nearest neighbor couplings $J_2$ are both antiferromagnetic. The Hamiltonian of the system is given by

$$H_{1D} = J_1 \sum_{i=1}^{N} \hat{\sigma}_i \hat{\sigma}_{i+1} + J_2 \sum_{i=1}^{N} \hat{\sigma}_i \hat{\sigma}_{i+2}$$

(4)

Here, $N$ represents the number of sites present in the spin chain, $J_1$ and $J_2$ are antiferromagnetic coupling coefficients of nearest and next nearest neighbor interactions and $\hat{\sigma} = \sigma^x \hat{z} + \sigma^y \hat{y} + \sigma^z \hat{x}$ where $\sigma^x, \sigma^y, \sigma^z$ are the Pauli spin matrices. Some solid state systems like SrCuO$_2$ may be described by this Hamiltonian [24]. Periodic boundary condition, $\sigma_{N+1} = \sigma_1$, has been imposed on all systems that have been investigated in this paper. It was known previously that this spin system goes from spin-fluid phase to dimer phase around $\alpha = J_2/J_1 \approx 0.241$. In the weakly frustrated region, $0 < \alpha < 0.24$ the system is gapless while it enters a gapped region for higher values of the coupling parameter [25–27].

It may be noted that for a two qubit state $\rho$, concurrence $C$ is defined as [18] $max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$, where $\lambda_1, \lambda_2$ are the square roots of eigenvalues of $\rho(\sigma^y \otimes \sigma^y)\rho^*(\sigma^y \otimes \sigma^y)$ in decreasing order and $\rho^*$ is complex conjugate of $\rho$. We perform exact diagonalization of the system Hamiltonian for system sizes $N = 8$ to $N = 15$. For large spin chains ($N > 15$) we are unable to use the exact diagonalization technique to calculate the eigenvalues and eigenvectors due to memory constraint of the computers used for computation. For $N = 16$, we use ARPACK (available in MATLAB that uses Lanczos algorithm) to calculate first 6 low lying eigen states. The results obtained using the Lanczos algorithm is compared with exact diagonalization results for system sizes up to $N = 15$ and both the eigenvalues and eigenvectors are found to be fairly accurate. We find the ground state and the low lying excited states and calculate the nearest neighbor concurrence, after tracing out the other qubits. In Fig. 1(a), we plot the nearest neighbor concurrence for the first excited states for the systems with even number of qubits from $N = 8$ to $N = 16$ and notice discontinuities in the plots in the vicinity of the quantum phase transition point. In Fig. 1(b), we plot the nearest neighbor concurrence for the first excited states for the systems with odd number of qubits from $N = 9$ to $N = 15$ and notice a pair of discontinuities in the plots in the vicinity of the quantum phase transition point. Finite size scaling analysis is done for data obtained for both even and odd qubits. In Fig. 2 we plot the nearest neighbor concurrence of the ground state as well as of the first excited state for the spin chain with $N = 16$. The plot of nearest neighbor concurrence for qubits is continuous across the QPT point for the ground state of the system whereas we notice a sudden drop in the value of concurrence in the vicinity of the quantum critical point at $\alpha_{16}^c = 0.24248$. The discontinuity of the bipartite entanglement of the first excited state of the system indicates the quantum phase transition point whereas a similar probe applied to the ground state of the same system fails to detect the quantum phase transition.

| $N_{(even)}$ | $\alpha_c$ | $N_{(even)}$ | $\alpha_{c,R}$ | $\alpha_{c,L}$ |
|-------------|----------|-------------|---------------|--------------|
| 8           | 0.24630  | 9           | 0.10855       | 0.33049      |
| 10          | 0.24449  | 11          | 0.14910       | 0.29944      |
| 12          | 0.24349  | 13          | 0.17465       | 0.28243      |
| 14          | 0.25288  | 15          | 0.19145       | 0.27199      |
| 16          | 0.24248  |             |               |              |

TABLE I. The driving parameter corresponding to the discontinuities in the nearest neighbor concurrence is listed against the appropriate number of qubits.

In Table I we have listed the values of the driving parameters at the discontinuities of the nearest neighbor concurrence of the first excited states for spin chains of $N = 8$ to $N = 16$ qubits. Similar results for even number of qubits were found earlier using conformal field theory by K. Okamoto and K. Nomura [22] for the QPT point, and our calculated values match with their results up to the fourth decimal place. The discontinuities associated with even spin chains are closer to the quantum phase transition point. The numerical values of $\alpha_c^N$ decrease with increasing $N$ for even number of qubits and asymptotically tend towards a fixed value $\alpha_c$. We fit a rational function $F(N)$ with second degree polynomials in numerator and denominator through the tabulated values associated with even spin chains:

$$F(N) = \frac{p_1 N^2 + p_2 N + p_3}{N^2 + q_1 N + q_2}$$

(5)
FIG. 1. (color online) Nearest neighbor concurrence in ebits of the first excited state of the 1-D $J_1 - J_2$ Hamiltonian is plotted with respect to the dimensionless system parameter $\alpha$, (a) for spin chains with even number of qubits and (b) for spin chains with odd number of qubits.

where $p_1 = 0.2412$, $p_2 = 0.1477$, $p_3 = 0.4848$, $q_1 = 0.6151$, and $q_2 = 0.5081$. In Fig. 3 we plot the position of discontinuities of the nearest neighbor concurrence $\alpha_{N_{\text{even}}}$ with respect to system size $N$. We choose the rational function because of its known advantages in extrapolation. The QPT point is estimated to be at $\alpha_c \approx 0.24116$ from the extrapolated function.

It may be noted that there are two discontinuities in nearest neighbor concurrence of odd spin chains which appear to asymptotically converge to some point of the system parameter $\alpha$. We have listed the right shifting as well as left shifting discontinuities for spin chains with odd number of particles from $N = 9$ to $N = 15$ in Table. From the previous equation we note that $\alpha_{N_{\text{even}}}^{(\text{odd})}$ approaches $\alpha_c$ as $N^{-1.962}$. The scaling exponent obtained, using this method of detection of QPT point, $\beta = -1.962$ is significantly high. We use the value of $\alpha_c$ obtained by analysing the even spin chains for the scaling analysis of odd spin chains. In Fig. 3 (b) and Fig. 3 (c) we plot $\log_2 \left( \frac{\alpha_{c_{R}}^{N_{\text{odd}}}}{\alpha_c} \right)$ and $\log_2 \left( \frac{\alpha_{c_{L}}^{N_{\text{odd}}}}{\alpha_c} \right)$ with respect to $\log_2 (N)$, to study the right-shifting and left-shifting discontinuities of odd spin chains. The SSE associated with the plots are $7.2094 \times 10^{-5}$ and $1.3726 \times 10^{-4}$ respectively and the corresponding equations may be written
FIG. 4. (color online) (a) $\log_2(N_{\text{even}}/\alpha_c)$ versus $\log_2(N)$ plot, (b) $\log_2(N_{\text{odd}}/\alpha_c)$ versus $\log_2(N)$ plot and (c) $\log_2(N_{\text{odd}}/\alpha_c)$ versus $\log_2(N)$ plot.

As

$$\alpha_{c,R}^{N_{\text{odd}}} = \alpha_c + 9.082 \times N^{-1.92}$$

$$\alpha_{c,L}^{N_{\text{odd}}} = \alpha_c + 8.64 \times N^{-2.082}.$$  

The data points for the odd spin chains fit very well in the finite size scaling plot and the right and left shifting discontinuities approach $\alpha_c$ as $N^{-1.92}$ and $N^{-2.082}$ respectively.

FIG. 5. (color online) Nearest neighbor concurrence in ebits of the ground state and first excited state of the 2-D $J_1 - J_2$ Hamiltonian is plotted with respect to dimensionless system parameter $\alpha$ for system size $N = 16$ (using partial ARPACK diagonalization). The solid black dots represent first excited state concurrence ($C_{16}^{1\text{e}}$) and smaller blue dots represent ground state concurrence ($C_{16}^{0\text{e}}$).

III. THE TWO DIMENSIONAL HEISENBERG J$_1$ - J$_2$ SPIN SYSTEM

We consider an arrangement of qubits in two dimensional square lattice, where the nearest neighbor spins are coupled by Heisenberg interactions, with coupling strength $J_1$ and the next nearest neighbor or diagonal spins are coupled by the same interactions with coupling strength $J_2$. The coupling strengths $J_1$ and $J_2$ are positive. Magnetic materials such as $\text{Li}_2\text{VOSiO}_4$ and $\text{Li}_2\text{VOGeO}_4$ can be described by this Hamiltonian \[28-32\]. We measure first excited state nearest neighbor concurrence in a square lattice with $(4 \times 4)$ sites. The system Hamiltonian is given by

$$H_{2D} = J_1 \sum \sigma_i \sigma_j + J_2 \sum \sigma_i \sigma_k (10)$$

where $i, j$ are nearest neighbors (horizontal or vertical) and $i, k$ are next nearest neighbors or diagonal spins. $J_1$ and $J_2$ are antiferromagnetic. Periodic boundary condition is imposed during computation. The spin model has been studied using exact diagonalization, field theory methods \[33-35\], but the exact phase boundaries are not known. It is predicted that there are two long range ordered phases separated by quantum paramagnetic phase without long range order, in the system. It has also been predicted that quantum phase transitions exist from ordinary-\textit{Néel} order to intermediate phase and from that intermediate phase to collinear-\textit{Néel} order at $\alpha \approx 0.4$ and $\alpha \approx 0.6$ respectively \[36, 37\]. The intermediate phase \[38\] is predicted as plaquette or columnar dimer phase \[39, 47\] as well as spin fluid phase \[48, 50\].

It can be seen from Fig. 5 that the nearest neighbor concurrence of the ground state goes to zero and indicates the columnar-dimer to collinear-\textit{Néel} QPT at $\alpha = 0.58$. Further, there is a sudden disappearance of nearest neighbor concurrence of the first excited state at $\alpha = 0.4078$, indicating the ordinary-\textit{Néel} to columnar-
FIG. 6. The Shastry-Sutherland lattice with 16 sites. The horizontal and vertical lines represent nearest neighbor coupling strength $J_1$ and the specific diagonal lines represent next nearest neighbor coupling strength $J_2$.

dimer QPT point. Note that the ground state nearest neighbor concurrence does not detect the ordinary-Néel to columnar-dimer QPT point.

IV. THE SHASTRY-SUTHERLAND SPIN SYSTEM

We study the entanglement properties of the first excited state of the Shastry-Sutherland quantum spin Hamiltonian for a $(4 \times 4)$ square lattice, the schematic diagram of which is shown in Fig. 6.

The Hamiltonian of the spin system is given by

$$H_{SS} = J_1 \sum_i \vec{\sigma}_i \cdot \vec{\sigma}_j + J_2 \sum_k \vec{\sigma}_k \cdot \vec{\sigma}_l \quad (11)$$

where $i, j$ are the nearest neighbors (horizontal and vertical) and $k, l$ are the specific diagonal pairs shown in Fig. 6. The coupling strengths $J_1$ and $J_2$ are both positive. Periodic boundary condition is imposed during computation.

It is predicted that the system goes through two quantum phase transitions from Néel to intermediate phase and from intermediate phase to dimer, driven by quantum fluctuations. The nature of the intermediate phase is not yet known. The quantum phase transition from an intermediate phase to dimer phase has been predicted by multipartite as well as multipartite entanglement measures applied on the ground state of the system at $\alpha \approx 1.53$. However, for this system a multipartite entanglement measure, namely the generalised geometric measure applied on the ground state of the system detects both the quantum critical points, from Néel to intermediate phase at $\alpha \approx 1.05$ and from intermediate phase to dimer at $\alpha \approx 1.53$.

In Fig. 7 we note that for $\alpha \geq 1.52798$ the nearest neighbor concurrence of the first excited eigenstate of the Hamiltonian $H_{SS}$ ($C_{16}^{16}$) suddenly becomes zero. The drop in the value of concurrence is sudden indicating the quantum phase transition.

V. DISCUSSIONS AND CONCLUSIONS

We have investigated the 1-D Heisenberg $J_1 - J_2$ spin chain, the 2D Heisenberg $J_1 - J_2$ spin system and the Shastry-Sutherland spin system from the viewpoint of bipartite entanglement of their low-lying eigen states. The quantum phase transition points and the phase diagrams of the above mentioned many-body spin systems have often been studied in the past. However, there remains a few unanswered questions regarding the behavior of such systems with respect to their quantum phase diagrams. We find that the bipartite quantum entanglement measure, concurrence of nearest neighbors in first excited states, is discontinuous with the variation of the driving parameter across the quantum phase transition points. It may be noted that bipartite and multipartite quantum entanglement measures applied on the ground state of the system Hamiltonian are unable to detect the quantum phase transition point for the 1D Heisenberg $J_1 - J_2$ spin system. This paper is not the first one to use first excited state. Prior to us Okamoto and Nomura in 1992, then, S. Chen and group in 2007 and may be more used the first excited state to detect the quantum phase transition of 1-dimensional frustrated $J_1 - J_2$ spin chain. G.-S. Tian and H.-Q. Lin in 2003 shows that level crossing of low lying excited states are actual reason of continuous quantum phase transitions when ground state level crossing is absent. As discussed in section-1 the paper by Okamoto and Nomura used singlet-triplet energy gap and singlet-singlet energy gap for their calculation. Although their calculation involves ground state energy but it is not sufficient to calculate energy gap. The singlet and triplet states with which the energy gap from ground state was calculated are actually some low lying excited states.
states with different total spin subspaces. So the low lying excited states necessarily included. However S. Chen and group \(5\) used fidelity of the first excited state.

\[
F(\alpha, \delta) = |\langle \psi(\alpha) | \psi(\alpha + \delta) \rangle|
\]  

(12)

Where \(\delta\) is the increment in \(\alpha\). Their results are direct outcome of energy level crossing between the first and second excited states. Fidelity actually measures how close two quantum states are. When there is a level crossing in between the two adjacent states (with increment in \(\alpha\)) are not close any more and fidelity drops for that single point only, after that the next adjacent state again close to the previous one (as no level crossing in between them) and fidelity catches its higher value onwards. Our present results actually in agreement with them. From Fig. 8 (b) we have seen several level crossing between the low lying excited states of 1-dimensional frustrated \(J_1 - J_2\) spin chain with even number of qubits, out of which the level crossing between \(1_{st}\) and \(2_{nd}\) excited states is exactly at the point of the qpt, which is the origin of the detection of qpt in all three methods discussed so far.

Although we used a different physical observable (entanglement) we may say that our results are actually a good extension of the idea of previous works. All three methods of detecting qpt of 1-dimensional frustrated \(J_1 - J_2\) spin chain with even number of qubits are originates from energy level crossing but level crossing is not a physical observable. The method of fidelity and entanglement are easier as the consideration of total spin sub spaces are not required. Fidelity shows a drop only for a single point but entanglement shows two different curves discontinuous at the qpt point. In case of entanglement we find where the curve is discontinuous and provide a table of the qpt points up to 5\(th\) decimal places using the bisection method (Table 1).

For the case of odd number of qubits we find two discontinuities and observed that both the discontinuities approaching towards the same qpt point, this portion is a new addition to the previous works. We may clearly see the reason of the two discontinuities from the energy level diagram of 15 qubits spin chain (Fig. 8(a)), i.e., there are actually two level crossing between the first and second excited states. This extension from the previous results picturize the situation much more clearly.

We further extend our method for the case of 2-dimensional frustrated \(J_1 - J_2\) spin model with 16 (4 \(\times\) 4) qubits and 2-dimensional Shastry-Sutherland spin model with 16 (4 \(\times\) 4) qubits. And detects qpt in both of them. We guess the method of fidelity is also applicable in these two spin models as well but we can not say now for the method of singlet-triplet energy gap and singlet-singlet energy gap as we do not consider total spin subspace.

For better understanding the energy level diagrams of these two models are depicted in Fig. 8(c) and Fig. 8(d). At last we say that the finite size scaling exponents, obtained using the present investigation for the 1D Heisenberg \(J_1 - J_2\) model, are quite high. The investigation of

![FIG. 8. (color online) Energy levels of ground and low lying excited state is plotted with respect to the dimensionless system parameter \(\alpha\) of the (a) 1-dimensional frustrated \(J_1 - J_2\) spin chain with odd number of qubits. (b) 1-dimensional frustrated \(J_1 - J_2\) spin chain with even number of qubits. (c) 2-dimensional frustrated \(J_1 - J_2\) spin model with 16 (4 \(\times\) 4) qubits. (d) 2-dimensional Shastry-Sutherland spin model with 16 (4 \(\times\) 4) qubits.](image-url)
low-lying excited states of such many-body Hamiltonians promises to shed more light on the behavior of quantum spin systems.

ACKNOWLEDGMENTS

We sincerely acknowledge the PARAM-Kanchenjunga High Performance Computer Centre, National Institute of Technology Sikkim for the support to conduct this research. We thank Ujjwal Sen for critical comments.
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