CHANGING ENTANGLEMENT STRUCTURES IN A FRUSTRATED TETRAMERIC SPIN SYSTEM WITH AN 'ENTANGLEMENT TRANSITION' POINT

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Abstract: *Exchange interactions in spin systems can bring about quantum entanglement in the ground and thermal states of the systems, which has been proved to be a resource for Quantum Information and Computation protocols. In this paper, we consider a spin tetramer, with spins of magnitude 1/2, in which the spins interact via nearest neighbour, and diagonal interactions* J_1, *and* J_2 *respectively. This kind of geometry is responsible for a phenomenon called frustration in a physical system. The ground and thermal state entanglement properties of the tetramer are calculated analytically. Both bipartite and multipartite entanglements are studied and a signature of quantum phase transition, which can also termed as 'entanglement transition", is detected.*

Keywords: **Molecular Magnets, Entanglement, Quantum Phase Transition**

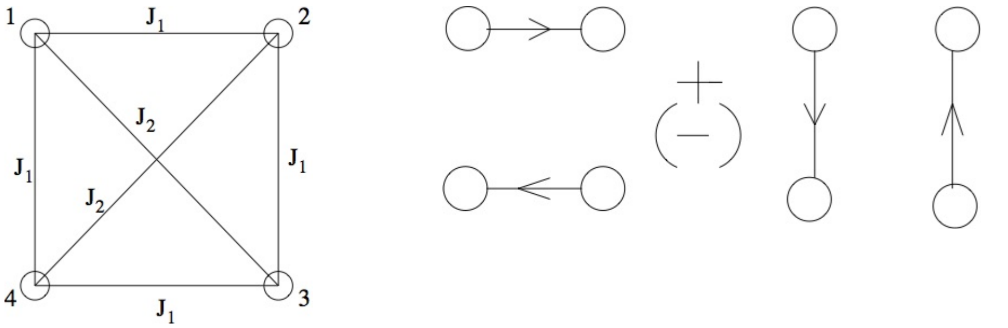
1. INTRODUCTION

Entanglement is a rudimentary property of quantum mechanical systems and gives rise to correlations in a physical system, which cannot be expected from classical considerations [1]. A pure state is said to be entangled if it cannot be written as a product of individual wave functions. For example, the singlet state of two spin- 1/2 particles, 1/2 (| ↑↓ 〉 -| ↓↑ 〉) , which cannot be written as a product of the spin states of individual spins. In the case of a mixed state, inseparability occurs if the density matrix is not a convex sum of product states. Entanglement plays an crucial role in applications related to quantum information and communication. Candidate systems for practical implementation of the said protocols include quantum spin systems in which exchange interactions are found to be responsible for entanglement [2].

Entanglement in a physical system can be classified as two types, bipartite and multipartite.. Bipartite (multipartite) entanglement involves two (more than two) subsystems. A number of appropriate quantification measures are available for bipartite entanglement, for both pure and mixed states of a composite system. The entanglement between a pair of spins, belonging to a chain of interacting spins, provides an example of bipartite entanglement. Bipartite and to a lesser extent multipartite entanglement properties of a variety of spin models have been studied so far at both zero and finite temperatures and including a tuning parameter like an external magnetic field or exchange inhomogeneity or anisotropy [3,4]. An issue of considerable interest is whether entanglement, a feature of pure quantum origin, develops special features in the vicinity of a quantum phase transition (QPT). A QPT occurs at T=0 and is brought about by tuning some system parameter, say, the exchange interaction strength or an external variable like the magnetic field to a critical value [5]. Some recent studies have explored the relation between entanglement and QPT in a variety of spin models and the main conclusion is that certain entanglement-related quantities exhibit features like scaling and singularity in the vicinity of a quantum critical point (QCP) [6]. In the case of first-order QPTs, the ground state concurrences may change discontinuously at the transition point [7]. A recent work on the ground state level crossings has coined the term 'entanglement transitions' where the transition from one state with a specific entanglement structure to another state with a different entanglement structure happens [8].

Studies on finite quantum spin systems acquire significant relevance in the context of molecular or nano-magnets. In such magnetic systems, the dominant exchange interactions are often confined to small spin clusters. The intercluster exchange interactions are much weaker in comparison so that the compounds can be assumed to consist of independent spin clusters. A recent study provides a number of examples of molecular magnets the thermodynamic and neutron scattering properties of which can be well described by small spin clusters like dimers, trimers and tetramers [9].

In this paper, we consider a spin cluster system of four (tetramer) spins in which pairwise entanglement between individual spins does not exhaust the total entanglement. The ground state and thermal entanglement properties of the tetramers are determined analytically. The system exhibits a QPT at special values of the exchange interaction strengths. This transition point can also be termed as the so-called 'entanglement transition' because the system exhibits very different entanglement structures and properties at the two sides of the said transition point [10]. The magnetic properties of the polyoxovanadate compound, (NHEt) 3 [V_8 IV V_4 V A s_8 O_{40} (H_2O)] . H_2O (designated as V12) are well explained by spin–1/2 AFM tetramers, with only nearest-neighbour (n.n.) interactions, and described by the isotropic Heisenberg exchange interaction Hamiltonian [9]. Also, this kind of model Hamiltonians for spin systems can be realized in ultra-cold atomic systems in optical lattices [11].



(a)

(b)

Figure 1: Tetramer with n.n. and diagonal interactions and Resonating Valence Bond (ψ_{RVB1} and ψ_{RVB2}) states of the 4-spin plaquette..

2. Entanglement properties of S= ½ AFM tetramer

We consider a tetramer of spins of magnitude ½ (Fig. 1(a)) described by the AFM Heisenberg exchange interaction Hamiltonian

$$H = \overline{J}_1(\vec{S}_1.\vec{S}_2 + \vec{S}_2.\vec{S}_3 + \vec{S}_3.\vec{S}_4 + \vec{S}_4.\vec{S}_1) + \overline{J}_2(\vec{S}_1.\vec{S}_3 + \vec{S}_2.\vec{S}_4) \quad (1)$$

where S_i is the spin operator at the ith site of the square plaquette, J_1 is the strength of the n.n. exchange interaction, J_2 that of the diagonal exchange interaction. The eigenvalue problem can be solved in the separate subspaces corresponding to the different values of $S_{z\ tot}$, which is a good quantum number. The results are displayed in the following:

$S_{z\ tot}$ =+2

$\psi_1 = |\uparrow\uparrow\uparrow\uparrow\rangle$

$$E_1 = (\overline{J}_1 + \overline{J}_2/2\ ) \quad (2)$$

$S_{z\,tot} = +1$

$\psi_2 = 1/2\,(|\uparrow\uparrow\uparrow\downarrow\rangle - |\uparrow\downarrow\uparrow\uparrow\rangle)$

$E_2 = -(\bar{J}_2/2)$ (3)

$\psi_3 = 1/2\,(|\uparrow\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\uparrow\rangle)$

$E_3 = -(\bar{J}_2/2)$ (4)

$\psi_4 = 1/4\,(|\uparrow\uparrow\uparrow\downarrow\rangle + |\uparrow\uparrow\downarrow\uparrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\uparrow\rangle)$

$E_4 = (\bar{J}_1 + \bar{J}_2/2)$ (5)

$\psi_5 = 1/2\,(|\uparrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\uparrow\rangle)$

$E_5 = (-\bar{J}_1 + \bar{J}_2/2)$ (6)

$S_{z\,tot} = 0$

$\psi_6 = 1/2\,(|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle)$

$E_6 = -(\bar{J}_2/2)$ (7)

$\psi_7 = 1/2\,(|\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle)$

$E_7 = -(\bar{J}_2/2)$ (8)

$\psi_8 = 1/2\,(|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle)$

$E_8 = (-\bar{J}_1 + \bar{J}_2/2)$ (9)

$\psi_9 = 1/\sqrt{6}\,(|\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle)$

$E_9 = (\bar{J}_1 + \bar{J}_2/2)$ (10)

$\psi_{10} = 1/2\,(|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle)$

$E_{10} = -3\bar{J}_2/2$ (11)

$\psi_{11} = 1/\sqrt{12}\,(2|\uparrow\downarrow\uparrow\downarrow\rangle + 2|\downarrow\uparrow\downarrow\uparrow\rangle - |\uparrow\uparrow\downarrow\downarrow\rangle - |\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle)$

$E_{11} = (-2\bar{J}_1 + \bar{J}_2/2)$ (12)

$S_{z\,tot} = -1$

$\psi_{12} = 1/\sqrt{2}\,(|\downarrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\downarrow\downarrow\rangle)$

$E_{12} = -(\bar{J}_2/2)$ (13)

$\psi_{13} = 1/\sqrt{2}\,(|\downarrow\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\downarrow\rangle)$

$E_{13} = -(\bar{J}_2/2)$ (14)

$\psi_{14} = 1\ 4\,(|\downarrow\downarrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\downarrow\downarrow\rangle)$

$E_{14} = (\bar{J}_1 + \bar{J}_2/2$ (15)

$\psi_{15} = 1/2\,(|\downarrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\downarrow\rangle - |\uparrow\downarrow\downarrow\downarrow\rangle)$

$E_{15} = (-\bar{J}_1 + \bar{J}_2/2)$ (16)

$S_{z\,tot} = -2$

$\psi_{16} = |\downarrow\downarrow\downarrow\downarrow\rangle$

$E_{16} = \bar{J}_1 + \bar{J}_2/2$ (17)

There are five distinct eigenvalues:

$e_1 = E_1 = E_4 = E_9 = E_{14} = E_{16} = \bar{J}_1 + \bar{J}_2/2$

$e_2 = E_2 = E_3 = E_6 = E_7 = E_{12} = E_{13} = -\bar{J}_2/2$

$e_3 = E_5 = E_8 = E_{15} = (-\bar{J}_1 + \bar{J}_2/2)$

$e_4 = E_{10} = -3\bar{J}_2/2$

$e_5 = E_{11} = (-2\bar{J}_1 + \bar{J}_2/2)$ (18)

When $J_2 < J_1$, the ground state is non-degenerate with eigenvalue e_5. When J1 < J 2, the ground state is non-degenerate with eigenvalue e_4. A QPT occurs at $J_1 = J_2$ when the ground state changes from ψ_{11} to ψ_{10} . In this paper, we focus our attention on this last QPT. The states ψ_{11} and ψ_{10} describe two resonating valence bond (RVB) states,

. A measure of entanglement between the spins at sites k and l is given by the quantity termed concurrence. A knowledge of the two-site reduced density matrix $\rho(i,j)$, obtained from the full density matrix by tracing out the spins other than the ones at sites i and j, enables one to calculate concurrence, a measure of entanglement between two spins at sites i and j [Hill et al, 1997]. Let $\rho(i,j)$ be defined as a matrix in the standard basis. One can define the spin-reversed density matrix as $\tilde{\rho} = (\sigma_y \times \sigma_y)\rho^*(\sigma_y \times \sigma_y)$, where σ_y is the Pauli matrix. The concurrence is given by $C = Max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}$ where λ_i 's are square roots of the eigenvalues of the matrix $\rho\tilde{\rho}$ in descending order. An equivalent way of writing C is $C = Max\{|\rho(3,2)| - \sqrt{\rho(1,1)\rho(4,4)}, 0\}$ where the matrix elements used in the formula are of the pairwise reduced density matrix in the standard basis { | ↑↑ ⟩, | ↑↓ ⟩, |↓↑ ⟩ ,| ↓ ↓ ⟩ }. *C=0* implies a separable state whereas *C=1* corresponds to maximum entanglement.

If the ground state is degenerate, the T=0 ensemble is described by a density matrix which is an equal mixture of contributions from all possible ground states. The density matrix is a limiting case of the thermal density matrix as T → 0 . The state ψ_{RVB1} is the ground state for $J_2 < J_1$. In this case, the n.n. concurrences $C_{12} = C_{23} = C_{34} = C_{41} = 0.5$, i.e., the n.n. spin pairs are entangled in equal amounts. The concurrences C_{13} and C_{24} are zero, i.e., the spins at the ends of a diagonal are un-entangled. At the QCP, $J_1 = J_2 = J$, the concurrences C_{12} , C_{23}, C_{34} , C_{41} and C_{13} , C_{24} are all equal to zero. The ground state at this point is doubly degenerate with wave functions ψ_{RVB1} and ψ_{RVB2} . For $J_2 > J_1$, the ground state is given by ψ_{RVB2} . The n.n. concurrences C 12 , C 23 , C 34 and C 41 are now zero whereas $C_{13} = C_{24} = 1$.

We now discuss the finite temperature entanglement properties of the spin tetramer. For the four-spin cluster, the thermal density matrix is $(T) \quad \frac{1}{Z} e^{H/k_B T}$. One can define a critical temperature T_c beyond which the entanglement between n.n. spins disappears. One can show that in the parameter regime of interest, the thermal entanglement between the diagonal spins is zero so that T_c can be taken as the critical temperature beyond which the entanglement between any two spins is zero. T_c tends to zero we approach the QCP $J_2/J_1 = 1$ (figure 2). For $J_2 > J_1$, the n.n. concurrences are zero.

We next calculate the concurrence for pairwise entanglement between the spins located at the ends of a diagonal. The critical entanglement temperature T_c , beyond which the entanglement between spins located at the ends of a diagonal disappears, is also the temperature beyond which the pairwise entanglement between any two spins vanishes, since in the parameter regime of interest, the n.n. concurrences are zero at all T . Conclusively, in the T=0 case, the two sets of concurrences (i) C_{12} , C_{23} , C_{34} , C_{41} and (ii) C_{13}, , C_{24} are mutually exclusive. For finite values of the concurrences belonging to the first set, the values of the concurrences belonging to the second set are zero and vice versa.

We now examine whether four-spin entanglement exists in the thermal state of the tetramer. This is done by calculating the state preparation fidelity F defined as

$F(\rho) = \langle \psi_{GHZ} | \rho(T) | \psi_{GHZ} \rangle$ where | ψ GHZ ⟩ = 1 2 (| ↑ ↓ ↑ ↓ ⟩ +| ↓ ↑ ↓ ↑ ⟩) is the four-spin Greenberger-Horne-Zeilinger (GHZ) state [12]. The sufficient condition for the four-particle (N=4) entanglement is given by F(ρ) > ½. F(ρ) = 2/3 ,i.e., > 1/2 as T → 0 indicating the presence of four-spin entanglement in the ground state of the tetramer. The critical entanglement temperature, T_c^{GHZ}, beyond which the four-spin GHZ-type entanglement vanishes is obtained from a solution of the equation F(ρ) = 1/2 . The value obtained is less than the critical temperature beyond which the pairwise entanglement between individual spins vanishes. We next consider a tetramer with n.n., diagonal and four-spin exchange interactions. Fig. 2 (solid circles) shows a plot of the said critical temperature with the inhomogeneity ratio J_2/J_1.

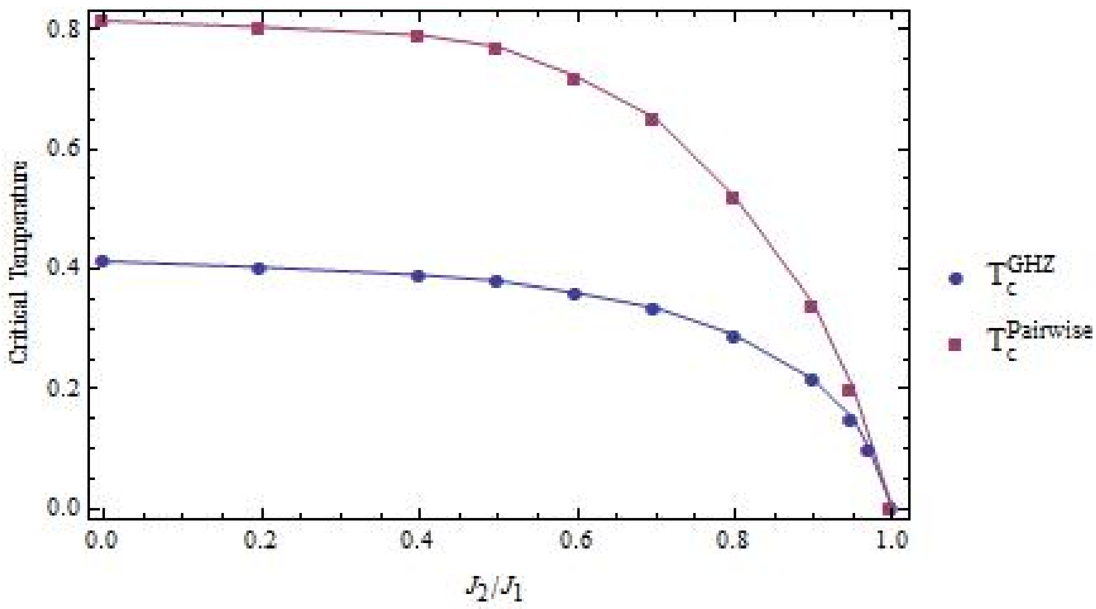


Figure 2: Plot of different critical temperatures versus J $_2$/J$_1$.

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3. Summary and Discussion

In this paper, we consider a spin tetramer (S= 1/2) with n.n., and diagonal AFM exchange interactions of strength J_1 , and J_2 respectively. We study the ground state and thermal entanglement properties of the tetramer in the various limiting cases. At T=0 , QPTs occur as the exchange interaction strengths are tuned to certain critical values. The QCP, which can also be termed as an 'entanglement transition point', $J_1 = J_2 = J$ separates two RVB ground states, ψ_{RVB1} and ψ_{RVB2} . The n.n. concurrences are non-zero only in ψ_{RVB1} and the other two concurrences associated with diagonal spins, are non-zero only in ψ_{RVB2} . The validity of the result needs to be tested in the case of other spin models.

The study of finite temperature entanglement properties again shows the existence of two distinctive parameter regimes with completely different entanglement structures. The n.n. concurrences are non-zero only when $J_2 < J_1$ and the concurrences associated with diagonal spins are non-zero only when $J_1<J_2$. At $J_1 = J_2$, all the six concurrences are zero. This is because the system becomes exactly non-bipartite in nature at that point, i.e, we can not separate the system into two subsystems where spins of one subsystem only interacts with the spins of the other one. The critical entanglement temperature, $T_c^{pairwise}$,, beyond which entanglement between two spins disappears is computed. The magnitude of $T_c^{pairwise}$ is highest when $J_2 = 0$. A measure of the four-spin entanglement in the thermal state of the tetramer is obtained by calculating the State preparation fidelity F(ρ) . The critical temperature, T_c^{GHZ}, beyond which the GHZ-type four-spin entanglement disappears is calculated and one finds that the critical temperature successfully signals the onset of the entanglement transition point, i.e., the QCP. Aslo, this temperature is lesser than its pairwise counterpart, which shows that the GHZ-type multipartite correlations vanishes at a lower temperature but we still have pairwise correlations upto a higher temperature.

There is a host of experimental data on molecular magnets and other magnetic systems which are yet to be analysed in terms of the entanglement properties of the systems [13]. Appropriate finite temperature measures of the different types of entanglement need to be developed so that contact between theory and experiments can be made. A challenging task ahead is to develop suitable measures of multipartite entanglement, which can encompass the different types of multipartite quantum correlations in a quantum system.

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