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Pairwise Entanglement in the Thermal State of a linear 4-spin Plaquette with Exchange Inhomogeneity

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Abstract

In this paper, we study different aspects of entanglement in a Four-spin cluster compound. We study the effect of inhomogeneous exchange coupling strengths and temperature on the entanglement properties of the S= 1/2 antiferromagnetic linear chain tetramer compound $NaCuAsO_4$ and an extended model system. We find some nontrivial phenomenon like non-monotonic behavior and enhancement of entanglement with temperature in case of the linear tetramer for a range for an exchange inhomogeneity parameter.

INTRODUCTION

In the past few years, quantum spin systems have been extensively studied to gain knowledge on the different aspects of entanglement, which is not only a key feature of quantum mechanical systems from theoretical interest, but also a resource for quantum information and computation protocols [1]. The spins in quantum spin systems interact via the exchange interaction and also with an external field, if any. Several studies show that the amount of entanglement can be varied by varying the temperature T, the magnitude of the external field or similar type of parameters [2-10]. In the case of entangled thermal states, when the ground state is entangled, one usually finds gradual decrease in the entanglement content with increasing temperature and eventual vanishing the entanglement at a critical temperature at which the system becomes separable.

The weak inter-cluster coupling between the spin cluster systems allows us to treat each system as a collection of effectively independent clusters. Since the clusters contain a small number of spins, the exact theoretical calculations of thermodynamic and entanglement-related quantities become possible. A number of molecular magnets are known which are well-described in terms of small spin clusters such as dimers, trimers, tetramers, tetrahedra etc [11]. In this paper, we consider the S= 1/2 AFM linear tetramer compound $NaCuAs\ O_4$ [12] in which the linear tetramer consisting of four spins is described by the Heisenberg Hamiltonian

$$H = \bar{J}(\vec{S}_1\vec{S}_2 + \vec{S}_3\vec{S}_4) + \alpha\bar{J}(\vec{S}_2\vec{S}_3)$$

$\bar{J}$ is the Exchange interaction strength between 1-2 and 3-4 pairs of the open 4-spin chain and α is an exchange inhomogeneity parameter which provides the relative strength of the exchange interaction of the 2-3 pair compared to the other two pairs.

In this paper, we have studied and compared the variations of thermal concurrence between different pairs of spins with temperature and the exchange inhomogeneity.

LINEAR CHAIN TETRAMER

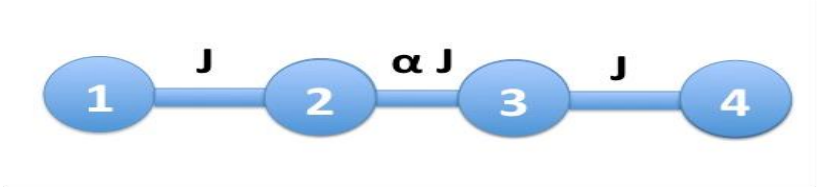

Figure 1: Schematic picture of a Linear Chain tetramer

The S= 1 2 AFM compound *Sodium Cupric Arsenate* ($NaCuAsO_4$) has a linear chain tetrameric structure (as shown in figure 1) described by the Hamiltonian, in Eq. (1) with $\alpha = 0.4$ The term "linear" refers to the pattern of exchange couplings and not to the spatial structure of the tetramer [12]. The total spin S tot of the tetramer has the values 2, 1 and 0. There are five S tot =2 states, nine $S_{tot} = 1$ states and two S tot =0 states. The different eigenvalues and eigenvectors are displayed below. The first index in the subscript of an eigenvector refers to the eigenvalue and the second to $S_{z\,tot}$, the z-component of the total spin.

$S_{tot} = 2$:

$E_1 = (1/2 + \alpha/4) J$ (2)

$\psi_{1,2} = |\uparrow\uparrow\uparrow\uparrow\rangle$

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

$\psi_{1,0} = (1/\sqrt{6}) (|\uparrow\uparrow\downarrow\downarrow\rangle + |\uparrow\downarrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\downarrow\uparrow\downarrow\uparrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle)$

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

$\psi_{1,-2} = |\downarrow\downarrow\downarrow\downarrow\rangle$ (3)

$S_{tot} = 1$:

$E_2 = (-1/2 + \alpha/4) J$ (4)

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

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

$\psi_{2,0} = (1/\sqrt{2}) (|\uparrow\downarrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\downarrow\rangle)$ (5)

$E_3 = (-\alpha/4 + 1/2 (1+\alpha^2) J$ (6)

$\psi_{3,1} = (1/N_1)(|\downarrow\uparrow\uparrow\uparrow\rangle - |\uparrow\uparrow\uparrow\downarrow\rangle - (\alpha - \sqrt{(1+\alpha^2)} (|\uparrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\uparrow\rangle)$

$\psi_{3,-1} = (1/N_1)(|\uparrow\downarrow\downarrow\downarrow\rangle - |\downarrow\downarrow\downarrow\uparrow\rangle \rangle - (\alpha - \sqrt{(1+\alpha^2)} (|\downarrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\downarrow\rangle)$

$\psi_{3,0} = (1/N_2) (|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle - (1/\alpha - \sqrt{(1+1/\alpha^2)} (|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle)$ (7)

$E_4 = (-\alpha/4 - 1/2 \sqrt{(1+\alpha^2)}$ (8)

$\psi_{4,1} = (1/N_3) (|\downarrow\uparrow\uparrow\uparrow\rangle - |\uparrow\uparrow\uparrow\downarrow\rangle - (\alpha + \sqrt{(1+\alpha^2)} (|\uparrow\downarrow\uparrow\uparrow\rangle - |\uparrow\uparrow\downarrow\uparrow\rangle)$

$\psi_{4,-1} = (1/N_3) (|\uparrow\downarrow\downarrow\downarrow\rangle - |\downarrow\downarrow\downarrow\uparrow\rangle - (\alpha + \sqrt{(1+\alpha^2)} (|\downarrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\downarrow\rangle)$

$\psi_{4,0} = (1/N_4) (|\uparrow\uparrow\downarrow\downarrow\rangle - |\downarrow\downarrow\uparrow\uparrow\rangle - (1/\alpha - \sqrt{(1+1/\alpha^2)} (|\uparrow\downarrow\uparrow\downarrow\rangle - |\downarrow\uparrow\downarrow\uparrow\rangle)$ (9)

$S_{tot} = 0$:

$E_5 = \{ -(1/2 + \alpha/4) + \sqrt{(1-\alpha/2+\alpha^2/4)} \} J$ (10)

$\psi_{5,0} = (1/N_5) (a_1 |\uparrow\uparrow\downarrow\downarrow\rangle + b_1 |\uparrow\downarrow\uparrow\downarrow\rangle + c_1 |\uparrow\downarrow\downarrow\uparrow\rangle + d_1 |\downarrow\uparrow\uparrow\downarrow\rangle + e_1 |\downarrow\uparrow\downarrow\uparrow\rangle + f_1 |\downarrow\downarrow\uparrow\uparrow\rangle)$ (17)

$E_6 = \{ -(1/2 + \alpha/4) - \sqrt{(1-\alpha/2+\alpha^2/4)} \} J$ (11)

$\psi_{5,0} = 1/N_6 (a_2 |\uparrow\uparrow\downarrow\downarrow\rangle + b_2 |\uparrow\downarrow\uparrow\downarrow\rangle + c_2 |\uparrow\downarrow\downarrow\uparrow\rangle + d_2 |\downarrow\uparrow\uparrow\downarrow\rangle + e_2 |\downarrow\uparrow\downarrow\uparrow\rangle + f_2 |\downarrow\downarrow\uparrow\uparrow\rangle)$ (12)

where $a_1 = f_1 = a_2 = f_2 = 1$, $b_1 = -2/\alpha + 2\sqrt{(1/4 - 1/2\alpha + 1/\alpha^2)} = e_1$, $b_2 = -2/\alpha + 2\sqrt{(1/4 - 1/2\alpha + 1/\alpha^2)} = e_2$, $c_1 = -1 + 2/\alpha - 2\sqrt{(1/4 - 1/2\alpha + 1/\alpha^2)} = d_1$, $c_2 = -1 + 2/\alpha + 2\sqrt{(1/4 - 1/2\alpha + 1/\alpha^2)} = d_2$

N_1 , N_2 , N_3 , N_4 , N_5 and N_6 are the appropriate normalization constants.

We now discuss the finite-temperature entanglement properties of the linear chain tetramer. The thermal density matrix $\rho (T)$ is given by

$$\rho(T) = \frac{1}{Z} e^{-H/k_B T} \quad (13)$$

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 $C = Max\{|\rho(3,2)| - \sqrt{\rho(1,1)\rho(4,4)}, 0\}$. C=0 implies an un-entangled state whereas *C=1* corresponds to maximum entanglement.

For the linear chain tetramer, the partition function Z is

$$Z=5\, e^{-\beta E1} + 3\, e^{-\beta E2} + 3\, e^{-\beta E3} + 3\, e^{-\beta E4} + e^{-\beta E5} + e^{-\beta E6} \quad (24)$$

With a knowledge of the eigenvalues and eigenvectors of the linear chain tetramer, the matrix elements of the reduced density matrix can be easily calculated. One can further define a critical temperature T_C^{kl} above which the entanglement between the spins at the sites k and l disappears. Figure 1 shows the variation of C_{12} as a function of temperature and J/k_B =92.7K , the parameter value relevant for $NaCuAs\ O_4$. It is clear that concurrence between the spins 1 and 2 are entangled in the ground state (the system at T=0) of the tetramer for all positive values of the exchange inhomogeneity parameter α including the point α=0 (where the tetramer splits into two spin dimers) and the point α=1 where the inhomogeneity vanishes. The pairwise concurrence between the said pair monotonically decreases with increasing temperature and vanishes at a critical temperature. This value of the critical temperature slowly decreases as the value of α is increased. This is because the exchange interaction strength between the pair 2 and 3 increases with the value of α lessening the relative strength of the pair 1 and 2. In figure 3, we plot the variation of the thermal concurrence between the spin pair 2-3 with T and α. As evident from the picture, the 2-3 pair is not entangled at the ground state for smaller values of α. The α=0 is trivial because there is no bond between spin 2 and 3 at that point. But even if we switch on an interaction between that pair, we don't get any pairwise entanglement at the ground state in the parameter value range $0<\alpha<1$ point, which includes the point α=4, which is relevant for the real compound $NaCuAsO_4$. But if we start increasing the temperature for α>=.75, the thermal concurrence kicks in at a finite value of the temperature, it then increases with T, attains a maximum and then it decreases and vanishes at a critical temperature. This is a novel example of a physical system, where even if the ground state entanglement is vanishing, we get entanglement by enhancing the thermal excitations, which usually is seen to kill quantum correlations in a quantum system. At α=1, i.e., the exchange homogeneity point, the 2-3 pair becomes entangled at the ground state. But the amount of entanglement increases as we increase temperature upto a certain value and then starts to decrease as the thermal decoherence starts to kill quantum effects in the system and it becomes separable at a critical temperature.

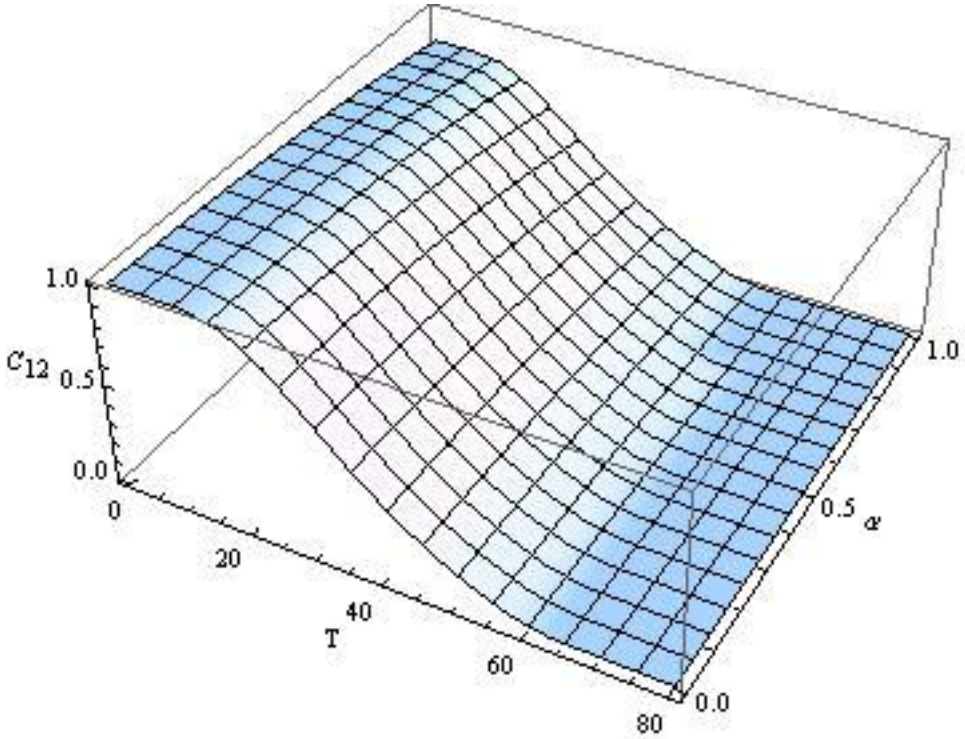

Figure 2: Variation of thermal concurrence C_{12} with T and α

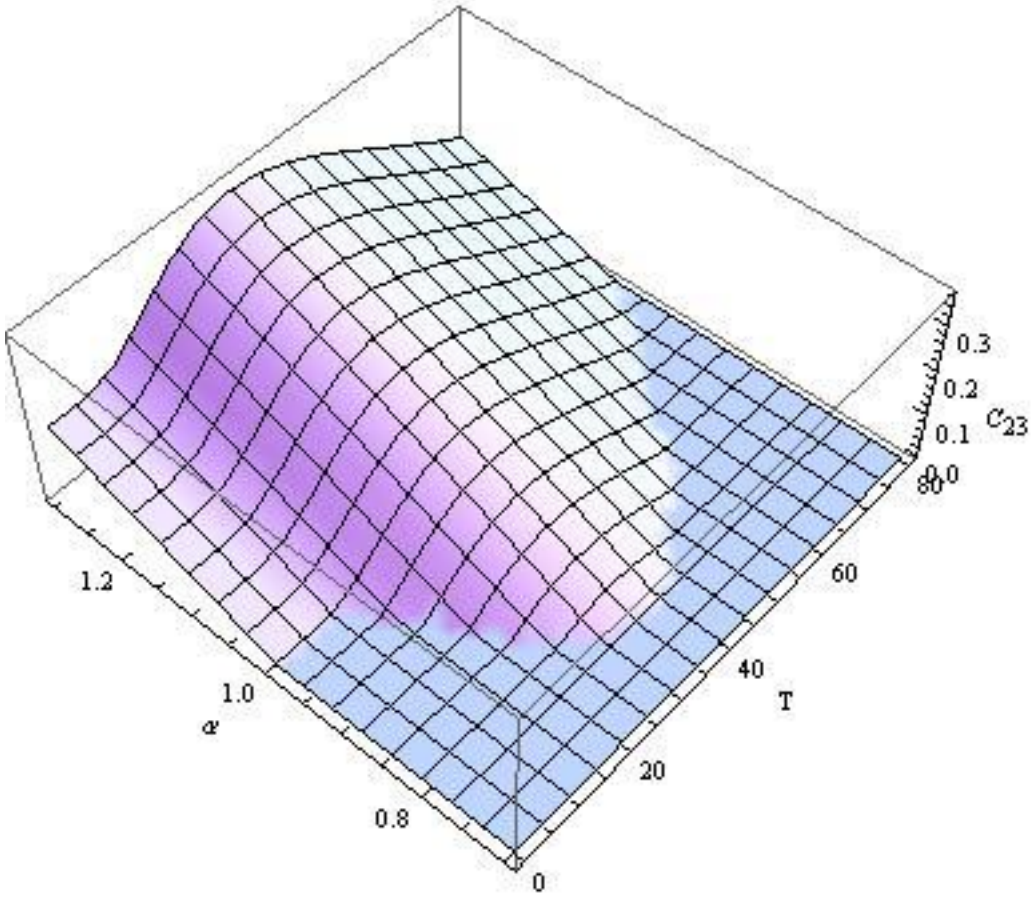

Figure 3: Variation of thermal concurrence C_{23} with T and α

SUMMARY AND DISCUSSION

In this paper, we study some special features of an entangled small spin cluster. We consider the S= 1/2 AFM linear chain tetramer compound, $NaCuAsO_4$, described by the Heisenberg exchange interaction Hamiltonian with inhomogeneous exchange coupling strengths (Eq. (1)) and show that the pairwise thermal entanglement between the spin pair 1 and 2 has a monotonic dependence on the temperature and the critical temperature at which the pair becomes separable, decreases slowly with the exchange coupling inhomogeneity parameter α, obeying the monogamy rule of entanglement. But as we consider the spin pair 2-3, there is no entanglement between the pair at T=0 and smaller values of α (0< α<1). But if we increase the temperature the pair becomes entangled at a finite

temperature. This is because of the mixing of the higher energy states with the separable ground state due to initial increase in thermal excitations. The entanglement structure of the higher energy states starts contributing as we increase the temperature from T=0. After this thermal kick-in, the thermal concurrence increases with T up to a certain value and then again starts to decrease due to the thermal decohering effect. This is in contrast with the result obtained when the Hamiltonian is translationally invariant, i.e., the rectangular tetramer. Where critical temperature of all the pairs behave in exactly the same fashion. The system we studied is a novel example of enhancement of quantum correlations by thermal excitations and non-monotonic variation of thermal entanglement with temperature. This work can be extended to many molecular magnetic systems which are available naturally like the Sodium Cupric Arsenate compound and also those which can be synthesized chemically or can be realized in ultra-cold atomic systems in optical lattices which can simulate any toy model we can imagine.

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