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Magnetization and concurrence on decorated zigzag ladder

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Abstract. Using Heisenberg model with two-, three- and four-site exchange interactions, by means of variational mean-field like treatment based on Gibbs-Bogoliubov inequality the magnetic properties and concurrence (measure of pairwise thermal entanglement) on decorated zigzag ladder are studied. We have found that in the antiferromagnetic region behaviour of the concurrence coincides with the magnetic susceptibility one. With absence of external magnetic field the dependence of magnetization from temperature plotted and shown that system undergo second order phase transition in some critical temperature.

1. Introduction

Entanglement [1, 2] is a fundamental property of quantum mechanical systems and gives rise to an excess of correlations in a system over and above those expected from classical considerations [3]. As one of the most intriguing features of quantum mechanics, it has become a subject of intense interest in recent years [1]-[13]. Besides being recognized as a crucial resource for quantum computing and quantum information processing [4] it has also provided new perspectives in problems of various many-body systems. In particular, the entanglement can well characterize the features of the quantum phase transition (QPT) [14]. Many works [10]-[19] have been devoted to understanding the relation between the QPT and entanglement in different systems. It has been observed that quantum phase transitions are signaled by critical behaviors of the concurrence [20, 21], a measure of entanglement for two-qubit systems. However, most of the previous works on QPT and entanglement were restricted to models with two-body interactions; the models with three- or four-body interactions are less investigated, [22]-[24] and the connections between entanglement and novel phases brought about by these multispin interactions are still less well understood by people. In fact a system with multibody interactions is important in both quantum information theory and condensed matter physics. It was pointed out that a small cluster of spins with three- or four-body interactions such as the four-spin ring exchange could be used for quantum computing [25, 26]. Moreover, four-spin ring exchange exists in many physical systems and plays an important role in understanding the magnetism in several quantum systems such as solid ³He and Wigner crystals [27]. Therefore, it is of importance to study the properties of the entanglement in those spin systems with multi-site interactions.

Statistical physical models on ladders may be considered as intermediate systems between one-dimensional (1D) and two-dimensional (2D) lattice models and have been a subject of increasingly intense research interest in recent decades [28, 29]. It is shown that materials like $Sr_{n-1}Cu_{n+1}O_{2n}$ contain ladder structures with a number of legs that depend on the value of n [31, 32]. The latter can also be used as a playground for theories of high- T_c superconductivity (two-leg Hubbard and t-J ladders) [33, 34]. Experimental properties of materials like $La_6Ca_8Cu_{24}O_{41}$ and $Cu_2(C_5H_{12}N_2)_2Cl_4(CuH_2P_2Cl_4)$ can be described by the two-leg Heisenberg antiferromagnetic ladder model [35, 36]. Zigzag ladders are also a good approximation of d -dimensional triangular ones for solid 3He [37, 38]. Especially excellent agreement is seen between the well known ladder compounds $(5IAP)_2CuBr_4 \cdot 2H_2O$, $Cu_2(C_5H_{12}N_2)_2Cl_4$ [39].

Determination of the entanglement properties of an interacting spin system is a theoretical challenge as the eigenstates and eigenvalues are not known exactly when the number of spins is large. Most of the calculations are confined to systems containing a few spins so that exact diagonalization is possible. Studies on finite quantum spin systems acquire significant relevance in the context of molecular or nanomagnets. In such magnetic systems, the dominant exchange interactions are often confined to small spin clusters. The inter-cluster exchange interactions are much weaker in comparison so that the compounds can be assumed to consist of independent spin clusters. With the help of a variational mean-field approach, based on the Gibbs-Bogoliubov inequality [40]-[43], one can reduce the system consisting of many particles to a limited cluster in self-consistent (effective) mean fields and calculate the quantum entanglement [44].

The key result of the paper is concentrated on the comparison of specific features in magnetization and thermal entanglement properties in the above mentioned model using variational mean-field like Gibbs-Bogoliubov inequality.

This paper is organized as follows: in section 2 we introduce the Heisenberg model with two-, three- and four- site exchange interactions. In section 3 mean-field like approximation, based on Gibbs-Bogoliubov inequality, has applied on decorated zigzag ladder. The magnetic properties as a measure of entanglement of the decorated zigzag ladder model are investigated in section 4. The conclusive remarks are given in section 5.

2. Heisenberg Hamiltonian with two-, three- and four-site exchange interactions

In our model we consider the quantum Heisenberg Hamiltonian with not only pair exchange interactions but also a three- and four-site exchange interactions [37, 45, 46]. This Hamiltonian consists of two parts:

$$H = H_{ex} + H_Z, \quad (1)$$

where H_{ex} is the Hamiltonian of exchange interactions and H_Z - is responsible for magnetism (Zeeman Hamiltonian). The expression for the Zeeman Hamiltonian is [45]:

$$H_Z = - \sum_i \frac{\gamma}{2} \hbar \mathbf{B} \sigma_i \equiv -h \sum_i \sigma_i^z, \quad (2)$$

where γ is gyromagnetic ratio for the fermions on zigzag ladder and \mathbf{B} is the magnetic field directed along the z axis. The exchange Hamiltonian with two-, three- and four-site exchange interactions has the following form [46]

$$H_{ex} = J_2 \sum_{\langle i,j \rangle} P_{i,j} - J_3 \sum_{\langle i,j,k \rangle} (P_{i,j,k} + P_{i,j,k}^{-1}) + J_4 \sum_{\langle i,j,k,l \rangle} (P_{i,j,k,l} + P_{i,j,k,l}^{-1}), \quad (3)$$

where $P_{i,j}$, $P_{i,j,k}$ and $P_{i,j,k,l}$ - operators of cyclic permutations, respectively, two, three and four particles, and summations are taken, respectively, over all edges, triangles and quadrangles. The

expression for $P_{i,j}$ has the form

$$P_{i,j} = \frac{1}{2} (1 + \sigma_i \sigma_j), \quad (4)$$

where $\sigma_i = \{\sigma_i^x, \sigma_i^y, \sigma_i^z\}$ – are Pauli matrices for the i -th particle. Using the latter, one can obtain an expression for $P_{i,j,k}$ and $P_{i,j,k,l}$. One can write

$$P_{i,j,k} + P_{i,j,k}^{-1} = \frac{1}{2} (1 + \sigma_i \sigma_j + \sigma_j \sigma_k + \sigma_k \sigma_i), \quad (5)$$

$$P_{i,j,k,l} + P_{i,j,k,l}^{-1} = \frac{1}{4} \left(1 + \sum_{\nu < \mu} \sigma_\nu \sigma_\mu + G(\sigma_i, \sigma_j, \sigma_k, \sigma_l) \right) \quad (6)$$

where

$$G(\sigma_i, \sigma_j, \sigma_k, \sigma_l) = (\sigma_i \sigma_j)(\sigma_l \sigma_k) + (\sigma_i \sigma_l)(\sigma_j \sigma_k) - (\sigma_i \sigma_k)(\sigma_l \sigma_j), \quad (7)$$

and the summation is over all $(\nu < \mu)$ pairs from (i, j, k, l) . Omitting irrelevant constants an expression for the Hamiltonian can be written

$$\begin{aligned} H &= \frac{J_2}{2} \sum_{i,j} \sigma_i \sigma_j - \frac{J_3}{2} \sum_{i,j,k} (\sigma_i \sigma_j + \sigma_j \sigma_k + \sigma_k \sigma_i) + \\ &+ \frac{J_4}{4} \sum_{i,j,k,l} \left(\sum_{\nu < \mu} \sigma_\nu \sigma_\mu + G(i, j, k, l) \right) - h \sum_i \sigma_i^z. \end{aligned} \quad (8)$$

3. Mean-field formalism for decorated zigzag ladder

We use a variational mean field theory based on the Gibbs-Bogoliubov inequality [40] in order to simplify the Hamiltonian (8) and find its eigenvalues and eigenvectors. Gibbs-Bogoliubov inequality has the form

$$F \leq F_0 + \langle H - H_0 \rangle_0, \quad (9)$$

where H is real Hamiltonian which describes the system and H_0 is trial Hamiltonian. F and F_0 is the free energy corresponding to H and H_0 and $\langle \dots \rangle_0$ denotes statistical averaging over the trial Hamiltonian H_0 . We introduce a trial Hamiltonian H_0 so that it contains some unknown parameters. Minimizing the right side of inequality (9) we obtain such a value of unknown parameters for which the trial Hamiltonian H_0 has best approximation.

Due to the nature of this method in the context of antiferromagnetic interaction the trial Hamiltonian should consist of two parts describing the two sublattices. For decorated zigzag ladder we introduce a trial Hamiltonian H_0 as a set of noninteracting clusters (rectangles) on two sublattices (see figure 1).

$$H_0 = \sum_{\diamond_i} H_v^{(i)}, \quad (10)$$

where

$$\begin{aligned} H_v^{(i)} &= \lambda_1 \cdot (\sigma_1^i \sigma_2^i + \sigma_2^i \sigma_3^i + \sigma_3^i \sigma_4^i + \sigma_1^i \sigma_4^i) + \lambda_2 \cdot \sigma_2^i \sigma_4^i + \\ &+ \lambda_3 \cdot \left(\sum_{\nu < \mu} \sigma_\nu^i \sigma_\mu^i + G^{(i)} \right) - \gamma_v \cdot \sum_{\alpha=1}^4 (\sigma_a^i)^z, \end{aligned} \quad (11)$$

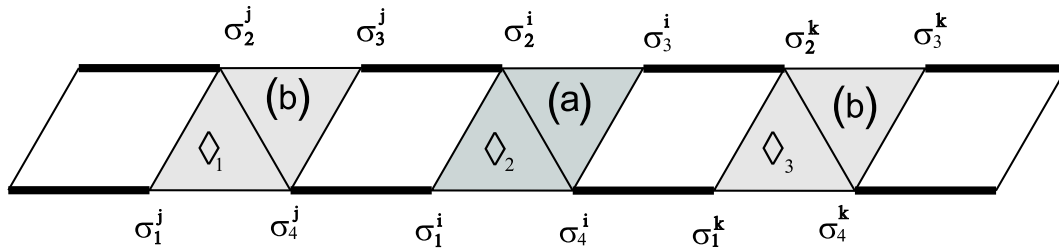


Figure 1. Zigzag ladder

where $\lambda_1, \lambda_2, \lambda_3$ and γ_v variational parameters, and the index of summation \diamond_i labels different noninteracting rectangles (see figure 1, the dark rectangles) and

$$\begin{aligned} \text{for even } i \quad \gamma_v &= \gamma_a \quad \text{sublattice (a),} \\ \text{for odd } i \quad \gamma_v &= \gamma_b \quad \text{sublattice (b).} \end{aligned} \quad (12)$$

Eigenvectors of the Hamiltonian $H_\nu^{(i)}$ does not depend on the parameters and can be found by diagonalization.

We emphasize that in context of a trial Hamiltonian spins σ_k^i of \diamond_i -th rectangle does not interact with spins σ_k^j \diamond_j -th rectangle if $i \neq j$, therefore these spins are statistically independent. Suppose the real Hamiltonian H (8) can be represented as a sum

$$H = \sum_{\diamond_i} H^{(i)}, \quad (13)$$

where $H^{(i)}$ is the contribution of one cluster in the Hamiltonian and the index of summation \diamond_i labels different noninteracting rectangles (see figure 1, the dark rectangles). Since the terms of the form $\sigma_a^i \sigma_b^i$ must appears only in the $H^{(i)}$, hence they have the same coefficient that in general H . In contrast, members of the form $\sigma_a^i \sigma_b^j$ (see figure 1 thick lines) should be included both in $H^{(i)}$ and $H^{(j)}$ and hence their coefficients are divided by two. The final form of $H^{(i)}$ is as follows:

$$\begin{aligned} H^{(i)} &= J'_1 \left(\sigma_1^i \sigma_2^i + \sigma_3^i \sigma_4^i + \sigma_1^i \sigma_4^i + \sigma_2^i \sigma_3^i \right) + J'_2 \left(\sigma_2^i \sigma_4^i \right) + J'_3 \left(\sigma_1^i \sigma_3^i + G^{(i)} \right) + \\ &+ \frac{J'_1}{2} \left(\sigma_4^i \sigma_1^k + \sigma_3^i \sigma_2^k \right) + \frac{J'_1}{2} \left(\sigma_4^j \sigma_1^i + \sigma_3^j \sigma_2^i \right) - h \sum_{a=1}^4 (\sigma_a^i)^z, \end{aligned} \quad (14)$$

where

$$J'_1 = \frac{J_2}{2} - \frac{J_3}{2} + \frac{J_4}{4}, \quad J'_2 = \frac{J_2}{2} - \frac{2J_3}{2} + \frac{J_4}{4}, \quad J'_3 = \frac{J_4}{4}. \quad (15)$$

Inequality (9) can be written for one rectangle on different sublattices:

$$f_v \leq (f_0)_v + \left\langle H^{(i)} - H_0^{(i)} \right\rangle_0, \quad (16)$$

where $H^{(i)}$ is a real and $H_0^{(i)}$ trial Hamiltonians of a rectangle, and $f_v, (f_0)_v$ are corresponding free energies of the sublattice (v). Taking into account that the spin σ_p^i belongs to sublattice (a) and spins $\sigma_p^{j,k}$ belong to sublattice (b) we have $\left\langle (\sigma_p^{i,j,k})^{x,y} \right\rangle = 0$, $m_a \equiv \left\langle (\sigma_p^i)^z \right\rangle / 2$,

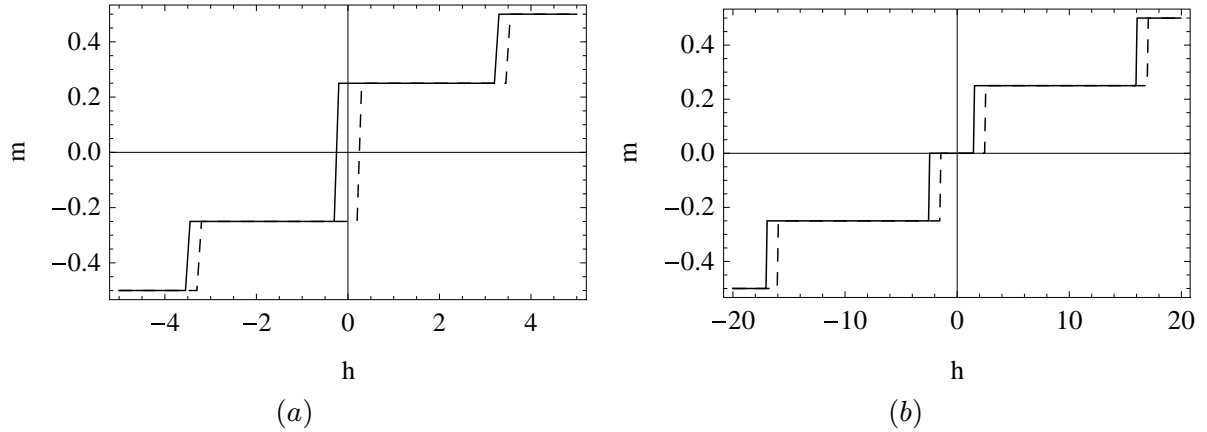


Figure 2. Magnetizations m_a, m_b versus magnetic field h for $J_3 = 2.5$ mK, $J_4 = 2$ mK, $T = 0.01$ mK and a) $J_2 = 2$ mK, b) $J_2 = 8$ mK.

$m_b \equiv \langle (\sigma_p^{j,k})^z \rangle / 2$. Since the spins σ_a^i and $\sigma_b^{j,k}$ are statistically independent we obtain $\langle \sigma_a^i \sigma_b^j \rangle = \langle (\sigma_a^i)^z \rangle \times \langle (\sigma_b^j)^z \rangle = 4m_a m_b$. Now we can rewrite (16) for (v) sublattice as follows

$$f_v \leq (f_0)_v + (J'_1 - \lambda_1 - \lambda_3) \langle \sigma_1^i \sigma_2^i + \sigma_2^i \sigma_3^i + \sigma_3^i \sigma_4^i + \sigma_1^i \sigma_4^i \rangle_0 + (J'_2 - \lambda_2 - \lambda_3) \langle \sigma_2^i \sigma_4^i \rangle_0 + (J'_3 - \lambda_3) \langle \sigma_1^i \sigma_3^i + G^{(i)} \rangle_0 + \frac{4J'_1}{2} (4m_a m_b) - 4(h - \gamma_v) 2m_v. \quad (17)$$

Minimizing the right side of inequality (17) with respect $\lambda_1, \lambda_2, \lambda_3$ and $\gamma_{a,b}$ one can obtain the following values for variational parameters

$$\begin{aligned} \lambda_1 &= J'_1 - J'_3, \quad \lambda_2 = J'_2 - J'_3, \quad \lambda_3 = J'_3 \\ \gamma_a &= h - J'_1 \cdot m_b, \quad \gamma_b = h - J'_1 \cdot m_a. \end{aligned} \quad (18)$$

4. Magnetic properties and quantum entanglement for decorated zigzag ladder

Hereafter all the Magnetization, by definition, is an average of the spin operator

$$m_v = \langle S_v \rangle = \frac{\text{Tr}(S_v \cdot \exp(-H_v^i/T))}{Z}, \quad (19)$$

where S_v is spin operator, H_v^i is Hamiltonian (11) with the found constants (18) and Z partition function of the system (coupling constants is determined in units of Boltzmann's constant, so that the new coupling constants have the dimension of temperature $J'_k = J'_k/k_B$, $h = h/k_B$). But according to (18) the expression m_a depends on m_b (by means of γ_a) and vice versa. Dependence of the magnetization m_a on the external magnetic field h can be found by solving the resulting recursive equation (19) for each value of the magnetic field. The experimental and theoretical studies suggest that three site exchanges are dominant in solid and fluid ^3He [47]–[50]. According to [45] the effective value of the exchange parameters $J_{eff} = J_2 - 2J_3$ on triangular lattice, which has been estimated experimentally from susceptibility and specific-heat data for solid ^3He is $J_{eff} = -3$ mK. In figure 2(a) the dependence of the magnetizations m_a and m_b at $T = 0,001$ mK, $J_2 = 2$ mK, $J_3 = 2.5$ mK, $J_4 = 2$ mK. As can be seen from figure, there are areas where the $m_a \neq m_b$. Thus our system is really separated into two sublattices with different magnetizations. For small values of J_2 there are magnetization plateau at $1/4$ (see figure 2(a)), which corresponds to the stable phase $\uparrow\uparrow\downarrow$ but for large J_2 (see figure 2(b)) in system appears

also plateau at $m_a = 0$, which is a consequence of the fact that the energy stable phase $\uparrow\uparrow\downarrow\downarrow$ is minimal. The figure 3 solid line shows dependance of the zero-field m_0 versus temperature T . As can be seen from the figure in the absence of field magnetization of one sublattice gradually tends to zero at a certain critical temperature T_C . This point is a point of phase transition between an ordered and disordered phases.

Mean field method allows us to consider only one cluster of zigzag ladder in the effective mean field γ to study the quantum entanglement.

As a measure of quantum entanglement we will use the concurrence [20, 21]. Concurrence $C(\rho)$ for a given density matrix ρ defined as follows:

$$C(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \quad (20)$$

where λ_i is the square root of the following operator eigenvalues,

$$\tilde{\rho} = \rho_{12}(\sigma_1^y \otimes \sigma_2^y)\rho_{12}^*(\sigma_1^y \otimes \sigma_2^y), \quad (21)$$

where $\rho_{12} = Tr_{3,4}\rho$ corresponds to the reduced density matrix only one pairs in the cluster. The density matrix ρ defined as follows:

$$\rho = \frac{1}{Z} \sum_{i=1}^{16} e^{-\frac{E_i}{T}} |\psi_i\rangle\langle\psi_i|, \quad (22)$$

where Z is the partition function of the system and ψ_i , E_i - eigenfunctions and eigenvalues of the Hamiltonian $H_0^{(i)}$ (see. (11)). Them matrix ρ_{12} has the following form

$$\rho_{12} = \begin{pmatrix} u & 0 & 0 & 0 \\ 0 & w & y & 0 \\ 0 & y & w & 0 \\ 0 & 0 & 0 & v \end{pmatrix}, \quad (23)$$

where u, w, y and v are some functions of variables γ, λ_i and T . Using (20),(21) and (23) one can find expression for concurrence $C(\rho)$

$$C(\rho) = \max\{|y| - \sqrt{uv}, 0\}. \quad (24)$$

Since $\gamma_a = h - J'_1 \cdot m_b$ (see (18)), hence the concurrence $C(\rho)$ of the sublattice **(a)** is function of the magnetization m_b (sublattice **(b)**) and vice versa.

To calculate the concurrence, we must solve the recursive equation (19) for each set of parameters (J'_i, h, T) and put the resulting solution into (24).

It is important to consider the relation between the statistical and quantum characteristics of the system. In our case, the statistical characteristic is the magnetization m (19) and the quantum characteristic is the concurrence. In figure 3 by dashed (dotted) lines shown concurrence between the non-diagonal spins (diagonal spins) as a function of temperature T at zero external field and fixed $J_2 = 2\text{mK}$, $J_3 = 2.5\text{mK}$ and $J_4 = 2\text{mK}$ are plotted. Comparing with the similar plot for the magnetization (figure 3, solid line), one can conclude that in the absence of magnetic field concurrence for the non-diagonal spins vanishes at the same critical temperature T_C , that the magnetization, and the concurrence between the diagonal spins - at lower temperature. At $T > T_C$ and zero external field the concurrence between all pairs is equal to zero.

Figures 4 and 5 show the magnetization m (figure 4) and concurrence $C(\rho)$ for the non-diagonal (figure 5(a)) and diagonal (figure 5(b)) spins as a function of from J_2 and external field h (for fixed $J_3 = 2.5 \text{ mK}$, $J_4 = 2 \text{ mK}$ and $T = 0.5 \text{ mK}$). By comparing these graphs, one can detect the similarity between the behavior of magnetization and concurrence. Both the magnetization plateau and the plateau of concurrence observed with the same values of J_2 and h .

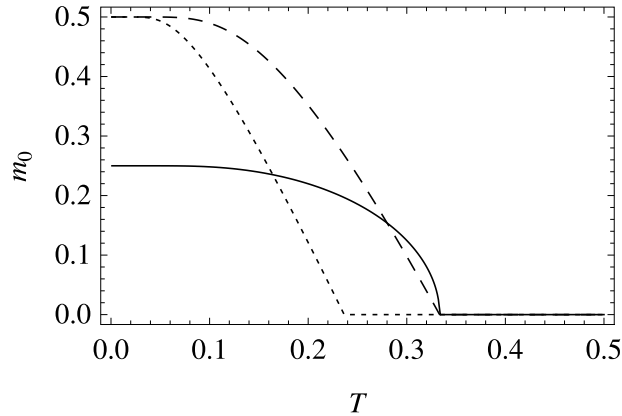


Figure 3. Dependence of the magnetization m_0 (solid line) and concurrence (dotted line - diagonal spins, dashed lines non-diagonal spins) at zero external field from temperature T at $J_2 = 2$ mK, $J_3 = 2.5$ mK and $J_4 = 2$ mK.

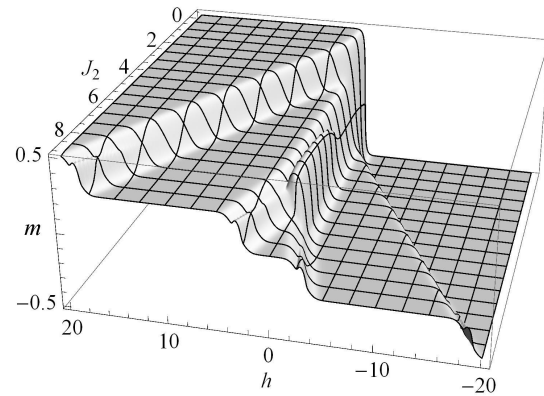


Figure 4. Dependence of the magnetization m on magnetic field h and the coupling constant J_2 at $J_3 = 2.5$ mK, $J_4 = 2$ mK and $T = 0.5$ mK Figure caption for second of two sided figures.

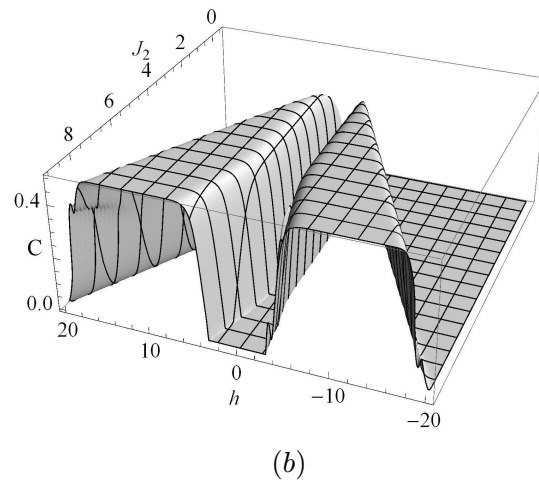
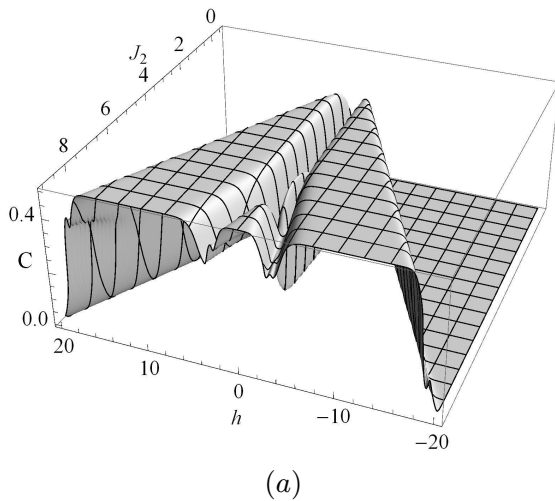


Figure 5. Dependence of (a) Concurrence $C(\rho)$ for nondiagonal spins and (b) Concurrence $C(\rho)$ for the diagonal spins on magnetic field h and the coupling constant J_2 at $J_3 = 2.5$ mK, $J_4 = 2$ mK and $T = 0, 5$ mK.

5. Conclusions

In this paper we found strong correlations between magnetic properties and quantum entanglement in the Heisenberg model with two-, three-, and four-site exchange interactions in strong magnetic field on the decorated zigzag ladder. By using variational mean-field-like treatment (based on the Gibbs-Bogoliubov inequality) we separated the zigzag ladder into clusters in effective magnetic fields and studied magnetic properties and concurrence as a measure of pairwise thermal entanglement. The system exhibits different magnetic behaviors, depending on the values of the exchange parameters (J_2, J_3, J_4) . We have obtained the magnetization plateaus at low temperatures. The comparison of magnetization and concurrence in antiferromagnetic region shows that regions corresponding to the magnetization plateaus, coincide with the plateaus on concurrence plot.

Acknowledgements

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