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Energy as an Entanglement Witnesses for One Dimensional *XYZ* Heisenberg Lattice: Optimization Approach

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Abstract
If energy ensemble average is less than the minimum energy of separable states, the system is entangled. In this study, we consider energy as an entanglement witness for one dimensional XYZ Heisenberg lattice up to ten qubits analytically. We find minimum of energy using Lagrange undetermined multipliers to construct the entanglement witness. We also find threshold temperature and magnetic field, for which below them the system is entangled. The results are in good agreement with the literature. For systems with more than six qubits, the results show temperature gets a stable value for a zero magnetic field.

Keywords Entanglement witness · Heisenberg lattice · Lagrange undetermined multipliers

1 Introduction

One of the important lattice models for quantum information [1–3] applications such as teleportation [4–6], dense coding [7] and quantum heat engine [8,9], is the *XYZ* Heisenberg lattice. In such applications, one must know the entanglement is present in the whole of the process or not, so the entanglement detection in such lattices needs to be investigated carefully.

Entanglement in lattices has been studied lately [10–12] as well as quantum Monte Carlo simulation [13]. One of the important approaches to entanglement detection is entanglement witness. An entanglement witness is an observable with the property that a negative expectation value give evidence of the entanglement [14–20]. It is very useful method to identify the entangled, ρ_{ent}, from the separable states, ρ_{sep}, for both bipartite and multipartite systems [21–23]. Due to measuring simplicity, energy as an entanglement witness is one of the important approaches [22,24–26], which can be applied for spin systems like XXX and XY Heisenberg spin lattices [27], where, it is shown if energy average (ensemble) is less than the minimum energy of separable states then, the system is entangled. The generalization of

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this approach to the multipartite case and frustrated systems has been done analytically in [28], where the authors using the definition of k-producibility, compute the desired energy bounds for one and two-dimensional Heisenberg model on a square lattice using the Cauchy-Schwarz inequality analytically. Other physical quantities can also be used for entanglement detection such as magnetic susceptibility [29–33], heat capacity [34,35] and proxy witnesses (where the entanglement can be certified at higher temperatures without access to any local observable) [36].

Significantly, energy was also proposed as a witness of non-locality in many-body systems, that is to say, as a Bell-like inequality [37]. In their study, they have shown that the ground states of some spin Hamiltonians are nonlocal and have assigned a Bell inequality to the Hamiltonian of the system which its classical bound can be calculated. As the Bell inequality is such that its quantum value corresponds to state energy, the presence of nonlocal correlations can be certified for states of low enough energy. Then, they optimize Bell inequalities for the translationally invariant case for a tight inequality for eight parties, quasi-translationally invariant uniparametric inequality for any even number of parties, ground states of spin-glass systems, and a nonintegrable interacting *XXZ*-like Hamiltonian. Their method is a good and efficient approach for entanglement detection of such systems.

In our study, we consider a one dimensional *XYZ* Heisenberg lattice in a uniform magnetic field. Our aim is to study energy as an entanglement witness for this model, analytically. If the energy ensemble average is less than the minimum energy of separable states, the system is entangled [27]. To do so, we minimize energy of separable states using Lagrange undetermined multipliers analytically and we construct the entanglement witnesses. Analytical results show for systems with spin numbers more than six, threshold temperature, the temperature after that the system is separable, will saturate. Also, we show, if we take the conditions of [27], our results will be as same as those ones. The results may be used for entanglement detection of related models such as in quantum memory studying problems [38].

Arranged in four sections, in Sect. 2, we introduce the energy as an entanglement witness for XYZ Heisenberg lattice and calculate the minimum energy using Lagrange undetermined multipliers to construct entanglement witness. Section 3, contains the examples, results and discussion. In Sect. 4, we briefly represent our results and its usefulness and disadvantages.

2 Entanglement Witness for One Dimensional *XYZ* Spin Lattice

Let us to consider a one dimensional lattice of N qubits in an external uniform magnetic field. The Hamiltonian can be written as

$$H = \sum_{i=1}^{N}(J_x\sigma_i^x\sigma_{i+1}^x + J_y\sigma_i^y\sigma_{i+1}^y + J_z\sigma_i^z\sigma_{i+1}^z + \mu h\sigma_i^z), \tag{1}$$

where $\sigma_i^a(a = x, y, z)$ are Pauli operators and $J_a(a = x, y, z)$ are coupling constants indicating the interaction strength between nearest neighbor spins, h denotes the uniform external magnetic field, and μ is the magnetic moment. Hereafter, we suppose $\mu = 1$ and the periodic boundary condition holds for the lattice, that is to say, $N + 1 = 1$. The chain is anti-ferromagnetic for $\mathrm{J} > 0$ and ferromagnetic for $\mathrm{J} < 0$.

How one can detect entanglement of this lattice? One of the entanglement detection approaches is considering energy as an entanglement witness [27,39]. In this approach, the system is entangled if the average energy, $\langle H\rangle$, is less than the minimum energy of the system (separable state), E_{min}^{sep}. In other words, if we define:

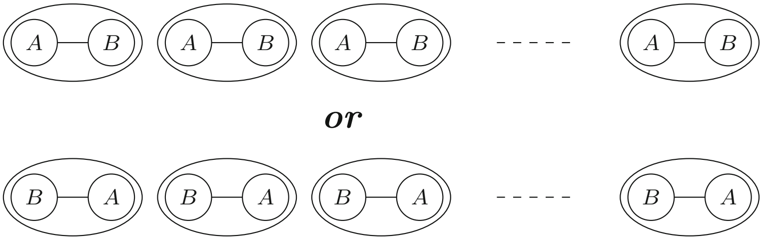

Fig. 1 Partitioning the N qubits lattice. Each pair with two qubits: A and B. In each pair, qubit A interacts with qubit B and each of them with the external magnetic field

$$\Delta E = \langle H \rangle - E_{min}^{sep} \tag{2}$$

then the system is entangled if $\Delta E < 0$. Therefore $|\Delta E|$ characterizes entanglement of the system.

We find E_{min}^{sep} by partitioning the lattice into pairs of qubits in a way that each pair contains two qubits A and B. As it can be seen in Fig. 1, there are two available partitioning, starting with A as the first qubit or B as the first one. In each pair qubit A interacts with qubit B and each of them interacts with the external magnetic field separately. With this in mind, we are going to find the minimum of the Hamiltonian (1). As a separable state can be written as a convex combination of pure product states, then it is enough to minimize only one pair. Then the lattice minimum energy will be equal to a pair minimum energy multiplied by the number of pairs, $N/2$, multiplied by 2 (because there are two distinct partitioning as it can be seen in Fig. 1). We apply this procedure in the following.

2.1 Minimizing Energy Using Lagrange Undetermined Multipliers

In order to minimize energy of each interacting pair, we parameterize the Hamiltonian (2), as follow

$$E_H = J_x \tau_x^A \tau_x^B + J_y \tau_y^A \tau_y^B + J_z \tau_z^A \tau_z^B + \frac{1}{2} h(\tau_z^A + \tau_z^B) \tag{3}$$

with constraints

$$\begin{aligned} \tau_{A,x}^2 + \tau_{A,y}^2 + \tau_{A,z}^2 = 1 \\ \tau_{B,x}^2 + \tau_{B,y}^2 + \tau_{B,z}^2 = 1 \end{aligned} \tag{4}$$

where τ_A and τ_B are Bloch sphere representations of qubits

$$\begin{aligned} &\tau_x^i = \cos\varphi_i \sin\theta_i, && \tau_y^i = \sin\varphi_i \sin\theta_i, && \tau_z^i = \cos\theta_i, \\ &0 \le \theta_i \le \pi, && 0 \le \varphi_i \le 2\pi, && i = A, B. \end{aligned} \tag{5}$$

Now our optimization problem is

$$\begin{aligned} &minimize \quad E_H = J_x \tau_x^A \tau_x^B + J_y \tau_y^A \tau_y^B + J_z \tau_z^A \tau_z^B + \frac{1}{2} h(\tau_z^A + \tau_z^B) \\ &subject \ \ to \quad \tau_{i,x}^2 + \tau_{i,y}^2 + \tau_{i,z}^2 = 1, \quad i = A, B. \end{aligned} \tag{6}$$

This is a nonlinear optimization problem. One of the effective methods for solving such nonlinear optimization problems is the so called Lagrange undetermined multipliers [40].

This method lets us to find minimum (or maximum) of a nonlinear multi variable function $f(x_1, x_2, \ldots)$, with nonlinear constraints, $g_k(x_1, x_2, \ldots) = v,\ k = 1, 2, \ldots$, on the variables $x_1, x_2, \ldots$.

To that end, we construct Lagrangian as follows

$$\mathcal{L} = L(\tau_A, \tau_B, \lambda_1, \lambda_2) = E_H - \sum_{j=A,B} \lambda_j(\tau_{j,x}^2 + \tau_{j,y}^2 + \tau_{j,z}^2 - 1) \tag{7}$$

where λ's is called Lagrange multipliers and there is no sign restriction on the value of λ. If we set the gradient of $\mathcal{L}$ equal to the zero vector, $\nabla\mathcal{L} = 0$, then the energy (3) extremum value solutions are

$$E = \begin{cases} J_z,\ \ J_z \pm h,\ \ \pm(J_x + h^2/4(J_x \mp Jz)),\ \ \pm(J_y + h^2/4(J_y \mp Jz)) \\ \pm(4J_x(J_x + Jz)^2 - h^2(3J_x + Jz))/(4(J_x \pm Jz)^2) \\ \pm(4J_y(J_y + Jz)^2 - h^2(3J_y + Jz))/(4(J_y \pm Jz)^2) \end{cases} \tag{8}$$

To determine which solution is the strict minimum, we use the Hessian matrix. If the Hessian matrix, $\nabla^2 f(x)$, be a positive definite matrix, then x is a strict local minimum of $f(x)$ [41]. For simplicity, we take $\mathrm{J_z} > \mathrm{J_y} > \mathrm{J_x}$ then the minimum energy of separable state pair becomes

$$E_{min}^{pair} = \begin{cases} -(M + h^2/4(M + J_z)) & \text{if } |h| \leq 2(M + J_z) \\ J_z - |h| & \text{if } |h| > 2(M + J_z) \end{cases} \tag{9}$$

Here $\mathrm{M} = \max\{\mathrm{J_x}, \mathrm{J_y}\}$ and so the lattice minimum energy of separable states can be written as follow

$$E_{min}^{lattice} = \begin{cases} -N(M + h^2/4(M + J_z)) & \text{if } |h| \leq 2(M + J_z) \\ N(J_z - |h|) & \text{if } |h| > 2(M + J_z) \end{cases} \tag{10}$$

where, N denotes the total number of spins.

In order to investigate the validity of our result, we consider two special cases. The first case is for $J_x = J_y = J_z = 1$ so $M = 1$, and $\mu = 1$, $h = B$, the so called Heisenberg lattice. In this case Eq. (10) is reduced to

$$E_{min}^{lattice} = \begin{cases} -N(B^2/8 + 1) & \text{if } |B| \leq 4 \\ -N(|B| - 1) & \text{if } |B| > 4 \end{cases} \tag{11}$$

The second case is for $J_z = 0$, and $\mu = 1$, $h = B$, the so called XY model. For this case Eq. (10) is reduced to

$$E_{min}^{lattice} = \begin{cases} -N(M + B^2/(4M)) & \text{if } |B| \leq 2M \\ -N|B| & \text{if } |B| > 2M \end{cases} \tag{12}$$

In both cases, the results are in complete agreement with [27].

The next step to construct entanglement witness using energy (2), is finding energy ensemble average, $\langle H\rangle$. For a given lattice Hamiltonian, the corresponding density matrix in thermal equilibrium is given by

$$\rho = \frac{exp(-H/k_B T)}{Tr[exp(-H/k_B T)]}$$

and the energy average is $\langle H\rangle = Tr[\rho H]$ where k_B is the Boltzmann constant. In the following section, we calculate energy average and entanglement witnesses for systems with low, even number of spins without loss of generality.

3 Examples and Results

Here we apply the previous section results for the one dimensional XYZ lattice with two, four, six, eight and ten spins (qubits).

3.1 Lattice with Two Spins

For two spins XYZ Heisenberg lattice, the Hamiltonian is

$$H = J_x\sigma_1^x\sigma_2^x + J_y\sigma_1^y\sigma_2^y + J_z\sigma_1^z\sigma_2^z + \frac{1}{2}h(\sigma_1^z + \sigma_2^z), \tag{13}$$

and the corresponding density matrix is

$$\rho = \frac{1}{Z}\begin{pmatrix} \Gamma\, e^{-\beta J_z} & 0 & 0 & \left(\frac{\delta}{\alpha}\sinh\alpha\beta\right) e^{-\beta J_z} \\ 0 & \frac{1}{2}(e^{-\beta\Omega} + e^{\beta\Delta}) & \frac{1}{2}(e^{-\beta\Omega} - e^{\beta\Delta}) & 0 \\ 0 & \frac{1}{2}(e^{-\beta\Omega} - e^{\beta\Delta}) & \frac{1}{2}(e^{-\beta\Omega} + e^{\beta\Delta}) & 0 \\ \left(\frac{\delta}{\alpha}\sinh\alpha\beta\right) e^{-\beta J_z} & 0 & 0 & \Lambda\, e^{-\beta J_z} \end{pmatrix}, \tag{14}$$

where $\beta = 1/k_B T$,

$$\begin{aligned} \Omega &= J_x + J_y - J_z, & \delta &= J_y - J_x, \\ \alpha &= \sqrt{h^2 + \delta^2}, & \Delta &= J_x + J_y + J_z, \\ \Gamma &= \cosh\beta\alpha - \tfrac{h}{\alpha}\sinh\beta\alpha, & \Lambda &= \cosh\beta\alpha + \tfrac{h}{\alpha}\sinh\beta\alpha, \end{aligned} \tag{15}$$

where, Z, the partition function of the system, is given by

$$Z = e^{-\beta\Omega} + e^{\beta\Delta} + 2e^{-\beta J_z}\cosh\beta\alpha \tag{16}$$

The energy ensemble average is

$$\begin{aligned} \langle H\rangle =&Tr(\rho H) = \frac{1}{Z\,\alpha}[-h^2 e^{\beta\omega}(-1 + e^{2\alpha\beta}) - e^{\beta(2\alpha+\delta)}(-J_z\,\alpha + \delta^2) \\ &+ e^{\beta\omega}(J_z\,\alpha + \delta^2) + \alpha\,\Delta\, e^{(2J_z+\alpha)\beta} - \alpha\,\Omega\, e^{\beta(\alpha+2\Omega)}] \end{aligned} \tag{17}$$

where $\omega = J_x + J_y$. The corresponding entanglement witness becomes $\Delta E = \langle H\rangle - E_{sep}$. Fig. 2a shows this witness in terms of the external magnetic field, h, at several temperatures. Now we are in the position that we can compare our results with the PPT, or so called Peres-Horodecki criterion which gives the necessary and sufficient condition of entanglement for two qubits systems. According to this criterion, if the least eigenvalue of ρ^{T_B} is negative, then the two qubits system is entangled. To do so, we calculate the partial transpose of the density matrix (13), which is

$$\rho^{T_B} = \frac{1}{Z}\begin{pmatrix} \Gamma\, e^{-\beta J_z} & 0 & 0 & \frac{1}{2}(e^{-\beta\Omega} - e^{\beta\Delta}) \\ 0 & \frac{1}{2}(e^{-\beta\Omega} + e^{\beta\Delta}) & \frac{\delta}{\alpha}\sinh\beta\alpha & 0 \\ 0 & \frac{\delta}{\alpha}\sinh\alpha\beta & \frac{1}{2}(e^{-\beta\Omega} + e^{\beta\Delta}) & 0 \\ \frac{1}{2}(e^{-\beta\Omega} - e^{\beta\Delta}) & 0 & 0 & \Lambda\, e^{-\beta J_z} \end{pmatrix} \tag{18}$$

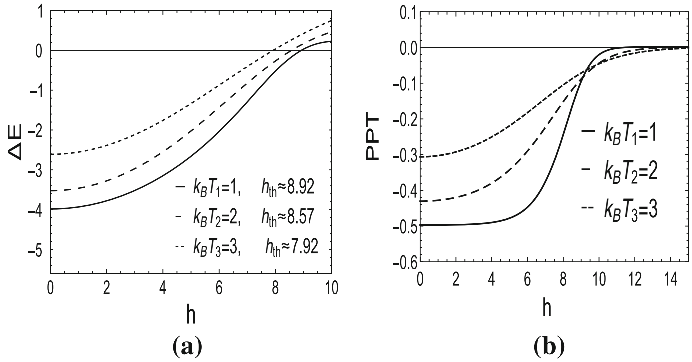

Fig. 2 **a** The entanglement witnesses, ΔE, of two qubits system and **b** The PPT criterion for two qubits system. Here $J_x = 1$, $J_y = 2$, $J_z = 3$. Threshold magnetic field, h_{th}, for which below them the entanglement can be detected, has been calculated for some temperatures

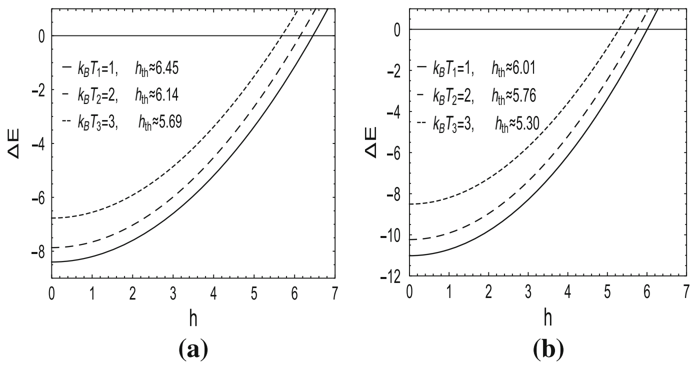

Fig. 3 The entanglement witnesses ΔE for **a** four and **b** six qubit system in terms of external magnetic field, h for $J_x = 1$, $J_y = 2$, $J_z = 3$

The least eigenvalue of the partial transposed matrix, is plotted in terms of h in Fig. 2b. However, due to Fig. 2, it is clear that there is a good agreement between our, Fig. 2a, and the PPT criterion results, Fig. 2b.

3.2 System with More Than Two Spins

Now we extend our results to even qubits systems up to ten qubits. Figure 3a, b represents the results for four and six qubits systems respectively. As seen, with increasing h, the entanglement witness ΔE, goes to zero so the entanglement can not be detected. The thresholds values of h, for which below them the entanglement can be detected, are given in Fig. 3a, b for four and six qubits respectively, where $k_B T = 1$, $h_{th} \approx 6.45$ is for four and $h_{th} \approx 6.01$ is for six qubits.

Figure 4 illustrates entanglement witnesses in terms of temperature for zero magnetic field, $h = 0$. When the number of particles becomes more than six, $N \geq 6$, It seems that the system takes a saturated state so that for $h = 0$ the threshold temperature becomes $k_B T_{th} \approx 7$ and does not change any more.

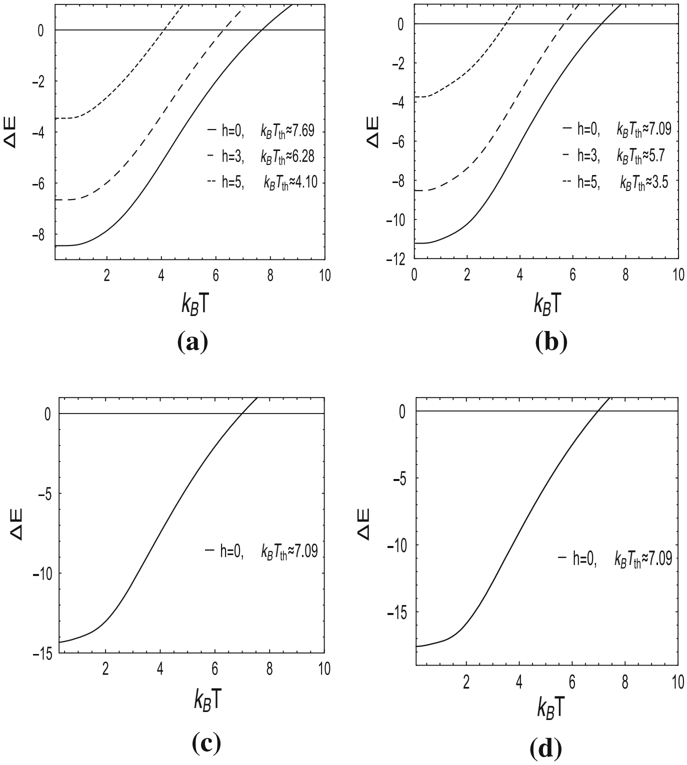

Fig. 4 The entanglement witnesses ΔE of **a** four, **b** six, **c** eight, and **d** ten qubits systems in terms of temperature $k_B T$. For $N \geq 6$ the threshold temperature is nearly $T_{th} \approx 7.09$. Here $J_x = 1$, $J_y = 2$, $J_z = 3$

For a special case $J_x = J_y = J_z$, the Hamiltonian reduce to Heisenberg XXX model, and the threshold temperature for $h = 0$ and $N \geq 8$ becomes $T_{th} = 3.1833$ which is in complete agreement with the threshold temperature in [42,43].

4 Conclusion and Discussion

If energy ensemble average is less than the minimum energy of separable states, the system is entangled so one can consider this condition as an entanglement witness specially for low dimensional systems. Here we have investigated this condition for one dimensional XYZ Heisenberg lattice with the external magnetic field. We found the minimum energy of separable states analytically using the Lagrange undetermined multipliers method. Lattices with two qubits have been studied with details. Comparison of results with the PPT criterion shows there is good agreement between them. We also applied the approach for systems up to ten qubits. The results show when spin number is greater than six, threshold temperature, the temperature after that the system is separable, will be saturated for zero magnetic field. As two special cases of our results, there are complete agreement with ref [27] for both the Heisenberg lattice and XY model. The temperature thresholds for XXX lattices, as a special case of our approach, is also in compatible with [42,43].

In spite of the fact that this method may be used for different Hamiltonians and gives the temperature dependence of the entanglement, our study has its limitations. First, it cannot be applied to systems with long-range couplings where, in this case one must consider the coupling with not only between nearest neighbors but also, with other qubits. Second, there is an analytical form of density matrix only for systems with low qubits. In other words, the minimum energy of the separable states is valid for any qubit systems (analytic form) but, there is the computational complexity of calculating the energy ensemble average for many qubits systems. Although, there are numerical solutions usually. To overcome this disadvantage one may use other methods to calculate the energy average such as Monte–Carlo methods which are under investigation.

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