

Entanglement witnesses in spin models

Géza Tóth

Theoretical Division, Max Planck Institute for Quantum Optics, Hans-Kopfermann-Straße 1, D-85748 Garching, Germany

(Received 21 July 2004; published 6 January 2005)

We construct entanglement witnesses using fundamental quantum operators of spin models which contain two-particle interactions and have a certain symmetry. By choosing the Hamiltonian as such an operator, our method can be used for detecting entanglement by energy measurement. We apply this method to the Heisenberg model in a cubic lattice with a magnetic field, the XY model, and other familiar spin systems. Our method provides a temperature bound for separable states for systems in thermal equilibrium. We also study the Bose-Hubbard model and relate its energy minimum for separable states to the minimum obtained from the Gutzwiller ansatz.

DOI: 10.1103/PhysRevA.71.010301

PACS number(s): 03.65.Ud, 03.67.-a, 05.50.+q

I. INTRODUCTION

Entanglement lies at the heart of quantum mechanics and also plays an important role in the field of quantum information theory (QIT) [1]. While for pure quantum states it is equivalent to correlations, for mixed states the two notions differ. In this general case, a quantum state is entangled if its density matrix cannot be written as a convex sum of product states. Based on this definition, several sufficient conditions for entanglement have been developed [1]. In special cases, e.g., for 2×2 (two-qubit) and 2×3 bipartite systems [2], and for multimode Gaussian states [3], even necessary and sufficient conditions are known.

However, in an experimental situation, usually only limited information about the quantum state is available. Only those approaches for entanglement detection can be applied, which require the measurement of not too many observables. One such approach is using entanglement witnesses. They are observables which have a positive expectation value or one that is zero for all separable states. Thus a negative expectation value signals the presence of entanglement. The theory of entanglement witnesses has recently been rapidly developing [4]. It has been shown how to generate entanglement witnesses that detect states close to a given one, even if it is mixed or a bound entangled state [5]. It is also known how to optimize a witness operator in order to detect the most entangled states [6].

Beside constructing entanglement witnesses, it is also important to find a way to measure them. For example, they can easily be measured by decomposing them into a sum of locally measurable terms [7]. In this paper we follow a different route. We will construct witness operators of the form

$$W_O := O - \inf_{\Psi \in S} [\langle \Psi | O | \Psi \rangle], \quad (1)$$

where S is the set of separable states, “inf” denotes infimum, and O is a fundamental quantum operator of a spin system which is easy to measure. In the general case $\inf_{\Psi \in S} \langle \Psi | O | \Psi \rangle$ is difficult, if not impossible, to compute [8]. Thus we will concentrate on operators that contain only two-particle interactions and have certain symmetries. We derive a general method to find bounds for the expectation value of such operators for separable states. This method will be applied to

spin lattices. We will also consider models with a different topology.

If observable O is taken to be the Hamiltonian, then our method can be used for detecting entanglement by energy measurement [9]. While our approach does not require that the system is in thermal equilibrium, it can readily be used to detect entanglement for a range of well-known systems in this case. The energy bound for separable states correspond to a temperature bound. Below this temperature the thermal state is necessarily entangled. Numerical calculations have been carried out for some familiar spin models. They show that for the parameter range in which substantial entanglement is present in the thermal ground state, our method detects the state as entangled. Thus our work contributes to recent efforts connecting QIT and the statistical physics of spin models [10].

II. ENERGY BOUND FOR SEPARABLE STATES

We consider a general observable O on a spin lattice defined in terms of the Pauli spin operators $\vec{\sigma}^{(k)}$ $= [\sigma_x^{(k)}, \sigma_y^{(k)}, \sigma_z^{(k)}]$ as

$$O := \mathcal{O}(\{\vec{\sigma}^{(k)}\}_{k=1}^N), \quad (2)$$

where \mathcal{O} is some multivariable function [11]. We will discuss how to find the minimum expectation value of such an operator for separable states of the form

$$\rho = \sum_l p_l \rho_l^{(1)} \otimes \rho_l^{(2)} \otimes \dots \otimes \rho_l^{(N)}. \quad (3)$$

The minimum of $\langle O \rangle$ for pure product states is obtained by replacing the Pauli spin matrices by real variables $s_{x/y/z}^{(k)}$ in Eq. (2) and minimizing it with the constraint that $s^{(k)}$ are unit vectors [12]. The minimum obtained this way is clearly valid also for mixed separable states, since the set of separable states is convex

$$O_{\text{sep}} := \inf_{\Psi \in S} \langle \Psi | O | \Psi \rangle = \inf_{\{s^{(k)}\}} \mathcal{O}(\{s^{(k)}\}_{k=1}^N). \quad (4)$$

In the most general case many-variable minimization is needed for obtaining O_{sep} . In some cases, to which many of the most studied lattice Hamiltonians belong, it is possible to

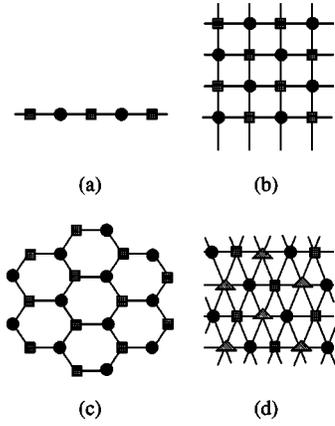


FIG. 1. Some of the most often considered lattice models: (a) Chain, (b) two-dimensional cubic, (c) hexagonal, and (d) triangular. Different symbols at the vertices indicate a possible partitioning into sublattices.

find a simple recipe for computing the minimum of \mathcal{O} .

(i) Let us consider an operator \mathcal{O} which is the sum of two-body interactions. It can be described by a lattice or a graph. The vertices $V := \{1, 2, \dots, N\}$ correspond to spins and the edges between two vertices indicate the presence of interaction.

(ii) Let us assume that this lattice can be partitioned into sublattices in such a way that interacting spins correspond to different sublattices. Figure 1 shows lattices of some common one- and two-dimensional spin models. The different symbols at the vertices indicate a possible partitioning into sublattices with the above property. For simplicity, next we will consider the case with only two disjoint sublattices, A and B , and assume that \mathcal{O} can be written in the form

$$\mathcal{O}(\{\vec{s}^{(k)}\}_{k=1}^N) = \sum_{\vec{s}_k^A \in A, \vec{s}_k^B \in B} f(\vec{s}_k^A, \vec{s}_k^B), \quad (5)$$

where f is some two-spin function, and $\vec{s}_k^{A/B}$ denotes spins of sublattice A/B .

If conditions (i) and (ii) are met, then it is enough to find spins \vec{s}^A and \vec{s}^B corresponding to the minimum of $f(\vec{s}^A, \vec{s}^B)$. Then, setting all the spins in sublattice A to \vec{s}^A and in sublattice B to \vec{s}^B , respectively, gives a solution which minimizes

III. EXAMPLES

In the following we will use the Hamiltonian H for constructing entanglement witnesses. The energy minimum for separable states is the same as the ground state of the corresponding classical spin model. Our method detects entanglement if

$$\Delta E := \langle H \rangle - E_{\text{sep}} < 0. \quad (6)$$

If $\Delta E < 0$ then $|\Delta E|$ characterizes the state of the system from the point of view of the robustness of entanglement. It is a lower bound on the energy that the system must receive to become separable.

We will use the previous results to detect entanglement in thermal states of spin models. In thermal equilibrium the

state of the system is given as $\rho_T = \exp(-H/k_B T) / \text{Tr}[\exp(-H/k_B T)]$, where T is the temperature and k_B is the Boltzmann constant. For simplicity we will set $k_B = 1$. Using Eq. (6) a temperature bound, T_E , can be found such that when $T < T_E$, then the system is detected as entangled.

A. Heisenberg lattice

Let us consider an antiferromagnetic Heisenberg Hamiltonian with periodic boundary conditions on a d -dimensional cubic lattice

$$H_H := \sum_{\langle k, l \rangle} \sigma_x^{(k)} \sigma_x^{(l)} + \sigma_y^{(k)} \sigma_y^{(l)} + \sigma_z^{(k)} \sigma_z^{(l)} + B \sigma_z^{(k)}. \quad (7)$$

The strength of the exchange interaction is set to be $J=1$, B is the magnetic field, and $\langle k, l \rangle$ denotes spin pairs connected by an interaction. The expectation value of Eq. (7) for separable states is bounded from below

$$\langle H_H \rangle \geq E_{H, \text{sep}} := \begin{cases} -dN(B^2/8 + 1) & \text{if } |B| \leq 4 \\ -dN(|B| - 1) & \text{if } |B| > 4 \end{cases}, \quad (8)$$

where N is the total number of spins. This bound was obtained using two sublattices, minimizing the expression $f_H(\vec{s}^A, \vec{s}^B) := \vec{s}^A \vec{s}^B + B(s_z^A + s_z^B)/2$. Based on this, $E_{H, \text{sep}} = dN \inf[f_H]$ [13].

Let us now consider a one-dimensional spin-1/2 Heisenberg chain of even number of particles. If $B=0$ then Eq. (8) corresponds to

$$\frac{1}{N} \sum_{\langle k, l \rangle} \langle \vec{\sigma}^{(k)} \vec{\sigma}^{(l)} \rangle \geq -1, \quad (9)$$

which is simply a necessary condition for separability in terms of nearest-neighbor correlations. The energy minimum for entangled states can be obtained using the Bethe ansatz as $E_{\text{min}} = -4N(\ln 2 - 1/4) \approx -1.77N$ [14]. The energy gap between the minimum for separable states and the ground-state energy of H_H is thus $\Delta E_{\text{gap}} \approx 0.77N$, which increases linearly with the number of spins. As shown in Refs. [16,17], when $B=0$ the concurrence of the two-qubit reduced density matrix in the thermal state is obtained as $C = \max[-\langle H_H \rangle / N + 1, 0]$. Hence $C > 0$ if $\langle H_H \rangle < -N$ and $E_{H, \text{sep}}$ coincides with the energy bound for nonzero concurrence.

Let us now consider the case $B > 0$. Figure 2(a) shows the nearest-neighbor entanglement versus B and T . The entanglement of formation was computed from the concurrence [15]. Light color indicates the region where the thermal ground state is detected as entangled. There are regions with $C > 0$ which are not detected. However, it is clear that when the system contains at least a small amount of entanglement (~ 0.07) the state is detected as entangled. Note that the sharp decrease of the nearest-neighbor entanglement around $B_{\text{crit}}=4$ for $T=0$ is due to a *quantum phase transition*.

Another important question is how the temperature bound T_E depends on the number of particles. For the Heisenberg model of even number of spins with $B=0$ this temperature decreases slowly with N and saturates at $T \approx 3.18$. Reference [17] finds the same bound temperature for nonzero concurrence for an infinite system.

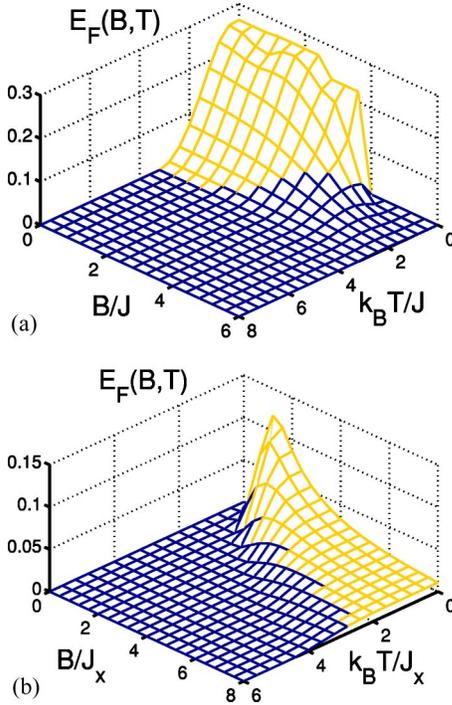


FIG. 2. (a) Heisenberg chain of eight spins. Nearest-neighbor entanglement as a function of magnetic field B and temperature T . (b) The same for an Ising spin chain. Here k_B is the Boltzmann constant, J and J_x are coupling constants. Light color indicates the region where entanglement is detected by our method.

B. XY model

The XY Hamiltonian on a d -dimensional cubic lattice with periodic boundary conditions is

$$H_{XY} := \sum_{\langle k,l \rangle} J_x \sigma_x^{(k)} \sigma_x^{(l)} + J_y \sigma_y^{(k)} \sigma_y^{(l)} + B \sum_k \sigma_z^{(k)}. \quad (10)$$

The energy of separable states is bounded from below

$$\langle H_{XY} \rangle \geq E_{XY, \text{sep}} := \begin{cases} -dNM(1 + b^2/4) & \text{if } b \leq 2, \\ -dNmb & \text{if } b > 2. \end{cases} \quad (11)$$

Here $J_{x/y}$ is the nearest-neighbor coupling along the x/y direction, B is the magnetic field, $M := \max(|J_x|, |J_y|)$ and $b := |B|/M$. This bound is simply the mean-field ground-state energy. It was obtained using two sublattices and minimizing $f_{XY}(\vec{s}^A, \vec{s}^B) := J_x s_x^A s_x^B + J_y s_y^A s_y^B + B(s_z^A + s_z^B)/2$.

A one-dimensional spin-1/2 Ising chain is a special case of an XY lattice with $J_x = 1$ and $J_y = 0$. Figure 2(b) shows the nearest-neighbor entanglement as a function of B and T for this system. According to numerics, T_E (computed for $B = 1$) decreases with increasing N . For $N = \infty$ we obtain $T_E \approx 0.41$ [18].

C. Heisenberg coupling between all spin pairs

From a theoretical point of view, it is interesting to consider a system in which the interactions are described by a complete graph rather than a lattice [19]. For the following Hamiltonian of N spin-1/2 particles,

$$H_S := J_x^2 + J_y^2 + J_z^2, \quad (12)$$

the expectation value for separable states is bounded [20]

$$\langle H_S \rangle \geq E_{S, \text{sep}} := 2N. \quad (13)$$

Here $J_{x/y/z} = \sum_k \sigma_{x/y/z}^{(k)}$ and for simplicity N is taken to be even.

Now we could not use the method for partitioning the spins into sublattices. The proof of Eq. (13) is based on the theory of entanglement detection with uncertainty relations [20,21]. For separable states one obtains [20]

$$\begin{aligned} & (\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 \\ & \geq \sum_l p_l \sum_k [(\Delta \sigma_x^{(k)})_l^2 + (\Delta \sigma_y^{(k)})_l^2 + (\Delta \sigma_z^{(k)})_l^2] \geq NL_S, \end{aligned} \quad (14)$$

where index l denotes the l th subensemble and $L_S = \inf_{\Psi} [(\Delta \sigma_x)_{\Psi}^2 + (\Delta \sigma_y)_{\Psi}^2 + (\Delta \sigma_z)_{\Psi}^2] = 2$. Hence Eq. (13) follows. The measured energy even gives information on the entanglement properties of the system. Based on the previous considerations, it can be proved that the number of unentangled spins is smaller than $\langle H_S \rangle / 2$.

Following the approach of Ref. [16], the concurrence can be computed as a function of the energy. For even N the concurrence is $C = \max\{-[\langle H_S \rangle + N(N-4)]/[2N(N-1)], 0\}$. Since for all quantum states $\langle H_S \rangle \geq 0$, the concurrence is zero for any temperature if $N \geq 4$. Thus our condition can detect multiqubit entanglement even when two-qubit entanglement is not present.

The thermodynamics of H_S can be obtained by knowing the energy levels and their degeneracies [22],

$$E_j = 2j(j+2), \quad d_j = \frac{(2j+1)^2}{N/2+j+1} \binom{N}{N/2+j}, \quad (15)$$

where $0 \leq j \leq N/2$. Approximating the binomial in Eq. (15) by a Gaussian, and taking the limit $N \rightarrow \infty$ while keeping T/N constant, we obtain $\langle H_S \rangle \approx 3NT/(T+2N)$ and $T_E \approx 4N$, which is in agreement with our numerical calculations. Thus T_E increases linearly with N , the reason being that the number of two-body interaction terms increases quadratically with the system size.

D. Bose-Hubbard model

Consider now a lattice model, the one-dimensional Bose-Hubbard model, in which the number of particles can vary on the lattice sites. We use the language of second quantization. Each lattice site corresponds to a bosonic mode with a destruction operator a_k . The Hamiltonian is [24]

$$H_B := -J \sum_{\langle k,l \rangle} a_k^\dagger a_l + a_l a_k^\dagger + U \sum_k a_k^\dagger a_k^\dagger a_k a_k, \quad (16)$$

where J is the intersite tunneling and U is the onsite interaction. Let us consider the case when there is at most a single particle per lattice site ($U \gg J$) [25]. Then, for separable states the energy is bounded from below as

$$\langle H_B \rangle \geq E_{B,\text{sep}} := -2JN_b(1 - N_b/N), \quad (17)$$

where N is the number of lattices sites and $N_b := \langle \sum_k a_k^\dagger a_k \rangle$ is the number of bosonic particles. For $N=10$ and $N_b=N/2$ (half filling) we obtain $T_E \approx 0.69J$.

Equation (17) can be proved as follows. Let us consider a site in a pure state $|\Psi\rangle = \alpha|0\rangle + \beta|1\rangle$ such that $|\alpha|^2 + |\beta|^2 = 1$. For this single-site state $\langle a \rangle = |\alpha\beta|$ and $\langle a^\dagger a \rangle = |\beta|^2$. Hence $|\langle a \rangle|^2 = \langle a^\dagger a \rangle (1 - \langle a^\dagger a \rangle)$. Now using $\sum_{\langle k,l \rangle} \langle a_k^\dagger \rangle \langle a_l \rangle + \text{H.c.} \leq 2 \sum_k |\langle a_k \rangle|^2$ one can show that $E_{B,\text{sep}}$ is an energy bound for product states. It is a bound also for mixed separable states of the form Eq. (3) since $E_{B,\text{sep}}(N_b)$ is a convex function.

Remarkably, the energy minimum for separable states equals the minimum for translationally invariant product states. In other words, it equals the energy minimum obtained from the Gutzwiller ansatz [23] if the expectation value of the particle number is constrained to N_b . Note that for our calculations we assumed that there is at most a single atom per lattice site.

E. Physical realization

The above methods can be used for entanglement detection in the following ways: (i) Energy can be directly measured in some systems (e.g., optical lattices of cold atoms

[24] when used to realize the Bose-Hubbard model). (ii) The temperature can be measured and used for entanglement detection. (iii) The expectation value of the Hamiltonian can be obtained indirectly if the correlation terms of the Hamiltonian are measured. For example, average correlations $\sum_k \langle \sigma_a^{(k)} \sigma_a^{(k+1)} \rangle / N$; $a=x,y,z$ can be measured in a Heisenberg chain realized with two-state bosonic atoms [26]. From these correlations $\langle H_H \rangle$ can be computed.

IV. CONCLUSION

In summary, we used the Hamiltonian for witnessing entanglement in spin models. We also considered bosonic lattices. Our further results concerning this system will be presented in a future publication [27]. While our method works for nonequilibrium systems, we have shown that entanglement can efficiently be detected by measuring energy in a thermal equilibrium.

We thank J.I. Cirac, A.C. Doherty, O. Gühne, P. Hyllus, V. Murg, and M.M. Wolf for useful discussions. We also thank J.J. García-Ripoll for helpful discussions on the Bose-Hubbard model, and K. Hammerer for suggesting Ref. [22]. We also acknowledge the support of the European Union (Grant No. MEIF-CT-2003-500183), the EU projects RESQ and QUPRODIS, and the Kompetenznetzwerk Quanteninformativonsverarbeitung der Bayerischen Staatsregierung.

-
- [1] D. Bouwmeester, A. Ekert, and A. Zeilinger, *The Physics of Quantum Information* (Springer, Berlin, 2000).
- [2] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996).
- [3] G. Giedke *et al.*, Phys. Rev. Lett. **87**, 167904 (2001).
- [4] M. Horodecki *et al.*, Phys. Lett. A **223**, 1 (1996); B.M. Terhal, *ibid.* **271**, 319 (2000); M. Lewenstein *et al.*, Phys. Rev. A **62**, 052310 (2000).
- [5] A. Acín *et al.*, Phys. Rev. Lett. **87**, 040401 (2001).
- [6] M. Lewenstein *et al.*, Phys. Rev. A **62**, 052310 (2000).
- [7] M. Bourennane *et al.*, Phys. Rev. Lett. **92**, 087902 (2004); G. Tóth and O. Gühne, e-print quant-ph/0405165.
- [8] J. Eisert *et al.*, e-print quant-ph/0407135; A.C. Doherty *et al.*, e-print quant-ph/0407143.
- [9] Independently, a preprint with a similar approach has recently appeared: Č. Brukner and V. Vedral, e-print quant-ph/040604.
- [10] A. Osterloh *et al.*, Nature (London) **416**, 608 (2002); T.J. Osborne and M.A. Nielsen, Phys. Rev. A **66**, 032110 (2002); G. Vidal *et al.*, Phys. Rev. Lett. **90**, 227902 (2003); F. Verstraete *et al.*, *ibid.* **92**, 027901 (2004); M.C. Arnesen *et al.*, *ibid.* **87**, 017901 (2001); V. Vedral, New J. Phys. **6**, 22 (2004).
- [11] \mathcal{O} is a sum of products of spin coordinates. These products have the form $\prod_k s_{a_k}^{(k)}$, where $a_k \in \{0,x,y,z\}$ and $s_0^{(k)} = 1$. Thus every spin can appear at most once. These restrictions are necessary if we want to use \mathcal{O} for getting the minimum for $\langle \mathcal{O} \rangle$. For example, $\mathcal{O} = (s_x^{(1)})^2$ is not of the required form. Its minimum is zero, while the corresponding quantum operator is $O = [\sigma_x^{(1)}]^2 = 1$.
- [12] Although we consider the spin-1/2 case, our approach can straightforwardly be generalized for spin-1 lattices.
- [13] If the number of sites along one dimension is odd, then a lattice with periodic boundary conditions cannot be partitioned into two sublattices such that neighboring sites correspond to different sublattices. In this case E_{sep} given in this paper is still a lower bound for the energy of separable states, but not necessarily the highest possible lower bound.
- [14] M. Takashi, *Thermodynamics of One-Dimensional Solvable Models* (Cambridge University Press, Cambridge, England, 1999).
- [15] C.H. Bennett *et al.*, Phys. Rev. A **54**, 3824 (1996); W.K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998); V. Coffman *et al.*, Phys. Rev. A **61**, 052306 (2000).
- [16] K.M. O'Connor and W.K. Wootters, Phys. Rev. A **63**, 052302 (2001).
- [17] X. Wang, Phys. Rev. A **66**, 044305 (2002); X. Wang and P. Zanardi, Phys. Lett. A **301**, 1 (2002).
- [18] P. Pfeuty, Ann. Phys. (N.Y.) **57**, 79 (1970).
- [19] T. Eggeling, R.F. Werner, and M.M. Wolf (unpublished); T. Eggeling, Ph.D. thesis, Technical University of Braunschweig, Germany, 2003 (unpublished); M. Plesch and V. Bužek, Phys. Rev. A **67**, 012322 (2003).
- [20] H.F. Hofmann and S. Takeuchi, Phys. Rev. A **68**, 032103 (2003).
- [21] O. Gühne, Phys. Rev. Lett. **92**, 117903 (2004); G. Tóth, Phys. Rev. A **69**, 052327 (2004).
- [22] J.I. Cirac *et al.*, Phys. Rev. Lett. **82**, 4344 (1999); G. Chiribella *et al.*, *ibid.* **93**, 180503 (2004).
- [23] W. Krauth *et al.*, Phys. Rev. B **45**, 3137 (1992).
- [24] D. Jaksch *et al.*, Phys. Rev. Lett. **81**, 3108 (1998); M. Greiner *et al.*, Nature (London) **415**, 39 (2002).
- [25] B. Paredes *et al.*, Nature (London) **429**, 277 (2004).
- [26] J. J. Garcia-Ripoll *et al.*, e-print cond-mat/0404566.
- [27] G. Tóth and J.I. Cirac (unpublished).