

Spin squeezing and entanglement

Géza Tóth,^{1,2,3,4,*} Christian Knapp,^{5,†} Otfried Gühne,^{5,6,‡} and Hans J. Briegel^{5,6,§}

¹*Department of Theoretical Physics, The University of the Basque Country, P. O. Box 644, E-48080 Bilbao, Spain*

²*Ikerbasque-Basque Foundation for Science, Alameda Urquijo 36, E-48011 Bilbao, Spain*

³*Institute of Photonic Sciences, Mediterranean Technology Park, E-08860 Castelldefels (Barcelona), Spain*

⁴*Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary*

⁵*Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria*

⁶*Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, A-6020 Innsbruck, Austria*

(Received 7 July 2008; published 27 April 2009)

What is the relation between spin squeezing and entanglement? To clarify this, we derive the full set of generalized-spin-squeezing inequalities for the detection of entanglement. These are inequalities for the mean values and variances of the collective angular-momentum components J_k . They can be used for the experimental detection of entanglement in a system of spin- $\frac{1}{2}$ particles in which the spins cannot be individually addressed. We present various sets of inequalities that can detect all entangled states that can be detected based on the knowledge of (i) the mean values and variances of J_k in three orthogonal directions, or (ii) the variances of J_k in three orthogonal directions, or (iii) the mean values of J_k^2 in three orthogonal directions, or (iv) the mean values and variances of J_k in arbitrary directions. We compare our inequalities to known spin-squeezing entanglement criteria and discuss to which extent spin squeezing is related to entanglement in the reduced two-qubit states. Finally, we apply our criteria for the detection of entanglement in spin models, showing that they can be used to detect bound entanglement in these systems.

DOI: 10.1103/PhysRevA.79.042334

PACS number(s): 03.67.Mn, 03.65.Ud, 05.50.+q, 42.50.Dv

I. INTRODUCTION

Entanglement lies at the heart of many problems in quantum mechanics and has attracted an increasing attention in recent years [1,2]. Entanglement is needed in several quantum information processing tasks such as teleportation and certain quantum cryptographic protocols. It also plays an important role in quantum computing making it possible that quantum computers can outperform their classical counterparts for several problems such as prime factoring or searching. Moreover, entangled states and the creation of quantum entanglement naturally arise as goals in nowadays quantum control experiments when studying the nonclassical phenomena in quantum mechanics.

When in an experiment entanglement is created, it is important to detect it. Thus, in many quantum physics experiments the creation of an entangled state is followed by measurements. Based on the results of these measurements, the experimenters conclude that the produced state was entangled. However, in many-particle experiments the possibilities for quantum control are very limited. In particular, the particles cannot be individually addressed. In such systems, the entanglement can be created and detected with collective operations.

Spin squeezing is one of the most successful approaches for creating quantum entanglement in such systems [3–17]. Reference [3] defined spin squeezing in analogy with squeezing in quantum optics. Let us consider an ensemble of

N spin- $\frac{1}{2}$ particles and define the observables for the collective angular momentum as

$$J_l := \frac{1}{2} \sum_{k=1}^N \sigma_l^{(k)} \quad (1)$$

for $l=x,y,z$ and where $\sigma_l^{(k)}$ are Pauli matrices. Then, the variances of the angular-momentum components are bounded by the following uncertainty relation:

$$(\Delta J_z)^2 (\Delta J_y)^2 \geq \frac{1}{4} |\langle J_x \rangle|^2. \quad (2)$$

If $(\Delta J_z)^2 := \langle J_z^2 \rangle - \langle J_z \rangle^2$ is smaller than the standard quantum limit $\frac{1}{2} |\langle J_x \rangle|$ then the state is called spin squeezed [18]. In practice, this means that the mean angular momentum of the state is large, and in a direction orthogonal to it the angular-momentum variance is small. An alternative and slightly different definition of spin squeezing considered the usefulness of spin-squeezed states for reducing spectroscopic noise or to improve the accuracy of atomic clocks [4,19].

It has already been noted in Ref. [3] that the occurrence of spin squeezing is connected to the correlations between the spins. In fact, as shown in Ref. [8], there is an entanglement criterion for the detection of the entanglement of spin-squeezed states. If an N -qubit state violates the inequality

$$\frac{(\Delta J_z)^2}{\langle J_x \rangle^2 + \langle J_y \rangle^2} \geq \frac{1}{N}, \quad (3)$$

then the state is entangled (not separable); that is, it cannot be written as [20]

*toth@alumni.nd.edu

†christian.knapp@uibk.ac.at

‡otfried.guehne@uibk.ac.at

§hans.briegel@uibk.ac.at

$$\rho = \sum_k p_k \rho_k^{(1)} \otimes \rho_k^{(2)} \otimes \dots \otimes \rho_k^{(N)}, \quad (4)$$

where the p_k forms a probability distribution.

After this first entanglement criterion, several generalized-spin-squeezing criteria for the detection of entanglement appeared in the literature [21–23] and have been used experimentally [24,25]. In Ref. [22], a generalized-spin-squeezing inequality was presented that detects entanglement close to many-body spin singlets such as, for example, the ground state of an antiferromagnetic Heisenberg chain. In Ref. [21], a generalized-spin-squeezing criterion was presented detecting the presence of two-qubit entanglement. For symmetric systems, these criteria are necessary and sufficient. In Ref. [23], other criteria can be found that detect entanglement close to symmetric Dicke states. All these entanglement conditions were obtained using very different approaches. Therefore, one may ask: is there a systematic way of finding all such inequalities? Clearly, finding such optimal entanglement conditions is a hard task since one can expect that they contain complicated nonlinearities.

In Ref. [26], we have presented a set of spin-squeezing inequalities for the detection of entanglement. We showed that these inequalities are complete, in the sense that they can detect all entangled states that can be detected by the knowledge of $\langle J_l \rangle$ and $(\Delta J_l)^2$ for three orthogonal directions $l = x, y, z$. This completeness means the following. A state that is not detected by the inequalities cannot be distinguished from a separable state by knowing $\langle J_l \rangle$ and $(\Delta J_l)^2$ only.

In this paper, we present extensions of this approach in several directions. In Sec. II, we first present a detailed derivation of the optimal spin-squeezing inequalities from Ref. [26]. Then, we consider the case when only the variances $(\Delta J_l)^2$ (and not the mean values $\langle J_l \rangle$) are known or when only the mean values $\langle J_l^2 \rangle$ are known. We derive the optimal spin-squeezing inequalities also for this case. In Sec. III, we consider the case when $\langle J_l \rangle$ and $(\Delta J_l)^2$ are known not only in three orthogonal directions but also in arbitrary directions. In this case, we can reformulate the spin-squeezing inequalities as inequalities for correlation and covariance matrices. In Sec. IV, we compare our optimal spin-squeezing inequalities to other known entanglement criteria. In Sec. V, we discuss the issue of detecting entanglement of the multiqubit quantum state vs detecting entanglement in the reduced two-qubit density matrix. Finally, in Sec. VI we apply our inequalities to the investigation of spin models. We have shown already in Ref. [26] that the spin-squeezing inequalities can detect bound entanglement (a weak form of entanglement, which is at the heart of many fundamental problems in entanglement theory) in such models. Here, we present more examples for the applicability of the spin-squeezing inequalities.

II. OPTIMAL SPIN-SQUEEZING INEQUALITIES

Our aim is to characterize the separable states in terms of the values of $\langle J_l \rangle$ and $(\Delta J_l)^2$. Note that the knowledge of $\langle J_l \rangle$ and $(\Delta J_l)^2$ is equivalent to the knowledge of $\langle J_l \rangle$ and $\langle J_l^2 \rangle$. We now present our main result from Ref. [26]:

Observation 1. Let us assume that for a physical system the values of

$$\vec{J} := (\langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle) \quad (5)$$

and

$$\vec{K} := (\langle J_x^2 \rangle, \langle J_y^2 \rangle, \langle J_z^2 \rangle) \quad (6)$$

are known. For separable states all the following inequalities are fulfilled:

$$\langle J_x^2 \rangle + \langle J_y^2 \rangle + \langle J_z^2 \rangle \leq \frac{N(N+2)}{4}, \quad (7a)$$

$$(\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 \geq \frac{N}{2}, \quad (7b)$$

$$\langle J_k^2 \rangle + \langle J_l^2 \rangle - \frac{N}{2} \leq (N-1)(\Delta J_m)^2, \quad (7c)$$

$$(N-1)[(\Delta J_k)^2 + (\Delta J_l)^2] \geq \langle J_m^2 \rangle + \frac{N(N-2)}{4}, \quad (7d)$$

where k, l, m take all the possible permutations of x, y, z . While Eq. (7a) is valid for all quantum states, the violation of any of Eqs. (7b)–(7d) implies entanglement.

Proof. The variance defined as $(\Delta A)^2 := \langle A^2 \rangle - \langle A \rangle^2$ is concave in the state that is, if $\rho = p\rho_1 + (1-p)\rho_2$, then $(\Delta A)_\rho^2 \geq p(\Delta A)_{\rho_1}^2 + (1-p)(\Delta A)_{\rho_2}^2$. Thus, it suffices to prove that the inequalities of observation 1 are satisfied by pure product states. Based on the theory of angular momentum, inequality (7a) is valid for all quantum states and the equality holds for states of the symmetric subspace. However, for separable states, it can be proved easily without this knowledge using that for such states [27]

$$\langle \sigma_x^{(i)} \sigma_x^{(j)} \rangle + \langle \sigma_y^{(i)} \sigma_y^{(j)} \rangle + \langle \sigma_z^{(i)} \sigma_z^{(j)} \rangle \leq 1. \quad (8)$$

For Eq. (7b) one first needs that for product states

$$(\Delta J_k)^2 = \frac{N}{4} - \frac{1}{4} \sum_i \langle \sigma_k^{(i)} \rangle^2 \quad (9)$$

holds. Then, for a product state one has

$$(\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 = \frac{3N}{4} - \frac{1}{4} \sum_k x_k^2 + y_k^2 + z_k^2. \quad (10)$$

Here $x_i := \langle \sigma_x^{(i)} \rangle$, $y_i := \langle \sigma_y^{(i)} \rangle$, and $z_i := \langle \sigma_z^{(i)} \rangle$. Knowing that $x_i^2 + y_i^2 + z_i^2 \leq 1$, the right-hand side of Eq. (10) is bounded from below by $\frac{N}{2}$.

Concerning Eq. (7c), we have to show that

$$\mathfrak{Y} := (N-1)(\Delta J_x)^2 + \frac{N}{2} - \langle J_y^2 \rangle - \langle J_z^2 \rangle \geq 0. \quad (11)$$

This can be written as

$$\begin{aligned} \mathfrak{Y} &= (N-1) \left[\frac{N}{4} - \frac{1}{4} \sum_i x_i^2 \right] - \frac{1}{4} \sum_{i \neq j} (y_i y_j + z_i z_j) \\ &= (N-1) \left[\frac{N}{4} - \frac{1}{4} \sum_i x_i^2 \right] - \frac{1}{4} \left[\left(\sum_i y_i \right)^2 + \left(\sum_i z_i \right)^2 \right] \\ &\quad + \frac{1}{4} \sum_i (y_i^2 + z_i^2). \end{aligned} \quad (12)$$

Using

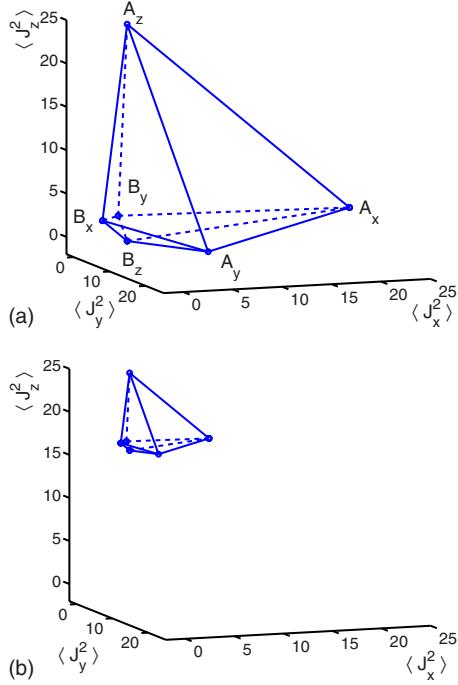


FIG. 1. (Color online) (a) The polytope of separable states corresponding to Eq. (7) for $N=10$ and for $\vec{J}=\vec{0}$. The origin of the coordinate system corresponds to a many-body singlet state. (b) The same polytope for $\vec{J}=(0,0,4)$. Note that this polytope is a subset of the polytope in (a).

$$\left(\sum_i s_i\right)^2 \leq N \sum_i s_i^2, \quad (13)$$

and the normalization of the Bloch vector, it follows that

$$\mathfrak{V} \geq \frac{N-1}{4} \sum_i (1 - x_i^2 - y_i^2 - z_i^2) \geq 0. \quad (14)$$

Equation (7d) can be proved in a similar way. We have to show that

$$\mathfrak{Z} := (N-1)[(\Delta J_k)^2 + (\Delta J_l)^2] - \langle J_m^2 \rangle - \frac{N(N-2)}{4} \geq 0. \quad (15)$$

This can be proved by rewriting \mathfrak{Z} with the individual spin coordinates and using Eq. (13),

$$\begin{aligned} \mathfrak{Z} &= (N-1) \left[\frac{N}{4} - \frac{1}{4} \sum_i x_i^2 + y_i^2 \right] - \frac{1}{4} \sum_{i \neq j} z_i z_j \\ &\geq \frac{N-1}{4} \sum_i (1 - x_i^2 - y_i^2 - z_i^2) \geq 0. \end{aligned} \quad (16)$$

■

For any value of \vec{J} the eight inequalities in Eq. (7) define a polytope in the three-dimensional $(\langle J_x^2 \rangle, \langle J_y^2 \rangle, \langle J_z^2 \rangle)$ space. Observation 1 states that separable states lie inside this polytope. The polytope is depicted in Figs. 1(a) and 1(b) for different values for \vec{J} . It is completely characterized by its extremal points. Direct calculation shows that the coordinates of the extreme points in the $(\langle J_x^2 \rangle, \langle J_y^2 \rangle, \langle J_z^2 \rangle)$ space are

$$A_x := \left[\frac{N^2}{4} - \kappa(\langle J_y \rangle^2 + \langle J_z \rangle^2), \frac{N}{4} + \kappa \langle J_y \rangle^2, \frac{N}{4} + \kappa \langle J_z \rangle^2 \right],$$

$$B_x := \left[\langle J_x \rangle^2 + \frac{\langle J_y \rangle^2 + \langle J_z \rangle^2}{N}, \frac{N}{4} + \kappa \langle J_y \rangle^2, \frac{N}{4} + \kappa \langle J_z \rangle^2 \right],$$

where $\kappa := (N-1)/N$. The points $A_{y/z}$ and $B_{y/z}$ can be obtained in an analogous way. Note that the coordinates of the points A_k and B_k depend nonlinearly on $\langle J_k \rangle$.

One might ask whether all points inside the polytope correspond to separable states. This would imply that the criteria of observation 1 are complete; that is, if the inequalities are satisfied then the first and second moments of J_k do not suffice to prove entanglement. In other words, it is not possible to find criteria detecting more entangled states based on these moments. Due to the convexity of the set of separable states, it is enough to investigate the extremal points.

Observation 2. (i) For any value of \vec{J} , there are separable states corresponding to A_k . (ii) If we define $J := N/2$,

$$c_x := \sqrt{1 - (\langle J_y \rangle^2 + \langle J_z \rangle^2)/J^2} \quad (17)$$

and $p := [1 + \langle J_x \rangle / (J c_x)]/2$ and if then Np is an integer then there is also a separable state corresponding to B_x . Similar statements hold for B_y and B_z . Note that this condition is always fulfilled, if $\vec{J}=\vec{0}$ and N is even.

(iii) There are always separable states corresponding to points B'_k such that their distance from B_k is smaller than $\frac{1}{4}$. In the limit $N \rightarrow \infty$ for a fixed normalized angular momentum $\vec{j} := \vec{J}/(N/2)$, the difference between the volume of polytope of Eq. (7) and the volume of set of points corresponding to separable states decreases with N at least as $\Delta V/V \propto N^{-2}$; hence in the macroscopic limit the characterization is complete.

Proof. A separable state corresponding to A_x is

$$\rho_{A_x} := p(|\psi_+\rangle\langle\psi_+|)^{\otimes N} + (1-p)(|\psi_-\rangle\langle\psi_-|)^{\otimes N}. \quad (18)$$

Here $|\psi_{+-}\rangle$ are the single qubit states with Bloch vector coordinates $(\langle \sigma_x \rangle, \langle \sigma_y \rangle, \langle \sigma_z \rangle) = (\pm c_x, \langle J_y \rangle/J, \langle J_z \rangle/J)$. If $M := Np$ is an integer, we can also define the state corresponding to the point B_x as

$$|\phi_{B_x}\rangle := |\psi_+\rangle^{\otimes M} \otimes |\psi_-\rangle^{\otimes (N-M)}. \quad (19)$$

Since there is a separable state for each extreme point of the polytope, for any internal point a corresponding separable state can be obtained by mixing the states corresponding to the extreme points. It is instructive to demonstrate this through a simple numerical experiment. Figure 2 shows that for $N=10$ and $\vec{J}=\vec{0}$, random separable states indeed fill the polytope.

If M is not an integer, we can approximate B_x by taking $m := M - \varepsilon$ as the largest integer smaller than M , defining

$$\begin{aligned} \rho' &:= (1 - \varepsilon)(|\psi_+\rangle\langle\psi_+|)^{\otimes m} \otimes (|\psi_-\rangle\langle\psi_-|)^{\otimes (N-m)} \\ &\quad + \varepsilon(|\psi_+\rangle\langle\psi_+|)^{\otimes (m+1)} \otimes (|\psi_-\rangle\langle\psi_-|)^{\otimes (N-m-1)}. \end{aligned} \quad (20)$$

This state has the same coordinates as B_x , except for the value of $\langle J_x^2 \rangle$, where the difference is $c_x^2(\varepsilon - \varepsilon^2) \leq 1/4$. The

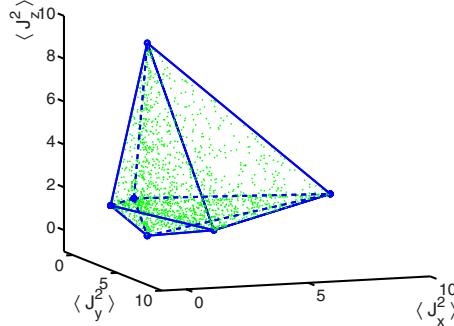


FIG. 2. (Color online) The polytope of separable states corresponding to Eq. (7) for $N=10$ and for $\vec{J}=\vec{0}$. The points corresponding to random separable states fill the polytope.

dependence of $\Delta V/V$ on N can be studied by considering the polytopes in the $(\langle J_x^2 \rangle, \langle J_y^2 \rangle, \langle J_z^2 \rangle)$ space corresponding to $\langle J_k \rangle = j_k \frac{N}{2}$, where j_k are the normalized angular-momentum coordinates. As N increases, the distance of the points A_k to B_k scales as N^2 , hence the volume of the polytope increases as N^6 . The difference between the polytope and the points corresponding to separable states scales like the surface of the polytope, hence as N^4 . ■

Let us analyze now our optimal spin-squeezing inequalities one by one and define the corresponding facets of the polytope on Fig. 1(a). Equation (7a) corresponds to the facet A_x - A_y - A_z . As we discussed, it is valid for all quantum states. The symmetric states correspond to states on this facet and saturate Eq. (7a).

Equation (7b) has already been presented in Ref. [22]. It corresponds to the facet B_x - B_y - B_z . For even N , it is maximally violated by many-body singlets. For such states

$$\begin{aligned}\vec{J} &:= (0,0,0), \\ \vec{K} &:= (0,0,0).\end{aligned}\quad (21)$$

That is, singlet states are states for which both the angular-momentum components and their variances are zero [28]. For large enough N , there are many states of this type. If we mix these states, the mixture still maximally violates this inequality and thus it is detected as entangled. This might be the reason that this criterion can detect states that are very weakly entangled in the sense that they are separable with respect to all bipartitions.

The violation of the criterion gives information about the number of spins that are unentangled with the rest in the following sense [27]. Let us consider a pure state for which the first M qubits are not entangled with other qubits, while the rest of the qubits are entangled with each other

$$|\Psi\rangle = (\otimes_{k=1}^M |\psi_k\rangle) \otimes |\psi\rangle_{M+1, \dots, N}. \quad (22)$$

For such a state, based on the theory of entanglement detection with uncertainties, we have [29]

$$(\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 \geq \frac{M}{2}. \quad (23)$$

Let us consider now a mixed state $\rho := \sum_k p_k |\Psi_k\rangle \langle \Psi_k|$. If it violates Eq. (23) then at least one of the components

$|\Psi_k\rangle \langle \Psi_k|$ must have M or more spins that are entangled with other spins. If the left-hand side of Eq. (23) is smaller than $\frac{1}{2}$ then the state cannot be created by mixing states that have one or more unentangled spins.

Equation (7c) corresponds to the facets A_y - A_z - B_x , A_x - A_z - B_y , and A_x - A_y - B_z . All entangled symmetric Dicke states violate this criterion [30]. This can be seen as follows. An N -qubit symmetric Dicke state with m excitations is defined as [31]

$$|m, N\rangle := \binom{N}{m}^{-1/2} \sum_k P_k (|1_1, 1_2, \dots, 1_m, 0_{m+1}, \dots, 0_N\rangle), \quad (24)$$

where $\{P_k\}$ is the set of all distinct permutations of the spins. $|1, N\rangle$ is the well-known N -qubit W state. For states of the form (24)

$$\vec{J} = (0, 0, m - \frac{N}{2}),$$

$$\vec{K} = \left(\frac{N}{4} + \frac{m(N-m)}{2}, \frac{N}{4} + \frac{m(N-m)}{2}, \left(m - \frac{N}{2}\right)^2 \right). \quad (25)$$

Using Eq. (25) one finds that Eq. (7c) is violated by all Dicke states except for the nonentangled ones with $m=0$ and $m=N$. For even N , it is maximally violated by the symmetric Dicke state $|\frac{N}{2}, N\rangle$.

Finally, Eq. (7d) corresponds to the facets A_y - B_z - B_x , A_x - B_z - B_y , and A_z - B_x - B_y . Note that these inequalities detect the singlet state with Eq. (21) as entangled.

Now we can ask the question, what happens if we only know \vec{K} from Eq. (6) and not \vec{J} from Eq. (5). Can we construct a polytope of the separable states similar to observation 1? Similarly, we can consider the case that we know the variances $[(\Delta J_x)^2, (\Delta J_y)^2, (\Delta J_z)^2]$ but not \vec{J} . The following observation gives the answer.

Observation 3. (i) Let us consider the set of points corresponding to separable states for even N in the $(\langle J_x^2 \rangle, \langle J_y^2 \rangle, \langle J_z^2 \rangle)$ space without constraining the value of \vec{J} . This set is the polytope from observation 1 for $\vec{J}=\vec{0}$, also shown in Fig. 1(a). (ii) Also, the set of points corresponding to separable states in the $[(\Delta J_x)^2, (\Delta J_y)^2, (\Delta J_z)^2]$ space is the same polytope. That is, Fig. 1(a) gives also the right polytope if the labels of the axes are changed from $\langle J_l^2 \rangle$ to $(\Delta J_l)^2$.

Proof. For the first part, it can be directly seen that Eq. (7) is least restrictive for $\vec{J}=\vec{0}$, for other \vec{J} the polytope is strictly smaller. For the second part, note that based on Eq. (7) the points corresponding to separable states must be within the same polytope shown in Fig. 1(a), even if we change the labels from $\langle J_l^2 \rangle$ to $(\Delta J_l)^2$. It is not clear, however, that the set of separable states is convex in the $[(\Delta J_x)^2, (\Delta J_y)^2, (\Delta J_z)^2]$ space. Thus, we have to show that for each separable state ρ with $\langle J_l^2 \rangle = S_l$ for $l=x, y, z$, there is a separable state $\tilde{\rho}$ for which $(\Delta J_l)^2 = S_l$. Let us use the decomposition $\rho = \sum p_k \rho_k$ where $\rho_k = \rho_k^{(1)} \otimes \rho_k^{(2)} \otimes \dots \otimes \rho_k^{(N)}$ are product states. Then, such a $\tilde{\rho} := \sum p_k \tilde{\rho}_k$ can be obtained by mixing

$$\tilde{\rho}_k := \frac{1}{4}(\rho_k + J_x \rho_k J_x + J_y \rho_k J_y + J_z \rho_k J_z). \quad (26)$$

The state $\tilde{\rho}$ has the same $\langle J_l^2 \rangle$ as ρ . However, the value of $\langle J_l \rangle^2$ is zero, hence $(\Delta J_l)_{\tilde{\rho}}^2 = \langle J_l^2 \rangle_{\rho}$. ■

III. OPTIMAL SPIN-SQUEEZING INEQUALITIES FOR THE CORRELATION MATRIX

We discuss some further features of our spin-squeezing inequalities. One can ask what happens if not only $\langle J_k \rangle$ and $\langle J_k^2 \rangle$ for $k=x,y,z$ are known but $\langle J_i \rangle$ and $\langle J_i^2 \rangle$ in arbitrary directions i . We will now first show how to find the optimal directions x', y', z' to evaluate observation 1.

Knowledge of $\langle J_i \rangle$ and $\langle J_i^2 \rangle$ in arbitrary directions is equivalent to the knowledge of the vector \vec{J} , the correlation matrix C , and the covariance matrix γ defined as [32–34]

$$\begin{aligned} C_{kl} &:= \frac{1}{2}\langle J_k J_l + J_l J_k \rangle, \\ \gamma_{kl} &:= C_{kl} - \langle J_k \rangle \langle J_l \rangle, \end{aligned} \quad (27)$$

for $k, l=x,y,z$. When changing the coordinate system to x', y', z' vector \vec{J} and the matrices C and γ transform as $\vec{J} \mapsto O\vec{J}$, $C \mapsto OCO^T$, and $\gamma \mapsto O\gamma O^T$ where O is an orthogonal 3×3 matrix. Looking at the inequalities of observation 1, one finds that the first two inequalities are invariant under a change in the coordinate system. Concerning Eq. (7c), we can reformulate it as

$$\langle J_i^2 \rangle + \langle J_j^2 \rangle + \langle J_k^2 \rangle - \frac{N}{2} \leq (N-1)(\Delta J_k)^2 + \langle J_k^2 \rangle. \quad (28)$$

Then, the left-hand side is again invariant under rotations, and we find a violation of Eq. (7c) in some direction if the minimal eigenvalue of

$$\mathfrak{X} := (N-1)\gamma + C \quad (29)$$

is smaller than $\text{Tr}(C) - \frac{N}{2}$. Similarly, we find a violation of Eq. (7d) if the largest eigenvalue of \mathfrak{X} exceeds $(N-1)\text{Tr}(\gamma) - N(N-2)/4$. Thus, the orthogonal transformation that diagonalizes \mathfrak{X} delivers the optimal measurement directions x', y', z' [35].

Observation 4. We can rewrite our condition (7) in a form that is independent from the choice of the coordinate system as

$$\text{Tr}(C) \leq \frac{N(N+2)}{4}, \quad (30a)$$

$$\text{Tr}(\gamma) \geq \frac{N}{2}, \quad (30b)$$

$$\lambda_{\min}(\mathfrak{X}) \geq \text{Tr}(C) - \frac{N}{2}, \quad (30c)$$

$$\lambda_{\max}(\mathfrak{X}) \leq (N-1)\text{Tr}(\gamma) - \frac{N(N-2)}{4}, \quad (30d)$$

where $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$ are the smallest and largest eigenvalues of matrix A , respectively. If Eq. (7) is violated by a quantum state for any choice of coordinate axes x, y and z then Eq. (30) are also violated.

The preceding observation shows how the optimal directions x, y, z can be chosen by diagonalizing the matrix \mathfrak{X} .

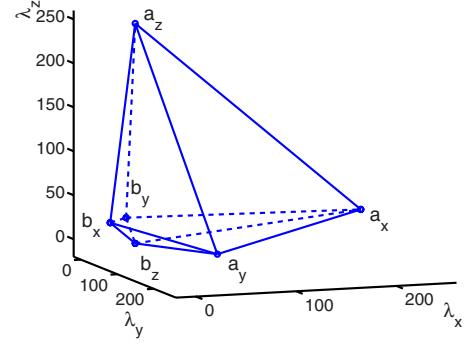


FIG. 3. (Color online) The polytope of separable states corresponding to Eq. (32) for the eigenvalues of \mathfrak{X} for $N=10$ and for $\vec{J}=\vec{0}$. Compare with Fig. 1(a).

However, if one diagonalizes \mathfrak{X} and does not find a violation of Eq. (30), this does not *a priori* imply that C , γ and \vec{J} are compatible with a separable state. The knowledge that for the diagonal \mathfrak{X} the off-diagonal entries vanish gives some additional information about the state, which may in principle be used as a signature for entanglement. We will prove now, however, that this is not the case and that diagonalizing \mathfrak{X} and applying Eq. (30) are the best that one can do if C , γ and \vec{J} are known.

Note first that Eq. (30) contains the following variables: the three eigenvalues of \mathfrak{X} , $\text{Tr}(C)$, and $\text{Tr}(\gamma)$. The latter two can be expressed with the trace of \mathfrak{X} and \vec{J} as

$$\begin{aligned} \text{Tr}(C) &= \frac{1}{N}\text{Tr}(\mathfrak{X}) + \frac{N-1}{N}|\vec{J}|^2, \\ \text{Tr}(\gamma) &= \frac{1}{N}\text{Tr}(\mathfrak{X}) - \frac{1}{N}|\vec{J}|^2. \end{aligned} \quad (31)$$

In this way, Eq. (30) can be rewritten with the eigenvalues of \mathfrak{X} and $|\vec{J}|^2$ as

$$\text{Tr}(\mathfrak{X}) \leq \frac{N^2(N+2)}{4} - (N-1)|\vec{J}|^2, \quad (32a)$$

$$\text{Tr}(\mathfrak{X}) \geq \frac{N^2}{2} + |\vec{J}|^2, \quad (32b)$$

$$\lambda_{\min}(\mathfrak{X}) \geq \frac{1}{N}\text{Tr}(\mathfrak{X}) + \frac{N-1}{N}|\vec{J}|^2 - \frac{N}{2}, \quad (32c)$$

$$\lambda_{\max}(\mathfrak{X}) \leq \frac{N-1}{N}\text{Tr}(\mathfrak{X}) - \frac{N-1}{N}|\vec{J}|^2 - \frac{N(N-2)}{4}. \quad (32d)$$

For fixed $|\vec{J}|$, these equations describe a polytope in the space of the three eigenvalues of \mathfrak{X} . The polytope is shown in Fig. 3. The coordinates of the extreme points in the $(\lambda_1, \lambda_2, \lambda_3)$ space of the eigenvalues of \mathfrak{X} are

$$a_x := \left(\frac{N^3}{4} - (N-1) \sum_k \langle J_k \rangle^2, \frac{N^2}{4}, \frac{N^2}{4} \right) \quad (33)$$

and

$$b_x := \left(\sum_k \langle J_k \rangle^2, \frac{N^2}{4}, \frac{N^2}{4} \right). \quad (34)$$

The other a_k and b_k points can be obtained by trivial relabeling the coordinates.

Let us now show that in the large N limit for any \mathfrak{X} and \vec{J} fulfilling Eq. (32), there is a corresponding quantum state. This would mean that the conditions with \mathfrak{X} and \vec{J} are complete and there is not another condition that could detect more entangled states based on knowing \mathfrak{X} and \vec{J} .

First, let us consider the case when \vec{J} and N fulfill the conditions for completeness from observation 2(ii), and there are quantum states corresponding to a_k and b_k . The states corresponding to a_x and b_x are ρ_{A_x} and $\rho_{B_x} := |\phi_{B_x}\rangle\langle\phi_{B_x}|$, respectively, defined in Eqs. (18) and (19). They are the same states that correspond to the points A_x and B_x in Fig. 1. The states corresponding to the other extreme points can be obtained straightforwardly from these formulas by relabeling the coordinates. Note that all these states have a diagonal \mathfrak{X} matrix. Now, let us take a \mathfrak{X} that fulfills Eq. (32) and diagonalize it and denote it \mathfrak{X}_D after the diagonalization. Then, it is clear that \mathfrak{X}_D can be obtained by “mixing” the \mathfrak{X} matrices corresponding to a_k and b_k as

$$\mathfrak{X}_D = \sum_{l=a_x, a_y, a_z, b_x, b_y, b_z} p_l \mathfrak{X}_l, \quad (35)$$

where $p_l > 0$ and $\sum_l p_l = 1$. Note that “mixing” \mathfrak{X} matrices is in general not equivalent to mixing the states, since \mathfrak{X} is a nonlinear function of the state. However, for all the states corresponding to a_k and b_k , the vector \vec{J} is the same and that all have diagonal \mathfrak{X} matrices. Therefore, the corresponding state is

$$\rho_D = \sum_{l=A_x, A_y, A_z, B_x, B_y, B_z} p_l \rho_l. \quad (36)$$

Then, if ρ_D is the quantum state corresponding to \vec{J} and \mathfrak{X}_D then the quantum state corresponding to \vec{J} and \mathfrak{X} can be obtained from ρ_D with coordinate rotations. Finally, if \vec{J} and N are such that no quantum state exists that corresponds to some of the points then an argument similar to the one in observation 2 can be applied showing that at least there is a quantum state corresponding to a point close to all b'_k s and because of that in the macroscopic limit, the characterization is complete even in this case. Thus, we can state the following.

Observation 5. The criteria from Eq. (30) are complete in the sense that under the conditions of observation 2 (ii) or for large N , they detect all entangled states that can be detected knowing \vec{J} and the correlation matrix C .

IV. COMPARISON WITH OTHER SPIN-SQUEEZING CRITERIA

In this section, we compare the optimal spin-squeezing inequality (7) to other spin-squeezing criteria. First, let us consider the original spin-squeezing criterion (3). This in-

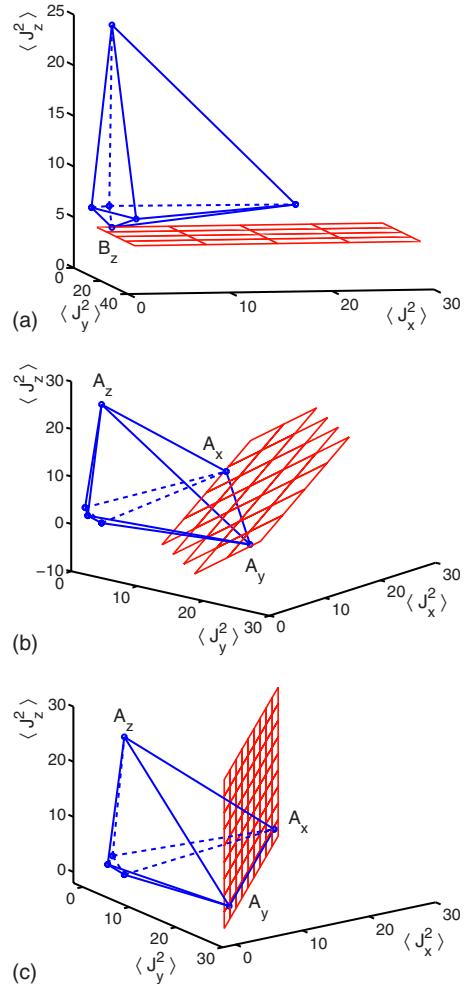


FIG. 4. (Color online) (a) Comparison of the optimal spin-squeezing inequalities and original spin squeezing for $(k, l, m) = (x, y, z)$, $N=10$, and $\vec{J}=(1, 0, 2)$. States detected by the latter are below the horizontal plane. (b) Optimal spin-squeezing inequalities and the inequality (40) for $N=10$ and $\vec{J}=(0, 0, 0)$. (c) Optimal spin squeezing and criterion (45) for $\vec{J}=(0, 0, 0)$.

equality is satisfied by all points A_k and B_k , for B_z even equality holds. It is instructive to compare the region detected by Eq. (3) to the region detected by the optimal spin-squeezing inequalities in the $(\langle J_x^2 \rangle, \langle J_y^2 \rangle, \langle J_z^2 \rangle)$ space. For a fixed \vec{J} , Eq. (3) corresponds to a horizontal plane in this space shown in Fig. 4(a). Equation (3) can be expressed in a way that is independent from the choice of the coordinate system

$$\lambda_{\min}(\mathfrak{X}) \geq |\vec{J}|^2. \quad (37)$$

Equation (37) is violated if Eq. (3) is violated for an optimal choice of coordinate axes x , y , and z .

For a state of many particles that has almost a maximal spin in some direction, the standard spin-squeezing inequality (3) is equivalent to our optimal spin-squeezing inequality (7c). To see that, let us now rewrite Eq. (7c) as

$$\frac{(\Delta J_z)^2}{\langle J_x^2 \rangle + \langle J_y^2 \rangle} \geq \frac{1}{N-1} - \frac{N}{2(N-1)(\langle J_x^2 \rangle + \langle J_y^2 \rangle)}. \quad (38)$$

This can be transformed into

$$\begin{aligned} \frac{(\Delta J_z)^2}{\langle J_x^2 \rangle + \langle J_y^2 \rangle} &\geq \left[\frac{1}{N-1} - \frac{N}{2(N-1)(\langle J_x^2 \rangle + \langle J_y^2 \rangle)} \right] \\ &\times \frac{\langle J_x^2 \rangle + \langle J_y^2 \rangle}{\langle J_x^2 \rangle + \langle J_y^2 \rangle}. \end{aligned} \quad (39)$$

Let us assume that N is large and the state has a large spin pointing to the x direction, that is, $\langle J_x^2 \rangle \approx \frac{N^2}{4}$ and $\langle J_y^2 \rangle \approx \frac{N}{4}$. In this case $\langle J_k^2 \rangle \approx \langle J_k \rangle^2$ and the right-hand side of Eq. (39) is very close to $\frac{1}{N}$. At this point, one can recognize Eq. (3).

Reference [22] presented a generalized-spin-squeezing inequality for the entanglement detection that is identical to Eq. (7b) of the optimal spin-squeezing inequalities. This inequality has been connected to susceptibility measurements in solid-state systems [26,36].

References [21,24] presented another generalized-spin-squeezing inequality, for detecting two-qubit entanglement. According to this criterion, for states with a separable two-qubit density matrix

$$\left(\langle J_k^2 \rangle + \langle J_l^2 \rangle - \frac{N}{2} \right)^2 + (N-1)^2 \langle J_m \rangle^2 \leq \left[\langle J_m^2 \rangle + \frac{N(N-2)}{4} \right]^2 \quad (40)$$

holds. This inequality is satisfied by all points A_k and B_k , while, when we choose $(k, l, m) = (x, y, z)$, for A_x and A_y even equality holds. Figure 4(b) shows the polytope of the optimal spin-squeezing inequality together with the plane corresponding to criterion (40). Any state below the plane is detected as two-qubit entangled by Eq. (40). Note that Eq. (7c) of the optimal spin-squeezing inequalities detects all states detected by Eq. (40). Note, however, that Eq. (40) detects only states with two-qubit entanglement while Eq. (7c) detects entangled states that can have separable two-qubit density matrices. Equation (40) can be expressed in a coordinate system independent way as

$$\begin{aligned} \lambda_{\max} \left\{ \left[\frac{1}{2} N^2 + 1 - 2 \text{Tr}(C) \right] C - (N-1)^2 \gamma \right\} \\ \leq \left[\frac{N(N-2)}{4} \right]^2 - \left[\text{Tr}(C) - \frac{N}{2} \right]^2. \end{aligned} \quad (41)$$

For states of the symmetric subspace, Eq. (40) can be simplified to [21,24]

$$\frac{4(\Delta J_n)^2}{N} \geq 1 - \frac{4\langle J_n \rangle^2}{N^2}. \quad (42)$$

Violation of Eq. (42) for some coordinate axis z is a necessary and sufficient condition for the two-qubit entanglement for symmetric states [37]. It can also be expressed in a form that is independent of the choice of coordinate axes [33]

$$\lambda_{\min} \left(\gamma + \frac{1}{N} \vec{J} \vec{J}^T \right) \geq \frac{N}{4}. \quad (43)$$

This can be rewritten with \mathfrak{X} as

$$\lambda_{\min}(\mathfrak{X}) \geq \frac{N^2}{4}. \quad (44)$$

Finally, Refs. [23,25] present a generalized-spin-squeezing inequality detecting entanglement close to symmetric Dicke states with $\langle J_z \rangle = 0$. For separable states, we have

$$\langle J_x^2 \rangle + \langle J_y^2 \rangle \leq \frac{N(N+1)}{4}. \quad (45)$$

The inequality is satisfied by all points A_k and B_k , for A_x and A_y even equality holds. Figure 4(c) shows the polytope of the optimal spin-squeezing inequality together with the plane corresponding to criterion (45). Any state corresponding to points on the right-hand side of the vertical plane is detected by Eq. (45) as entangled. Equation (45) can be rewritten in a coordinate system independent way as

$$\lambda_{\min}(C) \geq \text{Tr}(C) - \frac{N(N+1)}{4}. \quad (46)$$

V. TWO-QUBIT ENTANGLEMENT VS MULTIPARTITE ENTANGLEMENT

Next, it is interesting to ask what kind of entanglement is detected by our criteria knowing that they contain only two-body correlation terms of the form $\langle \sigma_k^{(i)} \sigma_k^{(j)} \rangle$ and do not depend on higher-order correlations. In fact, all quantities in our inequalities can be evaluated based on the knowledge of the average two-qubit density matrix

$$\rho_{av2} := \frac{1}{N(N-1)} \sum_{i \neq j} \rho_{ij}, \quad (47)$$

where ρ_{ij} is the reduced density matrix of qubits i and j . Do our criteria simply detect entanglement of the two-qubit reduced state of the density matrix? It will turn out that our criteria can detect entangled states with separable two-qubit density matrices.

Our entanglement detection scheme is related to the N -representability problem [38], i.e., to the problem of finding multipartite quantum states that have a given set of states as reduced states [39]. When detecting entanglement based on ρ_{av2} , we ask: is there a separable N -qubit state that has ρ_{av2} as the average two-qubit reduced state. If the answer is no then we know that the system is in an entangled state. Clearly, if ρ_{av2} is entangled then there is not an N -qubit separable quantum state that has it as a reduced state.

Interestingly, it turns out that it is also possible that ρ_{av2} is separable; however, there is not an N -qubit separable state that has ρ_{av2} as reduced state. In this case, we can conclude that the system is an entangled state even if ρ_{av2} is separable. A similar phenomenon can be observed in the theory of cluster states [40]. These are states that are defined as eigenstates of quasilocal operators. The total state is uniquely determined by these quasilocal properties of the reduced states, and it can happen that the reduced states are separable, while the total state is highly entangled [41].

Let us elaborate this point a little bit more. If ρ_{av2} is separable and it is in the symmetric subspace then it can always be written in the form [21]

$$\rho_{av2} = \sum_k p_k \rho_k \otimes \rho_k \quad (48)$$

with pure ρ_k matrices. In this case, there always can be found an N -qubit separable state that has this state as its reduced state

$$\rho_N = \sum_k p_k \rho_l^{\otimes N}. \quad (49)$$

Hence, we can make the following statement.

Observation 6. If any generalized-spin-squeezing criterion (i.e., an entanglement criterion containing only $\langle J_k \rangle$ and $\langle J_k^2 \rangle$) is violated by a symmetric state then the state is entangled and the reduced two-qubit density matrix of the state is also entangled. Note that this has already been known for the case of the original spin-squeezing criterion (3) [42].

On the other hand, if ρ_{av2} is not symmetric then it is possible that ρ_{av2} is separable but there is not an N -qubit symmetric separable state that has it as its reduced two-qubit state. This is the reason that entanglement conditions based on \vec{J} and \vec{K} can detect entangled states with a separable two-qubit density matrix. Next, we will examine all our entanglement criteria from this point of view.

First, we will rewrite Eq. (7) as an equation for the average two-qubit density matrix ρ_{av2} . All expectation values in these equations are computed for ρ_{av2} ,

$$\Sigma \leq 1, \quad (50a)$$

$$\Sigma \geq -\frac{1}{N-1} + \frac{N}{N-1} \sum_{i=x,y,z} \langle \sigma_i \otimes \mathbb{I} \rangle^2, \quad (50b)$$

$$\Sigma \leq 1 + N(\langle \sigma_m \otimes \sigma_m \rangle - \langle \sigma_m \otimes \mathbb{I} \rangle^2), \quad (50c)$$

$$\Sigma \geq -\frac{1}{N-1} + \frac{N}{N-1}(\langle \sigma_k \otimes \mathbb{I} \rangle^2 + \langle \sigma_l \otimes \mathbb{I} \rangle^2) + \frac{N}{N-1}\langle \sigma_m \otimes \sigma_m \rangle, \quad (50d)$$

where

$$\Sigma := \langle \sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y + \sigma_z \otimes \sigma_z \rangle. \quad (51)$$

The first of the four optimal spin-squeezing inequalities [Eq. (7a)] corresponds to Eq. (50a). Again, this inequality is valid for any quantum state and cannot be violated.

The second inequality (7b) corresponds to Eq. (50b). It is known that Eq. (7b) can detect states that have separable two-qubit density matrices as have been shown in Ref. [27]. Such a state is, for example, one of the many-body singlet states,

$$\rho_s \propto \lim_{T \rightarrow 0} \exp\left(-\frac{J_x^2 + J_y^2 + J_z^2}{T}\right). \quad (52)$$

For this state $\langle J_m^n \rangle = 0$ for any $m, n \geq 0$. For such a state for increasing N , the average two-qubit density matrix ρ_{av2} becomes arbitrarily close to the totally mixed state. Thus, Eq. (50b) is not a condition for detecting the entanglement of ρ_{av2} . Moreover, note that Eq. (7b) can even detect states that are separable with respect to all bipartitions [26].

The third inequality (7c) corresponds to Eq. (50c). Let us consider the state

$$\rho \propto \exp\left(-\frac{7J_z^2 - J_x^2 - J_y^2}{T}\right) \quad (53)$$

for $N=8$ and $T=3$. Direct calculation shows that this state is detected by Eq. (7c) for $(k, l, m) = (x, y, z)$. Thus, again, this is not a condition for the separability of the two-qubit density matrix.

The fourth condition is Eq. (7d) which corresponds to Eq. (50d). It detects the singlet state ρ_s . This state has a separable two-qubit density matrix, thus Eq. (7d) is not a condition on the separability of the reduced density matrix.

Let us consider now the original spin-squeezing inequality (3). It is known that the violation of this inequality implies two-qubit entanglement for symmetric states [42]. However, if the quantum state is not symmetric, Eq. (3) can detect states with separable two-qubit density matrices. For example, the following state violates Eq. (3), while it does not have two-qubit entanglement:

$$\rho_{sq} \propto \exp\left(-\frac{2J_x^2 - J_z}{T}\right) \quad (54)$$

for $N=8$ and $T=0.3$.

Finally, let us consider the generalized-spin-squeezing inequality (45). It can be proved that any state violating it has two-qubit entanglement. This is because it can be rewritten with expectation values computed for ρ_{av2} as

$$\langle \sigma_x \otimes \sigma_x \rangle + \langle \sigma_y \otimes \sigma_y \rangle \leq 1. \quad (55)$$

Any two-qubit state violating this criterion is entangled [27].

VI. SPIN SYSTEMS GIVING VIOLATIONS FOR THE OPTIMAL SPIN-SQUEEZING INEQUALITIES

In the recent years, considerable effort has been made to create large scale entanglement in various physical systems: in Bose-Einstein condensates of two-state bosonic atoms [8], in optical lattices of cold two-state atoms realizing the dynamics of an Ising spin chain [11,43,44], and in atomic clouds through interaction with light and appropriately chosen measurements [5,14,15]. In the future, it is expected that experimenters will also engineer the various ground states of well-known spin chains. Entanglement detection in such systems were considered, for example, in Refs. [22,45–47]. Note that there are methods available for measuring the variances of the collective spin components of atomic systems through the interaction with light [48,49].

In the light of the experiments, we ask the question: under what circumstances are our optimal spin-squeezing inequalities useful for detecting entanglement in the sense that they outperform other spin-squeezing entanglement criteria? In this section, we will show that our entanglement criteria are especially useful in situations in which the state has a small or zero mean spin \vec{J} and its reduced average two-qubit density matrix ρ_{av2} is separable.

A. Ground state of spin systems

These will be, on one hand, one-dimensional spin chains. On the other hand, we will consider spin systems corresponding to the completely connected graph. We will consider the following Hamiltonians. First let us consider the Heisenberg chain with the Hamiltonian

$$H_H := \sum_k \sigma_x^{(k)} \sigma_x^{(k+1)} + \sigma_y^{(k)} \sigma_y^{(k+1)} + \sigma_z^{(k)} \sigma_z^{(k+1)}. \quad (56)$$

Its ground state is a many-body singlet state. Thus, the optimal spin-squeezing inequality (7b) is ideal for its detection. Concerning how other criteria can detect its ground state as entangled, we can state the following.

Observation 7. The $T=0$ ground state of a spin system with a Hamiltonian without an external field cannot be detected by the original spin-squeezing criterion (3). The ground state of a spin chain Hamiltonian without an external field cannot be detected by the Korbicz-Cirac-Lewenstein criterion (40).

Proof. The first statement is true since criterion (3) cannot be used for states with $\vec{J}=\vec{0}$ since in Eq. (3) one has to divide with the length of the collective spin components. The other claim can be proved noting that for large N the two-qubit density matrix ρ_{av2} of the ground state of spin chains without an external field is unentangled. This can be seen realizing that for the ground state of an N -qubit translationally invariant chain

$$\rho_{av2} = \frac{1}{N-1} (\rho_{12} + \rho_{13} + \rho_{14} + \dots + \rho_{1N}), \quad (57)$$

where ρ_{kl} is the reduced two-qubit matrix of spins k and l . However, for a spin chain, distant sites are less and less correlated thus for large enough k we have $\rho_{1k} \approx \frac{1}{4} \mathbb{I}$. Hence, for large enough N , the reduced two-qubit density matrix ρ_{av2} is very close to the totally mixed state and it is separable [50]; thus, the state is not detected by the Korbicz-Cirac-Lewenstein criterion (40). ■

The Hamiltonian of the isotropic XY chain is

$$H_{XY} := \sum_k \sigma_x^{(k)} \sigma_x^{(k+1)} + \sigma_y^{(k)} \sigma_y^{(k+1)}. \quad (58)$$

This system is similar to Eq. (56) from the point of view of detecting its ground state by various entanglement criteria. That is, ρ_{av2} is unentangled for this system and the spin-squeezing criterion (3) cannot detect its ground state. Moreover, its ground state is detected by the optimal spin-squeezing inequalities. While the XY chain is exactly solvable [51], the latter statement can be understood based on simpler arguments using only qualitative properties of the ground state. Let us consider a chain with a periodic boundary condition. For the nondegenerate ground state of the XY chain for even N , one has $\langle J_z^2 \rangle = 0$ since J_z commutes with H_{XY} . The nearest-neighbor correlation is the strongest; that is for the ground state

$$\langle \sigma_l^{(m)} \sigma_l^{(n)} \rangle = (-1)^{m-n} c_{l,D(m,n)} \quad (59)$$

for $l=x,y$ where $D(m,n)$ is the distance of qubit m and n , and $c_{l,m} > 0$ is a monotonous decreasing function of m . Hence, due to translational invariance, it follows that

$$\langle J_l^2 \rangle = \frac{N}{4} + \frac{1}{4} \sum_{m \neq n} \langle \sigma_l^{(m)} \sigma_l^{(n)} \rangle < \frac{N}{4} - \frac{N}{2} \Delta_N \quad (60)$$

for $l=x,y$, where $\Delta_N := |\langle \sigma_l^{(1)} \sigma_l^{(2)} \rangle| - |\langle \sigma_l^{(1)} \sigma_l^{(3)} \rangle|$. Note that Δ_N converges to a nonzero value for $N \rightarrow \infty$. Using these arguments, one can see that for any even N the ground state of the XY chain violates Eq. (7b) and this violation is of order N in the large N limit; that is, the relative violation does not approach zero with increasing N . Hence it also follows that chains with odd N must also violate Eq. (7b) in this limit.

The Hamiltonian

$$H_S := J_x^2 + J_y^2 + J_z^2 = \frac{N}{4} + \frac{1}{2} \sum_{l=x,y,z} \sum_{m>n} \sigma_l^{(m)} \sigma_l^{(n)} \quad (61)$$

corresponds to a system that has a Heisenberg interaction between all spin pairs and has a very degenerate ground state. The two-qubit density matrix of its $T=0$ thermal ground state converges to the completely mixed state as N increases, thus for large enough N it is separable [27]. With respect to other qualitative statements about entanglement detection, it is similar to the Heisenberg chain.

The Hamiltonian of the Lipkin-Meshkov-Glick model is [52]

$$H_{LMG} := -\frac{\lambda}{N} (J_x^2 + \gamma J_y^2) - h J_z. \quad (62)$$

For $\lambda \geq 0$, $\gamma = 1$, and $h = 0$, the ground state is an N -qubit symmetric Dicke states with $\frac{N}{2}$ excitations. For $h \neq 0$ all the symmetric Dicke states given in Eq. (24) can be obtained as ground states of the system. These, except for the trivial $|0,N\rangle = |0000\dots\rangle$ and $|N,N\rangle = |1111\dots\rangle$ states, all have entangled reduced two-qubit density matrix. Using Eq. (25), one can show that they are detected both by our optimal spin-squeezing inequalities and the Korbicz-Cirac-Lewenstein criterion (40). However, they are not detected by the original spin-squeezing inequality as can be seen by substituting Eq. (25) into the original spin-squeezing inequality. For $\lambda \leq 0$, $\gamma = 1$, and $h = 0$, the ground state is the same as for the Hamiltonian (61).

Finally, the summary of the results in this section is shown in Table I.

B. Bound entanglement in spin chains

Next, we study spin models in thermal equilibrium. We give the threshold temperatures for various spin models for the Peres-Horodecki (PPT) criterion [53] and for our optimal spin-squeezing inequality (7). These temperatures are defined as the values, below which the spin-squeezing inequalities are violated of the state becomes NPT with respect to at least one partition. The results are given in Table II. The systems considered are the Heisenberg chain and the XY chain defined in Eqs. (56) and (58), the Heisenberg system on a fully connected graph with the Hamiltonian (61), the XY system on a fully connected graph with the Hamiltonian H_{LMG} defined in Eq. (62) for $h=0$, $\gamma=1$ and $\lambda=-1$, and the antiferromagnetic Ising spin chain in a transverse field defined as

TABLE I. Table showing for several spin Hamiltonians which entanglement condition can detect their $T=0$ thermal ground state in the large particle number limit. For the Hamiltonians, see text. For the Lipkin-Meshkov-Glick model $\gamma=1$ is assumed.

Hamiltonian	Spin squeezing Eq. (3)	Korbicz-Cirac-Lewenstein Eq. (40)	Optimal spin squeezing Eq. (7)
Heisenberg chain	–	–	+
XY chain	–	–	+
Heisenberg model fully connected	–	–	+
H_{LMG} $\lambda > 0$	–	+	+
H_{LMG} $\lambda < 0$, $h=0$	–	–	+

$$H_I := \sum_k \sigma_z^{(k)} \sigma_z^{(k+1)} + B \sum_k \sigma_x^{(k)}. \quad (63)$$

The thermal state of the system is computed as $\rho_{\text{th}} \propto \exp(-\frac{H}{kT})$ with $k=1$. In many cases, the temperature bound for the PPT criterion is lower than for our spin-squeezing criterion. This means that there is a temperature range in which the quantum state has a positive partial transpose with respect to all bipartitions while it is still detected as entangled. Such quantum states are bound entangled and since all bipartitions are PPT, no entanglement can be distilled from them with local operations and classical communications even if arbitrary number of parties is allowed to join [54]. In particular, the results show that Eq. (7) can detect fully PPT bound entanglement in Heisenberg and XY chains, moreover, in Heisenberg and XY systems on a completely connected graph. Note that the bound temperature for the optimal spin-squeezing inequalities for the Heisenberg model on a fully connected graph is $T_c \approx N$ for large N [27]. On the other hand, our criteria do not seem to detect fully PPT bound entanglement in Ising spin chains. Finally, Fig. 5 shows the results for the Heisenberg and XY and chains,

together with the bounds for the computable cross norm or realignment (CCNR) criterion [55]. The latter is often a good indicator of bound entanglement; however, in these systems it does not detect bound entanglement.

C. Bound entanglement in a nanotubular system

Let us finally investigate a finite system showing bound entanglement at high temperatures. The nanotubular system $\text{Na}_2\text{V}_3\text{O}_7$ is a prominent example of a low-dimensional quantum magnet. The compound was synthesized in 1999 by Millet *et al.* [56], who also provided a detailed description of its structure. Every nine V^{4+}O_5 pyramids form a ring, by sharing edges and corners; furthermore those rings accumulate to nanotubes with Na atoms located in the center of and between them. Due to the complex structure of this system some years passed, until an effective model for the exchange interactions could be found [57]. The coupling terms between the rings are considerably smaller than the inter-ring coupling and therefore can be neglected in a first approximation. Effectively the system can be described as a nine site antiferromagnetic spin- $\frac{1}{2}$ Heisenberg ring showing nearest-

TABLE II. Critical temperatures for the PPT criterion and Eq. (7) for Heisenberg, XY , and Ising spin chains of various size and for the Heisenberg any XY systems on a fully connected graph. For the definitions of the Hamiltonians, see text.

N		3	4	5	6	7	8	9
Heisenberg	Eq. (7b)	5.46	5.77	5.72	5.73	5.73	5.73	5.73
Chain	PPT	4.33	5.47	4.96	5.40	5.17	5.38	5.25
XY	Eq. (7b)	3.09	3.48	3.39	3.41	3.41	3.41	3.41
Chain	PPT	2.56	3.46	3.07	3.34	3.19	3.32	3.24
Heisenberg	Eq. (7b)	2.73	3.73	4.73	5.72	6.72	7.72	8.72
model f.c.	PPT	2.16	2.73	3.17	3.71	4.17	4.70	5.17
XY	Eq. (7b)	1.54	2.08	2.59	3.10	3.60	4.11	4.61
model f.c.	PPT	1.28	1.82	2.23	2.74	3.20	3.71	4.19
Ising chain	Eq. (7c)	0.67	0.89	0.55	0.78	0.50	0.71	0.46
$B=0.5$	PPT	1.08	1.26	1.17	1.26	1.21	1.26	1.22
Ising chain	Eq. (7c)	1.22	1.29	1.14	1.17	1.10	1.11	1.08
$B=1$	PPT	1.49	1.71	1.61	1.71	1.65	1.71	1.67
Ising chain	Eq. (7c)	2.01	1.97	1.90	1.87	1.85	1.83	1.82
$B=2$	PPT	2.15	2.43	2.30	2.43	2.36	2.43	2.38

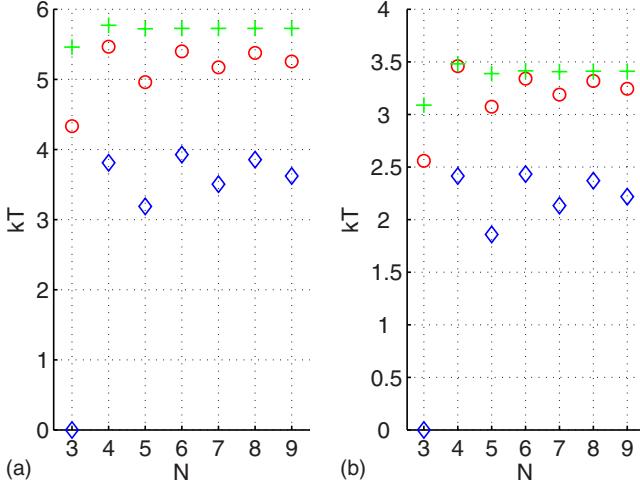


FIG. 5. (Color online) Comparison of the critical temperatures of separability criteria for different site numbers in the Heisenberg-(left) and the XY model (right). T_c of the spin-squeezing inequality (7b) (+) is higher than the critical temperatures of the PPT (○) criterion [53] or the CCNR (◊) criterion [55].

neighbor and next-to-nearest-neighbor interactions. The Hamiltonian can be written as

$$H := \sum_{k=1}^9 \frac{C_1}{4} \vec{\sigma}^{(k)} \cdot \vec{\sigma}^{(k+1)} + \frac{C_2^k}{4} \vec{\sigma}^{(k)} \cdot \vec{\sigma}^{(k+2)}, \quad (64)$$

with periodic boundary conditions and approximately homogeneous parameters for the nearest-neighbor interactions $C_1 = 200$ K and $C_2^k = 140$ K for $k=2, 3, 5, 6, 8, 9$, while $C_2^k = 0$ in all other cases (see Fig. 6). The magnetic susceptibility of this simplified model coincides well with the experimental results above a temperature of about 10 K [57].

For the given Hamiltonian, the thermal state is entangled for low temperatures and will become separable at a certain point when increasing the temperature. For every separability criterion, a critical temperature T_c can be found. Doing so for the spin-squeezing inequalities shows that the critical temperature of the inequality (7d) is $T_c^{(7d)} = 182.8$ K while the inequality (7b) gives $T_c^{(7b)} = 363.6$ K, the other ones do not detect any entanglement at all. The critical temperature of Eq. (7b) has already been known from Ref. [58], where the magnetic susceptibility of the system has been used as an entanglement witness, which effectively results in the same criterion [26,36]. Furthermore, we have computed the critical temperature of the PPT criterion according to all bipartite splittings, resulting in a maximal temperature of $T_c^{\text{PPT}} = 303.9$ K for the splitting $A = \{1, 3, 4, 6, 7, 9\}$ vs $B = \{2, 5, 8\}$. So we find a transition from free to bound entanglement at approximately room temperature.

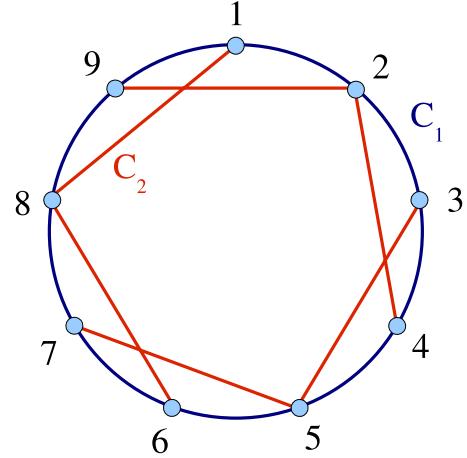


FIG. 6. (Color online) Schematic picture of the $\text{Na}_2\text{V}_3\text{O}_7$ system with coupling parameters C_1 and C_2 of the nine spin- $\frac{1}{2}$ Heisenberg ring model.

$=\{2, 5, 8\}$. So we find a transition from free to bound entanglement at approximately room temperature.

VII. CONCLUSIONS

We presented a family of entanglement criteria that detect any entangled state that can be detected based on the first and second moments of collective angular momenta. We also showed that these criteria can be extended such that they detect all entangled states that can be detected based on knowing the expectation values of the spin components and the correlation matrix. In spite of that, these criteria do not contain multiqubit correlation terms; they do not merely detect the entanglement of the two-qubit reduced state. They can even detect entangled states with separable two-qubit matrix. For further research, it would be very interesting to extend our results to ensembles of particles with a higher spin, e.g., spin-1 particles.

ACKNOWLEDGMENTS

We thank A. Acín, A. Cabello, M. Christandl, J. I. Cirac, S. R. de Echaniz, K. Hammerer, S. Iblisdir, M. Koschorreck, J. Korbicz, J. I. Latorre, M. Lewenstein, M. W. Mitchell, L. Tagliacozzo, and R. F. Werner for fruitful discussions. We also thank the support of the EU (OLAQUI, SCALA, and QICS), the National Research Fund of Hungary OTKA (Contract No. T049234), and the Hungarian Academy of Sciences (Bolyai Programme). This work was further supported by the FWF and the Spanish MEC (Ramon y Cajal Programme, Consolider-Ingenio 2010 project “QOIT”).

-
- [1] D. Bouwmeester, A. Ekert, and A. Zeilinger, *The Physics of Quantum Information* (Springer-Verlag, Berlin, 2000).
[2] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, e-print arXiv:quant-ph/0702225; M. Plenio and S. Virmani,

- Quantum Inf. Comput. **7**, 1 (2007); L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008); O. Gühne and G. Tóth, Phys. Rep. **474**, 1 (2009).
[3] M. Kitagawa and M. Ueda, Phys. Rev. A **47**, 5138 (1993).

- [4] D. J. Wineland, J. J. Bollinger, W. M. Itano, and D. J. Heinzen, Phys. Rev. A **50**, 67 (1994).
- [5] A. Kuzmich, N. P. Bigelow, and L. Mandel, Europhys. Lett. **42**, 481 (1998).
- [6] J. Hald, J. L. Sørensen, C. Schori, and E. S. Polzik, Phys. Rev. Lett. **83**, 1319 (1999).
- [7] A. Sørensen and K. Mølmer, Phys. Rev. Lett. **83**, 2274 (1999).
- [8] A. Sørensen, L.-M. Duan, J. I. Cirac, and P. Zoller, Nature (London) **409**, 63 (2001).
- [9] A. S. Sørensen and K. Molmer, Phys. Rev. Lett. **86**, 4431 (2001).
- [10] A. Sørensen, L.-M. Duan, J. I. Cirac, and P. Zoller, Nature (London) **409**, 63 (2001).
- [11] X. Wang, A. S. Sørensen, and K. Molmer, Phys. Rev. A **64**, 053815 (2001).
- [12] V. Meyer, M. A. Rowe, D. Kielpinski, C. A. Sackett, W. M. Itano, C. Monroe, and D. J. Wineland, Phys. Rev. Lett. **86**, 5870 (2001).
- [13] J. M. Geremia, J. K. Stockton, and H. Mabuchi, Science **304**, 270 (2004).
- [14] K. Hammerer, K. Mølmer, E. S. Polzik, and J. I. Cirac, Phys. Rev. A **70**, 044304 (2004).
- [15] K. Hammerer, E. S. Polzik, and J. I. Cirac, Phys. Rev. A **74**, 064301 (2006).
- [16] S. R. de Echaniz, M. W. Mitchell, M. Kubasik, M. Koschorreck, H. Crepaz, J. Eschner, and E. S. Polzik, J. Opt. B: Quantum Semiclassical Opt. **7**, S548 (2005).
- [17] S. R. de Echaniz, M. Koschorreck, M. Napolitano, M. Kubasik, and M. W. Mitchell, Phys. Rev. A **77**, 032316 (2008).
- [18] Note that for Eq. (2) we assume that the mean spin points to the x direction. Without this requirement, even a pure state in which all spins point into the same direction could violate Eq. (2) [3].
- [19] For a discussion about the differences of the two definitions, see K. Hammerer, A. S. Sørensen, and E. S. Polzik, e-print arXiv:0807.3358; For an analysis concerning the two-qubit case, see A. Messikh, Z. Ficek, and M. R. B. Wahiddin, Phys. Rev. A **68**, 064301 (2003).
- [20] R. F. Werner, Phys. Rev. A **40**, 4277 (1989).
- [21] J. K. Korbicz, J. I. Cirac, and M. Lewenstein, Phys. Rev. Lett. **95**, 120502 (2005); **95**, 259901(E) (2005), for detailed discussions see Ref. [24].
- [22] G. Tóth, Phys. Rev. A **69**, 052327 (2004).
- [23] G. Tóth, J. Opt. Soc. Am. B **24**, 275 (2007).
- [24] J. K. Korbicz, O. Guhne, M. Lewenstein, H. Haffner, C. F. Roos, and R. Blatt, Phys. Rev. A **74**, 052319 (2006).
- [25] N. Kiesel, C. Schmid, G. Tóth, E. Solano, and H. Weinfurter, Phys. Rev. Lett. **98**, 063604 (2007).
- [26] G. Tóth, C. Knapp, O. Guhne, and H. J. Briegel, Phys. Rev. Lett. **99**, 250405 (2007).
- [27] G. Tóth, Phys. Rev. A **71**, 010301(R) (2005).
- [28] This is the definition for singlets in condensed-matter physics. In quantum information science, the word singlet is used in a slightly different context. Singlets are pure states that are invariant under transformations of the type $U^{\otimes N}$. It can be shown that all such states have zero total angular momentum and zero angular-momentum variance. In general, states that are invariant under $U^{\otimes N}$ are called Werner states [20]. There are mixed Werner states that have nonzero angular-momentum variance. Finally, all multiqubit states with zero total angular momentum and zero angular-momentum variance are $U^{\otimes N}$ invariant. We thank A. Cabello and S. Iblisdir for discussions on this topic. See A. Cabello, J. Mod. Opt. **50**, 10049 (2003); T. Eggeling and R. F. Werner, Phys. Rev. A **63**, 042111 (2001).
- [29] H. F. Hofmann and S. Takeuchi, Phys. Rev. A **68**, 032103 (2003); O. Guhne, Phys. Rev. Lett. **92**, 117903 (2004).
- [30] For engineering Dicke states, see, for example, Ref. [25], R. G. Unanyan and M. Fleischhauer, Phys. Rev. Lett. **90**, 133601 (2003); C. Thiel, J. von Zanthier, T. Bastin, E. Solano, and G. S. Agarwal, *ibid.* **99**, 193602 (2007); A. Retzker, E. Solano, and B. Reznik, Phys. Rev. A **75**, 022312 (2007).
- [31] J. K. Stockton, J. M. Geremia, A. C. Doherty, and H. Mabuchi, Phys. Rev. A **67**, 022112 (2003).
- [32] O. Guhne, P. Hyllus, O. Gittsovich, and J. Eisert, Phys. Rev. Lett. **99**, 130504 (2007).
- [33] A. R. Usha Devi, M. S. Uma, R. Praphu, and A. K. Rajagopal, Phys. Lett. A **364**, 203 (2007); A. R. Usha Devi, R. Prabh, and A. K. Rajagopal, Phys. Rev. Lett. **98**, 060501 (2007).
- [34] Uncertainty relations expressed with the correlation matrix of the many-qubit system have appeared recently in Á. Rivas and A. Luis, Phys. Rev. A **77**, 022105 (2008). A related problem of finding criteria for physically allowed correlation matrices was considered in T. Moroder, M. Keyl, and N. Lütkenhaus, J. Phys. A: Math. Theor. **41**, 275302 (2008).
- [35] Command OPTSPINSQ.M of the QUBIT4MATLAB v3.0 package computes the violation of Eq. (7) in these optimal directions. See G. Tóth, Comput. Phys. Commun. **179**, 430 (2008).
- [36] M. Wieśniak, V. Vedral, and Č. Brukner, New J. Phys. **7**, 258 (2005).
- [37] Besides detecting entanglement, it is possible to obtain the two-qubit concurrence from measuring collective observables. See J. Vidal, Phys. Rev. A **73**, 062318 (2006).
- [38] A. J. Coleman, Rev. Mod. Phys. **35**, 668 (1963).
- [39] Note that a closely related problem is the symmetric extension problem, R. F. Werner, Lett. Math. Phys. **17**, 359 (1989); B. M. Terhal, A. C. Doherty, and D. Schwab, Phys. Rev. Lett. **90**, 157903 (2003).
- [40] M. Hein, J. Eisert, and H. J. Briegel, Phys. Rev. A **69**, 062311 (2004).
- [41] For example, the reduced states of three neighbored qubits of a ring cluster state are given by $\rho = (\mathbb{I} + \sigma_z \sigma_x \sigma_z)/8$, which is fully separable. However, the ring cluster state is the only global state that is compatible with these reduced states and is highly entangled.
- [42] X. Wang and B. C. Sanders, Phys. Rev. A **68**, 012101 (2003).
- [43] D. Jaksch, H. J. Briegel, J. I. Cirac, C. W. Gardiner, and P. Zoller, Phys. Rev. Lett. **82**, 1975 (1999); G. K. Brennen, C. M. Caves, P. S. Jessen, I. H. Deutsch, *ibid.* **82**, 1060 (1999).
- [44] O. Mandel, M. Greiner, A. Widera, T. Rom, T. W. Hansch, and I. Bloch, Nature (London) **425**, 937 (2003).
- [45] G. K. Brennen, Quantum Inf. Comput. **3**, 619 (2003).
- [46] C. M. Alves and D. Jaksch, Phys. Rev. Lett. **93**, 110501 (2004).
- [47] K. G. H. Vollbrecht and J. I. Cirac, Phys. Rev. Lett. **98**, 190502 (2007).
- [48] K. Eckert, O. Romero-Isart, M. Rodriguez, M. Lewenstein, E. S. Polzik, and A. Sanpera, Nat. Phys. **4**, 50 (2008).
- [49] I. de Vega, J. Ignacio Cirac, and D. Porras, Phys. Rev. A **77**, 051804(R) (2008).

- [50] K. Życzkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Phys. Rev. A **58**, 883 (1998).
- [51] E. Barouch, M. McCoy, and M. Dresden, Phys. Rev. A **2**, 1075 (1970); E. Barouch and M. McCoy, *ibid.* **3**, 786 (1971); **3**, 2137 (1971).
- [52] H. J. Lipkin, N. Meshkov, and A. J. Glick, Nucl. Phys. **62**, 188 (1965); T. Barthel, S. Dusuel, and J. Vidal, Phys. Rev. Lett. **97**, 220402 (2006).
- [53] A. Peres, Phys. Rev. Lett. **77**, 1413 (1996); M. Horodecki, P. Horodecki, and R. Horodecki, Phys. Lett. A **223**, 1 (1996).
- [54] On the other hand, there are multipartite bound entangled states that have a negative partial transpose with respect to some bipartitions. Recent papers studying bound entanglement that has a negative partial transpose with respect to some bipartitions are D. Patanè, R. Fazio, and L. Amico, New J. Phys. **9**, 322 (2007); A. Ferraro, D. Cavalcanti, A. García-Saez, and A. Acín, Phys. Rev. Lett. **100**, 080502 (2008). The latter obtains the temperature range for bound entanglement for a chain of oscillators in the thermodynamic limit. Fully PPT bound entanglement does not appear in this system.
- [55] O. Rudolph, Quantum Inf. Process. **4**, 219 (2005); K. Chen and L.-A. Wu, Quantum Inf. Comput. **3**, 193 (2003).
- [56] P. Millet, J. Y. Henry, F. Mila, and J. Galy, J. Solid State Chem. **147**, 676 (1999).
- [57] T. Saha-Dasgupta, R. Valentí, F. Capraro, and C. Gros, Phys. Rev. Lett. **95**, 107201 (2005).
- [58] T. Vértesi and E. Bene, Phys. Rev. B **73**, 134404 (2006).