Optimal Spin Squeezing Inequalities Detect Bound Entanglement in Spin Models

Géza Tóth,[1,2] Christian Knapp,[3] Otfried Gühne,[4] and Hans J. Briegel[3,4]

[1]*ICFO-Institut de Ciències Fotòniques, E-08860 Castelldefels (Barcelona), Spain*

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

[3]*Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria*

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

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We determine the complete set of generalized spin squeezing inequalities. These are entanglement criteria that 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. They can also be used to show the presence of bound entanglement in the thermal states of several spin models.

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Entanglement lies at the heart of many problems in quantum mechanics and has attracted increasing attention in recent years. However, in spite of intensive research, many of its intriguing properties are not fully understood. For example, it has been shown that there are entangled states from which the entanglement cannot be distilled again into the pure state form, even if many copies of the state are available [1]. The existence of these so-called bound entangled states has wide-ranging consequences for quantum cryptography [2] and classical information theory [3]. Since entangled states that are not recognized by the separability criterion of the positivity of the partial transpose (PPT) [4] are bound entangled, such states also serve as a test bed for new separability criteria [5–7]. However, bound entangled states are often considered to be rare, in the sense that they do not occur under natural conditions.

In physical systems such as ensembles of cold atoms [8] or trapped ions [9], spin squeezing [10,11] is one of the most successful approaches for creating large scale quantum entanglement. Since the variance of a spin component is small, spin squeezed states can be used for reducing spectroscopic noise or to improve the accuracy of atomic clocks [10,11]. Moreover, if an N-qubit state violates the inequality [12]

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

where $J_l := \frac{1}{2}\sum_{k=1}^{N} \sigma_l^{(k)}$ for $l = x, y, z$ are the collective angular momentum components, and $\sigma_l^{(k)}$ are Pauli matrices, then the state is entangled (i.e., not separable), which is necessary for using it in quantum information processing applications [12].

Recently, several generalized spin squeezing criteria for the detection of entanglement appeared in the literature [13–15] and have been used experimentally [16]. These criteria have a large practical importance since in many quantum control experiments, the spins cannot be individually addressed, and only collective quantities can be measured. In Ref. [13], a generalized spin squeezing criterion was presented detecting the presence of two-qubit entanglement. In Refs. [14,15], other criteria can be found that detect entanglement close to spin singlets and symmetric Dicke states, respectively. These entanglement conditions were obtained using very different approaches. At this point, two main questions arise: (i) 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. (ii) How strong are spin squeezing criteria? Can they detect entangled states that are not detected by the PPT criterion or other known entanglement criteria?

The goal of this Letter is twofold. First, we give a complete set of spin squeezing inequalities based on the first and second moments of collective observables. Second, we use them to show the presence of multipartite bound entanglement in several spin models in thermal equilibrium. In particular, we consider bound entanglement that has a positive partial transpose with respect to all bipartitions.

We can directly formulate our first main result:

Observation 1.—Let us assume that for a physical system, the values of $\vec{J} := (\langle J_x\rangle, \langle J_y\rangle, \langle J_z\rangle)$ and $\vec{K} := (\langle J_x^2\rangle, \langle J_y^2\rangle, \langle J_z^2\rangle)$ are known. Violation of any of the following inequalities implies entanglement:

$$\langle J_x^2\rangle + \langle J_y^2\rangle + \langle J_z^2\rangle \leq N(N+2)/4, \tag{2a}$$

$$(\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 \geq N/2, \tag{2b}$$

$$\langle J_i^2\rangle + \langle J_j^2\rangle - N/2 \leq (N-1)(\Delta J_k)^2, \tag{2c}$$

$$(N-1)[(\Delta J_i)^2 + (\Delta J_j)^2] \geq \langle J_k^2\rangle + N(N-2)/4, \tag{2d}$$

where i, j, k take all the possible permutations of x, y, z. The proof is given in the Appendix.

For any value of $\vec{J}$, these eight inequalities 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. For the case $\vec{J} = 0$ and $N = 6$, the polytope is depicted in Fig. 1. Such a polytope is completely charac-

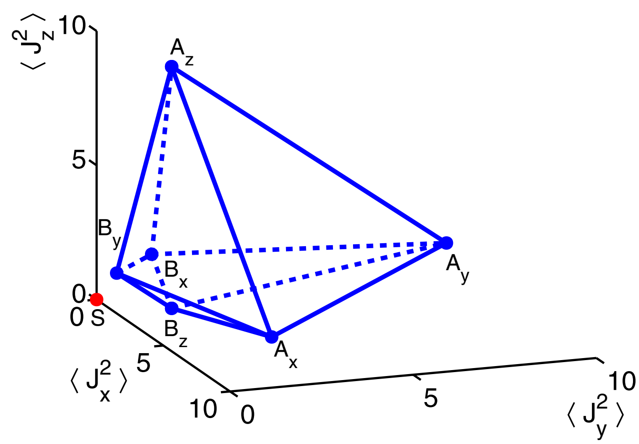

FIG. 1 (color online). The polytope of separable states corresponding to Eqs. (2) for $N = 6$ and $\vec{J} = 0$. S corresponds to a many-body singlet state.

terized by its extreme points. Direct calculation shows that they 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.

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. Because of the convexity of the set of separable states, it is enough to investigate the extreme points:

Observation 2.—For any value of $\vec{J}$, there are separable states corresponding to A_k. For certain values of $\vec{J}$ and N, there are separable states corresponding to points B_k. However, there are always separable states corresponding to points B_k' such that their distance from B_k is smaller than 1/4. In the limit $N \to \infty$ for a fixed normalized angular momentum $\vec{j} := \vec{J}/(N/2)$, the difference between the volume of polytope of Eqs. (2) 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

$$\rho_{A_x} := p(|\psi_+\rangle\langle\psi_+|)^{\otimes N} + (1-p)(|\psi_-\rangle\langle\psi_-|)^{\otimes N}. \quad (3)$$

Here, $|\psi_{+/-}\rangle$ are the single qubit states with Bloch vector coordinates $(\langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_z\rangle) = (\pm c_x, \langle J_y\rangle/J, \langle J_z\rangle/J)$ where $J := N/2$ and $c_x := \sqrt{1 - (\langle J_y\rangle^2 + \langle J_z\rangle^2)/J^2}$. The mixing ratio is defined as $p := [1 + \langle J_x\rangle/(Jc_x)]/2$. If $M := Np$ is an integer, we can also define the state corresponding to the point B_x as

$$|\phi_{B_x}\rangle := |\psi_+\rangle^{\otimes M} \otimes |\psi_-\rangle^{\otimes(N-M)}. \quad (4)$$

If M is not an integer, we can approximate B_x by taking $m := M - \varepsilon$ as the largest integer smaller than M, defining $\rho' := (1-\varepsilon)(|\psi_+\rangle\langle\psi_+|)^{\otimes m} \otimes (|\psi_-\rangle\langle\psi_-|)^{\otimes(N-m)} + \varepsilon(|\psi_+\rangle\langle\psi_+|)^{\otimes(m+1)} \otimes (|\psi_-\rangle\langle\psi_-|)^{\otimes(N-m-1)}$. 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 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 $\langle J_k\rangle = j_k \times N/2$, 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. □

Now we consider already known entanglement criteria and show how they can be derived from our theory. This can be done by showing that for any $\vec{J}$, the points A_k and B_k satisfy them.

Case 1.—The standard spin squeezing inequality is Eq. (1) from Ref. [12]. This inequality is valid for all A_k and B_k, for B_x even equality holds.

Case 2.—For separable states, $\langle J_x^2\rangle + \langle J_y^2\rangle \leq (N^2 + N)/4$ holds [15], as can be proved in the same way. This can be used to detect entanglement close to the N-qubit symmetric Dicke states with $N/2$ excitations.

Case 3.—Separable states fulfill Eq. (2b) which has already been shown in Ref. [14]. It is maximally violated by a many-body singlet, e.g., the ground state of an antiferromagnetic Heisenberg chain.

Case 4.—For symmetric states, it is known that $\langle J_x^2\rangle + \langle J_y^2\rangle + \langle J_z^2\rangle = N(N+2)/4$ [13]. From this and Eq. (2c), one can directly derive $1 - 4\langle J_i\rangle^2/N^2 \leq 4(\Delta J_i)^2/N$ from Ref. [13].

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 from $\langle\sigma_k^{(i)}\sigma_k^{(j)}\rangle$ and do not depend on higher order correlations. In fact, all quantities in our inequalities can be evaluated based on knowing the average two-qubit density matrix $\rho_{\text{av2}} := \frac{1}{N(N-1)} \times \sum_{i\neq j}\rho_{ij}$. Do our criteria simply detect entanglement of the two-qubit reduced state of the density matrix? We will now show that the criteria Eqs. (2) can detect entangled states that have a separable two-qubit density matrix. Even more surprisingly, they can detect bound entanglement in spin systems. While in the following we will use Eqs. (2) for the theoretical analysis of spin models, we stress that Eqs. (2) can also be used for the experimental detection of entanglement in a realization of these models in physical systems in which the collective angular momentum can be measured (e.g., Ref. [16]).

Let us first consider four spin-1/2 particles, interacting via the Heisenberg-type Hamiltonian [17]

$$H = \sum_{k=1}^{4} \vec{\sigma}_k \vec{\sigma}_{k+1} + J_2(\vec{\sigma}_1 \vec{\sigma}_3 + \vec{\sigma}_2 \vec{\sigma}_4), \tag{5}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. For the above Hamiltonian, we compute the thermal state $\varrho(T, J_2) \propto \exp(-H/kT)$ and investigate its separability properties. Hamiltonians of the type Eq. (5) are by no means artificial: They are used to describe cuprate and polyoxovanadate clusters [17,18]. For several separability criteria, we calculate the maximal temperature, below which the criteria find the states entangled. The results are summarized in Fig. 2. For $J_2 \gtrsim -0.5$, the spin squeezing inequality Eq. (2b) is the strongest criterion for separability. It allows us to prove the presence of entanglement even if the state is PPT with respect to all bipartitions [4]. This implies that the state is multipartite bound entangled: No pure entangled state can be distilled from it [19]. Note that introducing the next-to-nearest neighbor coupling made the PPT entangled temperature range larger.

For comparison, we investigated the computable cross norm or realignment criteria (CCNR, [5]) corresponding to all bipartitions, all the other criteria based on permutations [20], and the criterion based on covariance matrices [7]. None of them is able to find PPT entanglement in our spin system. Finally, we studied for each bipartition the separability test of symmetric extensions [21] that is strictly stronger than the PPT criterion. The critical temperatures, however, coincide within numerical accuracy with the ones from the PPT criterion, giving strong evidence that ϱ is indeed separable for the bipartitions. Indeed, we will see later that in some spin models, the spin squeezing inequalities signal the presence of entanglement even for states that are separable with respect to all bipartitions.

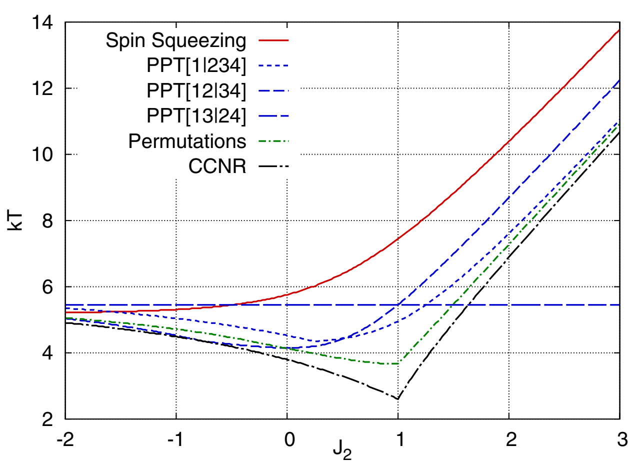

FIG. 2 (color online). Entanglement properties of the spin model with the Hamiltonian Eq. (5). The critical temperatures for several entanglement conditions are shown as a function of the next-to-nearest neighbor coupling J_2. For details see text.

After small spin clusters, we consider larger spin systems. Using Eqs. (2), we find bound entanglement that is PPT with respect to all bipartitions in Heisenberg and XY chains with a periodic boundary condition with up to 9 qubits. The critical temperatures are shown in Table I. Equations (2) also detect bound entanglement in Heisenberg and XY models with a complete graph topology [22]. Latter is a special case of the Lipkin-Meshkov-Glick model [23]. In all these cases, there is a considerable temperature range for which the thermal state is PPT with respect to all partitions but not yet separable [24]. Interestingly, since in the three-qubit Heisenberg model the thermal state is invariant under multilateral unitary transformations of the type $U \otimes U \otimes U$, for such states the PPT condition implies biseparability [25]. Thus, the spin squeezing inequalities can detect bound entanglement for which all bipartitions are separable.

Note that the bound entanglement that is PPT with respect to all bipartitions is perhaps the most intriguing type and the most challenging to detect. No pure state entanglement can be distilled from it with local operations and classical communication, even if an arbitrary number of parties join. However, an entangled state that is PPT with respect to only a single partition is already bound entangled since no GHZ state can be distilled from it [19]. Such entanglement can be found by the PPT criterion with respect to a different partition. It is expected to appear in many systems since as the temperature increases, not all the bipartitions become PPT at the same temperature [26].

Our study of the spin models has two general consequences. First, we realize that examination of spin models via the partial transposition or the investigation of bipartitions does not lead to a full understanding of the entanglement properties of condensed matter systems. Second, we note that the spin clusters and spin chains we studied are models of existing physical systems. Thus, multipartite bound entanglement that is PPT with respect to all partitions is not a rare phenomenon in nature.

Moreover, based on Ref. [27], it is possible to connect the variances of collective angular momenta to important thermodynamical quantities giving our inequalities a new physical interpretation. Let us consider a system with a Hamiltonian H and an additional magnetic interaction $H_I := \sum_{k=x,y,z} B_k J_k$, where $\vec{B}$ is the magnetic field. Moreover, assume that H commutes with $J_{x/y/z}$. Then the magnetic susceptibilities are $\chi_l := (\partial\langle J_l\rangle/\partial B_l)|_{\vec{B}=0}$ for

TABLE I. Critical temperatures for the PPT criterion and Eqs. (2) for Heisenberg and XY spin chains of various size.

	N	3	4	5	6	7	8	9
Heisenberg	Equations (2)	5.46	5.77	5.72	5.73	5.73	5.73	5.73
model	PPT	4.33	5.47	4.96	5.40	5.17	5.37	5.25
XY	Equations (2)	3.08	3.48	3.39	3.41	3.41	3.41	3.41
model	PPT	2.56	3.46	3.08	3.34	3.19	3.32	3.24

$l = x, y, z$ and the variances can be written as $(\Delta J_l)^2 = kT\chi_l$. Thus, our inequalities can be expressed with susceptibilities [28].

Finally, 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 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 [7,29] $C_{kl} := \langle J_k J_l + J_l J_k \rangle /2$ and $\gamma_{kl} := C_{kl} - \langle J_k \rangle \langle J_l \rangle$ 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 of the coordinate system. Concerning Eq. (2c), we can reformulate it as $\langle J_i^2 \rangle + \langle J_j^2 \rangle + \langle J_k^2 \rangle - N/2 \leq (N-1)(\Delta J_k)^2 + \langle J_k^2 \rangle$. Then, the left hand side is again invariant under rotations, and we find a violation of Eq. (2c) in some direction if the minimal eigenvalue of $\mathfrak{X} := (N-1)\gamma + C$ is smaller than $\mathrm{Tr}(C) - N/2$. Similarly, we find a violation of Eq. (2d) if the largest eigenvalue of $\mathfrak{X}$ exceeds $(N-1)\mathrm{Tr}(\gamma) - N(N-2)/4$. Thus, the orthogonal transformation that diagonalizes $\mathfrak{X}$ delivers the optimal measurement directions x', y', z' [30].

In summary, 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 applied our findings to examples of spin models, showing the presence of bound entanglement in these models.

Appendix—Proof of Observation 1.—Fully separable states are of the form $\rho = \sum_l p_l \rho_l^{(1)} \otimes \rho_l^{(2)} \otimes \ldots \otimes \rho_l^{(N)}$, where $\sum_l p_l = 1$ and $p_l > 0$. The variance, defined as $(\Delta A)^2 := \langle A^2 \rangle - \langle A \rangle^2$, is concave in the state; thus, it suffices to prove that the inequalities of Observation 1 are satisfied by pure product states. Based on the theory of angular momentum, Eq. (2a) is valid for all quantum states. For Eq. (2b), one first needs that for product states $(\Delta J_k)^2 = N/4 - (1/4)\sum_i \langle \sigma_k^{(i)} \rangle^2$ holds, then the statement follows form the normalization of the Bloch vector. Concerning Eq. (2c), we have to show that $\mathfrak{Y} := (N-1) \times (\Delta J_x)^2 + N/2 - \langle J_y^2 \rangle - \langle J_z^2 \rangle \geq 0$. Using the abbreviation $x_i = \langle \sigma_x^{(i)} \rangle$, $y_i = \langle \sigma_y^{(i)} \rangle$, etc., this can be written as $\mathfrak{Y} = (N-1)[N/4 - (1/4)\sum_i x_i^2] - (1/4)\sum_{i \neq j}(y_i y_j + z_i z_j) = (N-1)[N/4 - (1/4)\sum_i x_i^2] - (1/4)[(\sum_i y_i)^2 + (\sum_i z_i)^2] + (1/4)\sum_i (y_i^2 + z_i^2)$. Using the fact that $(\sum_i s_i)^2 \leq N \sum_i s_i^2$, and the normalization of the Bloch vector, it follows that $\mathfrak{Y} \geq 0$. Equation (2d) can be proven in the same way. □

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