Optimal spin squeezing inequalities detect bound entanglement in spin models

Géza Tóth,1,2 Christian Knapp,3 Otfried Gühne,4 and Hans J. Briegel3,4

1ICFO-Institut de Ciències Fotòniques, E-08860 Castelldefels (Barcelona), Spain
2Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O. Box 49, H-1525 Budapest, Hungary
3Institut für Theoretische Physik, Universität Innsbruck, Technikerstraße 25, A-6020 Innsbruck, Austria,
4Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, A-6020 Innsbruck, Austria

(Dated: September 14, 2018)

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-$1/2$ 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.

PACS numbers: 03.65.Ud, 03.67.Mn, 05.50.+q, 42.50.Dv

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, 6, 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

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

(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, 14, 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. [12] 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

![FIG. 1: The polytope of separable states corresponding to Eqs. (2) for $N = 6$ and $\vec{J} = 0$. $S$ corresponds to a many body singlet state.](image-url)
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 \( J := \{J_x, J_y, J_z\} \) and \( \bar{K} := \{J_x^2, J_y^2, J_z^2\} \) are known. Violation of any of the following inequalities implies entanglement:

\[
\begin{align*}
&J_x^2 + J_y^2 + J_z^2 \leq N(N+2)/4, \\
&(\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 \geq N/2, \\
&(\Delta J_y^2 + J_z^2)/N \leq (N-1)(\Delta J_y)^2, \\
&(N-1)[(\Delta J_x)^2 + (\Delta J_y)^2] \geq (J_x^2) + N(N-2)/4.
\end{align*}
\]

where \( i, j, k \) take all the possible permutations of \( x, y, z \).

*Proof.* A separable state corresponds to \( A_x \) and \( B_x \) 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. Due to the convexity of the set of separable states, it is enough to investigate the extreme points:

**Observation 2.** For any value of \( J \) there are separable states corresponding to \( A_x \). For certain values of \( J \) and \( N \) there are separable states corresponding to points \( B_x \).

However, there are always separable states corresponding to points \( B_x \) such that their distance from \( B_x \) is smaller than 1/4. In the limit \( N \to \infty \) for a fixed normalized angular momentum \( \bar{J} := J/(N/2) \) the difference between the volume of polytope of Eqs. (3) 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

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

\[ H = \sum_{k=1}^{4} \vec{\sigma}_k \vec{\sigma}_{k+1} + J_2 (\vec{\sigma}_1 \vec{\sigma}_3 + \vec{\sigma}_2 \vec{\sigma}_4). \]

(5)

where \( \vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \). For the above Hamiltonian, we compute the thermal state \( \rho(T, J_2) \propto \exp(-H/kT) \) 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 to prove the presence of entanglement even if the state is PPT with respect to all bipartitions [2]. 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 \( \rho \) 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.

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. Eqs. (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 [22]. 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 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 [10]. 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 [24].

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

\[ \text{Table I: Critical temperatures for the PPT criterion and Eqs. (2) for Heisenberg and XY spin chains of various size.} \]

| N   | 3     | 4     | 5     | 6     | 7     | 8     | 9     |
|-----|-------|-------|-------|-------|-------|-------|-------|
| Heisenberg model | Eqs. (2) | 5.46 | 5.77 | 5.72 | 5.73 | 5.73 | 5.73 |
| XY model       | Eqs. (2) | 3.08 | 3.48 | 3.39 | 3.41 | 3.41 | 3.41 |

FIG. 2: 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.
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 $H_1 := \sum_{k=x,y,z} B_k J_k$, where $B$ is the magnetic field. Moreover, assume that $H$ commutes with $J_k / g_{ik}$. Then the magnetic susceptibilities are

$$\chi_l := \langle \partial (J_l) / \partial B_l \rangle_{\beta = 0}$$

for $l = x, y, z$. 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 $\langle J_l \rangle$ and $\langle J_k^2 \rangle$ for $k = x, y, z$ are known, but $\langle J_l \rangle$ and $\langle J_k^2 \rangle$ in arbitrary directions $i$. We will now show how to find the optimal directions $x', y', z'$ to evaluate Observation 1. Knowledge of $\langle J_l \rangle$ and $\langle J_k^2 \rangle$ in arbitrary directions is equivalent to the knowledge of the vector $\vec{J}$, the correlation matrix $C$ and the covariance matrix $\Sigma$ of $J_l$

$$C_{kl} := \langle J_l J_k \rangle / 2$$

and $\gamma_{kl} := \langle J_l \rangle \langle J_k \rangle$ for $k, l = x, y, z$. When changing the coordinate system to $x', y', z'$, vector $\vec{J}$ and the matrices $C$ and $\gamma$ transform as $J \rightarrow O J$, $C \rightarrow OCO^T$ and $\gamma \rightarrow O \gamma O^T$ where $O$ is an orthogonal 3 x 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. (23), we can reformulate it as

$$\langle J_i^2 \rangle + \langle J_j^2 \rangle + \langle J_k^2 \rangle - N/2 \leq (N - 1) (\Delta J_i)^2 + \langle J_k^2 \rangle.$$

Then, the left hand side is again invariant under rotations, and we find a violation of Eq. (23) in some direction if the minimal eigenvalue of $\hat{X} := (N - 1) \gamma + C$ is smaller than $Tr(C) - N/2$. Similarly, we find a violation of Eq. (24) if the largest eigenvalue of $\hat{X}$ exceeds $(N - 1) Tr(\gamma) - N(N - 2)/4$. Thus the orthogonal transformation that diagonalizes $\hat{X}$ delivers the optimal measurement directions $x', y', z'$. [24]

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.

We thank A. Acín, J.I. Cirac, J. Korbicz, and M. Lewenstein for fruitful discussions. We thank the support of the EU (OLAQUI, SCALA, QICS), the National Research Fund of Hungary OTKA (Contract No. T049234), the Hungarian Academy of Sciences (Bolyai Programme), the FWF, and the Spanish MEC (Ramón y Cajal Programme, Consolider-Ingenio 2010 project "QOIT").

Appendix – Proof of Observation 1. Fully separable states are of the form $\rho = \sum_i p_i \rho_i^{(1)} \otimes \rho_i^{(2)} \otimes \ldots \otimes \rho_i^{(N)}$, where $\sum_i p_i = 1$ and $p_i > 0$. 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. (23) is valid for all quantum states. For Eq. (24) one first needs that for product states $(\Delta J_i)^2 = N/4 - (1/4) \sum_i (\sigma_i^{(i)})^2$ holds, then the statement follows form the normalization of the Bloch vector. Concerning Eq. (24), we have to show that $\tilde{\gamma} := (N - 1) (\Delta J_i)^2 + N/2 - (\langle J_i^2 \rangle - \langle J_i \rangle^2) \geq 0$. Using the abbreviation $x_i = \langle \sigma_i^{(i)} \rangle, \gamma_i = \langle \sigma_i^{(i)} \rangle$, etc. this can be written as $\tilde{\gamma} = (N - 1) [N/4 - (1/4) \sum_i x_i^2] - (1/4) \sum_i (y_i z_i + z_i y_i) = (N - 1) [N/4 - (1/4) \sum_i x_i^2] - (1/4) [\sum_i y_i^2 + (1/4) \sum_i z_i^2 + (1/4) \sum_i y_i z_i + z_i y_i]$. Using the fact that $(\sum_i s_i^2) \leq N \sum_i s_i^2_i$, and the normalization of the Bloch vector, it follows that $\tilde{\gamma} \geq 0$. Eq. (24) can be proved in the same way.

[1] M. Horodecki et al., Phys. Rev. Lett. 80, 5239 (1998); for a review see P. Horodecki in D. Bruß and G. Leuchs (eds.), Lectures on Quantum Information (Wiley-VCH, Berlin, 2006); see also P. Hyllus et al., Phys. Rev. A 70, 032316 (2004); U.V. Poulsen et al., ibid. 71, 063605 (2005).

[2] K. Horodecki et al., Phys. Rev. Lett. 94, 160502 (2005).

[3] A. Acín et al., Phys. Rev. Lett. 92, 107003 (2004).

[4] A. Peres, Phys. Rev. Lett. 77, 1413 (1996).

[5] O. Rudolph, quant-ph/0202121. K. Chen and L.-A. Wu, Quant. Inf. Comp. 3, 193 (2003).

[6] A.C. Doherty et al., Phys. Rev. A 69, 022308 (2004).

[7] O. Gühne et al., Phys. Rev. Lett. 99, 130504 (2007).

[8] J. Hald et al., Phys. Rev. Lett. 83, 1319 (1999).

[9] V. Meyer et al., Phys. Rev. Lett. 86, 5870 (2001).

[10] M. Kitagawa and M. Ueda, Phys. Rev. A 47, 5138 (1993).

[11] D.J. Wineland et al., Phys. Rev. A 50, 67 (1994).

[12] A. Sørensen et al., Nature 409, 63 (2001).

[13] J. Korbicz et al., Phys. Rev. Lett. 95, 120502 (2005).

[14] G. Tóth, Phys. Rev. A 69, 052327 (2004).

[15] G. Tóth, J. Opt. Soc. Am. B 24, 275 (2007).

[16] J. Korbicz et al., Phys. Rev. A 74, 052319 (2006); N. Kiesel et al., Phys. Rev. Lett. 98, 063604 (2007).

[17] I. Bose and A. Tribedi, Phys. Rev. A 72, 022314 (2005); T. Vertesi and E. Bene, Phys. Rev. B 73, 134404 (2006).

[18] See, e.g. R. Basler et al., Inorg. Chem. 41, 5675 (2002); J.T. Haraldsen et al., Phys. Rev. B 71, 064403 (2005).

[19] W. Dür et al., Phys. Rev. Lett. 83, 3562 (1999).

[20] L. Clarisse and P. Wocjan, Quant. Inf. Comp. 6, 277 (2006).

[21] We used the second step of the hierarchy of Ref. 6, available at http://www.iq.calkit.edu/documents/spedalleri/ppspsetest1.m

[22] G. Tóth, Phys. Rev. A 71, 010301(R) (2005).

[23] H.J. Lipkin et al., Nucl. Phys. B 62, 188 (1965); T. Barthel et al., Phys. Rev. Lett. 97, 220402 (2006).

[24] C. Knapp, diploma thesis, University of Innsbruck, 2007.

[25] T. Eggeling and R.F. Werner, Phys. Rev. A 63, 042111 (2001).

[26] Recent preprints studying bound entanglement that has a negative partial transpose with respect to some bipartitions: D. Patané et al., New J. Phys. 9 (2007) 322; D. Cavalcanti et al., arXiv:0705.3762. 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.

[27] M. Wieśniak et al., New J. Phys. 7, 258 (2005).

[28] Note that the condition $[H, M_i] = 0$ is difficult to guarantee in realistic situations.

[29] A.R. Usha Devi et al., Phys. Rev. Lett. 98, 060501 (2007).

[30] See the command `optspinsq.m` of the QUBIT4MATLAB program package described in G. Tóth, [arXiv:0709.0948](https://arxiv.org/abs/0709.0948).