Optimal spin squeezing inequalities detect bound entanglement in spin models

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We fully characterize the entangled states in a system of spin-$\frac{1}{2}$ particles which can be detected based on the first and second moments of collective angular momenta. Any generalized spin squeezing inequality can directly be derived from our approach. When applied to condensed matter systems, our results show the presence of bound entanglement in thermal states of several spin models.

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Spin squeezing [1, 2] is one of the most successful approaches for creating large scale quantum entanglement in various physical systems such as ensembles of cold atoms [3] or trapped ions [4]. A spin squeezed state of two-state particles, in the most general sense, has a small variance of the collective angular momentum in one direction, while in an orthogonal direction the angular momentum is large. For instance, if an $N$-qubit state violates the inequality [5]

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

(1)

where $J_{x/y/z} := \frac{1}{2} \sum_{k=1}^{N} \sigma_{x/y/z}^{(k)}$, are the collective angular momentum components and $\sigma_{x/y/z}^{(k)}$ are Pauli matrices, then the state is entangled (i.e., not separable), which is necessary for using it in quantum information processing applications [2, 6]. Moreover, spin squeezed states can also be used for reducing spectroscopic noise or to improve the accuracy of atomic clocks [1, 2].

Recently, several generalized spin squeezing criteria for the detection of entanglement appeared in the literature and have been used experimentally. 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 Refs. [7] a generalized spin squeezing criterion was presented which detects the presence of two-qubit entanglement and for symmetric states it is a necessary and sufficient condition. In Refs. [8, 9] other criteria can be found which detect entanglement close to spin singlets and symmetric Dicke states, respectively. Since up to now there is not a systematic way of deriving such inequalities, these entanglement conditions were obtained using very different approaches. Moreover, it is also not clear how to construct new criteria for detecting entanglement in the vicinity of various quantum states available in today’s experiments.

In this paper, we explicitly give the values of first and second order moments of collective observables allowed for fully separable states, i.e., for states of the form $\rho = \sum_{p} p_{l} \rho_{l}^{(1)} \otimes \rho_{l}^{(2)} \otimes ... \otimes \rho_{l}^{(N)}$, where $\sum_{l} p_{l} = 1$ and $p_{l} > 0$. Consequently, our conditions represent the optimal spin squeezing inequalities for the detection of entanglement, and any other spin squeezing inequality can be derived from our approach. Moreover, our methods make it possible to demonstrate the presence of bound entanglement in spin chains in thermal equilibrium. Bound entanglement, a special form of entanglement with intriguing properties, is often considered to be rare. However, it is at the heart of many problems in quantum information science and is hence under intensive research [10].

We can directly formulate our first main result:

**Observation 1.** Let us assume that for a physical system the values of $\mathbf{J} := \langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle$ and $\langle J_{x/y/z}^2 \rangle$ are known. If the system is in a separable state, the following

![Image](image.png)

**FIG. 1:** The polytope of separable states corresponding to Eq. (2) for $N = 6$ and for $\langle J_{x/y/z} \rangle = 0$. $S$ corresponds to a many body singlet state.
Inequalities hold:

\[
\begin{align*}
(J^2_x + J^2_y + J^2_z) &\leq N(N + 2)/4, \\
(\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 &\geq N/2, \\
(J^2_x + J^2_y - N/2 &\leq (N - 1)(\Delta J_m)^2, \\
(N - 1) [(\Delta J_k)^2 + (\Delta J_l)^2] &\geq (J^2_m + N(N - 2))/4, 
\end{align*}
\]

where \((\Delta A)^2 := (A^2 - \langle A \rangle^2)\) is the variance and \(k, l, m\) take all the possible permutations of \(x, y, z\). The proof is given in the appendix.

For any value of \(J\) these eight inequalities define a polytope in the three-dimensional \((J_x, J_y, J_z)\)-space. Observation 1 states that the separable states lie inside this polytope. If one of the inequalities is violated, then the separation states lie inside this polytope. Direct calculation shows that they are extremal points. Hence in the macroscopic limit the characterization is complete.

For any value of \(J\) the points corresponding to separable states are given in the appendix. For them we have:

\[
\begin{align*}
A_x := \left[ \frac{N^2}{4} - \kappa(\langle J_y \rangle^2 + \langle J_z \rangle^2), \frac{N}{4} + \kappa(\langle J_y \rangle^2, \frac{N}{4} + \kappa(\langle J_z \rangle^2) \right], \\
B_x := \left[ \frac{\langle J_x \rangle^2 + \langle J_y \rangle^2 + \langle J_z \rangle^2}{N}, \frac{N}{4} + \kappa(\langle J_y \rangle^2, \frac{N}{4} + \kappa(\langle J_z \rangle^2) \right],
\end{align*}
\]

where \(\kappa := (N - 1)/N\). The points \(A_{y/z}\) and \(B_{y/z}\) can be obtained from these by permuting the coordinates.

The question arises, whether all points inside the polytope correspond to separable states. This would imply that the criteria of Observation 1 are complete, in the sense that if the inequalities are fulfilled, then the first and second moments of \(J_x, J_y, J_z\) do not suffice to prove entanglement. Due to the convexity of the set of separable states, it is enough to investigate the extremal points. For them we have:

**Observation 2.** For any value of \(J\) there are separable states corresponding to \(A_{x/y/z}\). For certain values of \(J\) and \(N\) (e.g., \(J = 0\) and even \(N\)) there are separable states corresponding to points \(B_{x/y/z}\). However, there are always separable states corresponding to points \(B_{y/z}\) such that their distance from \(B_{x/y/z}\) is smaller than \(1/4\). In the limit \(N \to \infty\) for a fixed normalized angular momentum \(2J/N\) the difference between the volume of polytope of Eqs. [2] and the volume of sets of points corresponding to separable states decreases with \(N\) 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

\[
\rho_{A_x} = p|\psi_+\rangle\langle\psi_+|^{\otimes N} + (1 - p)|\psi_-\rangle\langle\psi_-|^{\otimes N}. \tag{3}
\]

Here \(|\psi_+/-\rangle\) are the single qubit states with Bloch vector coordinates \((\sigma_x, \sigma_y, \sigma_z) = (\pm c_x, 2J_x/N, 2J_z/N)\) where \(c_x := \sqrt{1 - 4\langle J_y \rangle^2 + \langle J_z \rangle^2}/N^2\). The mixing ratio is defined as \(p := 1/2 + |J_x|/(Nc_x)\). If \(N_1 := Np\) is an integer, we can also define the state corresponding to the point \(B_x\) as \(|\phi_{B_x}\rangle = |\psi_+\rangle^{\otimes N_1} \otimes |\psi_-\rangle^{\otimes (N - N_1)}\). In general, there is a separable state \(|\phi_{B_k}\rangle\) for \(J_x = (k_x - N/2)c_x\) where \(k_x\) is an integer. If \(N_1\) is not an integer, we can approximate \(B_x\) by taking \(N_1 = N_1 - \varepsilon\) as the largest integer smaller than \(N_1\), defining \(N_1 = N_1 + \varepsilon\) as the largest integer smaller than \(N_1\), defining \(N_1 = N_1 + 1\) and \(\varepsilon = (1 - \varepsilon)|\psi_+\rangle\langle\psi_+|^{\otimes(N - 1)} \otimes |\psi_-\rangle\langle\psi_-|^{\otimes(N - N_1)} + \varepsilon(|\psi_+\rangle\langle\psi_+|^{\otimes(N - 1)} \otimes |\psi_-\rangle\langle\psi_-|^{\otimes(N - N_1)}).\) This state has the same coordinates as \(B_x\), except for the value of \(\langle J_x^2\rangle\), where the difference is \(\varepsilon^2/(N^2) \leq 1/4\). The dependence of \(\Delta V/V\) on \(N\) can be studied by considering the polytopes in the \((J_x^2, J_y^2, J_z^2)\)-space corresponding to \(J_k = j_k \times N/2\), where \(j_k\) is the normalized angular momentum. As \(N\) increases, the distance of the points \(A_{x/y/z}\) to \(B_{x/y/z}\) 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 \(N^4\).

Having shown that Observation 1 gives a full characterization of the states without entanglement in the six-dimensional space of \((J_x, J_y, J_z)\) and \((J_x, J_y, J_z)^2\), the question arises, what can be said concerning entanglement in the three-dimensional spaces of \((J_x^2, J_y^2, J_z^2)\) or \((\Delta J_x)^2\). The following Observation gives the answer.

**Observation 3.** Let us consider the set of points corresponding to separable states for even \(N\) in the \((J_x^2, J_y^2, J_z^2)\)-space without constraining the values of \((J_x, J_y, J_z)\). This set is the polytope from Observation 1 for \(J = 0\), also shown in Fig. 1. Also, the set of points corresponding to separable states in the \((\Delta J_x)^2\)-space is the same polytope. That is, Fig. 1 gives also the right polytope if the labels of the axes are changed from \((J_x^2)\) to \((\Delta J_x)^2\).

**Proof.** For the first part, it can be directly seen that Eq. [2] are least restrictive for \(J = 0\), for other \(J\) the polytope is strictly smaller. For the second part, note that based on Eq. [2] the points corresponding to separable states must be within the same polytope shown in Fig. 1 even if we change the labels from \((J_x^2)\) to \((\Delta J_x)^2\). It is not clear, however, that the set of separable states is convex in the \((\Delta J_x)^2\)-space. So we have to show that for each separable state \(\rho\) with \((J_x^2) = S_l\) for \(l = x, y, z\) is there a separable state \(\hat{\rho}\) for which \((\Delta J_x)^2 = S_l\). Let us approximate 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 \(\hat{\rho} := \sum p_k \hat{\rho}_k\) can be obtained by mixing

\[
\hat{\rho}_k := \frac{1}{N} \sum_{\alpha, \beta, \gamma = 0, 1} M_{\alpha\beta\gamma}(M_{\alpha\beta\gamma}\langle\phi_{(j)}|)) \tag{4}
\]

where \(M_{\alpha\beta\gamma}(\rho)\) changes the sign of the \(x/y/z\)-coordinate of the Bloch vector by \((-1)^\alpha\). The state \(\hat{\rho}\) has the same \((J_x^2)\) as \(\rho\). However, the value of \((\Delta J_x)^2\) is zero, hence \((\Delta J_x)^2 = \langle J_x^2\rangle\).
we calculate the maximal temperature, below which the criteria detect the states as entangled. The results are summarized in Fig. 2. For $J_2 \geq -0.5$, the spin squeezing inequality Eq. (2d) is the strongest criterion for separability. It allows to detect entanglement, where the state has a positive partial transpose (PPT) with respect to each bipartition \[13\]. This implies that the state is multipartite bound entangled. No pure entangled state can be distilled from them \[14\]. Furthermore, we investigated for each bipartition the separability test of symmetric extensions \[13\], which 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. Finally, we investigated also the computable cross norm (CCN) criterion \[16\] and further criteria based on other permutations \[17\] and covariance matrices \[18\]. None of them is able to detect the entanglement in the critical regime. A full discussion will be given elsewhere \[19\].

Further remarks follow. First, it has been shown in Ref. \[20\] that if a magnetic interaction $H_I = B M_z$ is added to the Hamiltonian and if $H$ commutes with the magnetization $M_i = J_i$, then Eq. (2d) may be expressed in terms of the magnetic susceptibility $\chi_i = (\partial M_i/\partial B), i = x, y, z$ as

$$\chi_x + \chi_y + \chi_z \geq \frac{N}{2kT},$$

giving the spin squeezing inequality a new physical interpretation \[21\].

Second, we would like to stress that similar results hold also for other Hamiltonians. We found XY-, and Heisenberg-type Hamiltonians up to nine qubits for which our inequalities also detect multipartite bound entanglement. This encourages to conjecture that bound entanglement is also present in macroscopic systems.

In general, our study of the spin model has two consequences. First, we realize that studies of spin models via the partial transposition or investigations of bipartitions will not lead to a full understanding of the entanglement properties of condensed matter systems. Second, given the practical relevance of such spin clusters, we can conclude that bound entanglement is not a rare phenomenon in nature.

Finally, let us discuss some further features and consequences of our spin squeezing inequalities. First, one can ask what happens, if not only $\langle J_{x/y/z}\rangle$ and $\langle J^2_{x/y/z}\rangle$ are known, but $\langle J_i \rangle$ and $\langle J^2_i \rangle$ in arbitrary directions $i$. Then, the question arises how one can find the optimal directions $x', y', z'$ to evaluate Observation 1.

Knowledge of $\langle J_i \rangle$ and $\langle J^2_i \rangle$ in arbitrary directions is equivalent to the knowledge of the the vector $v := (\langle J_x \rangle, \langle J_y \rangle, \langle J_z \rangle)$, the correlation matrix C and the covariance matrix $\gamma$, which have the entries \[18\].

$$C_{kl} := \langle J_k J_l + J_l J_k \rangle/2; \quad \gamma_{kl} := C_{kl} - \langle J_k \rangle \langle J_l \rangle$$

Case 1. The standard spin-squeezing inequality for entanglement is Eq. (1) from Ref. \[3\]. This inequality is valid for all $A_k$ and $B_k$, for $B_k$ even equality holds.

Case 2. For separable states $\langle J^2_1 \rangle + \langle J^2_y \rangle \leq (N^2 + N)/4$ holds \[3\], 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 must fulfill Eq. (2b) which has already been shown in Ref. \[3\]. It is maximally violated by a many-body singlet, e.g., the ground state of an antiferromagnetic Heisenberg chain. A condition similar to Eq. (2b), however, needing fewer measurements is the following: For separable states $(\Delta J_x)^2 + (\Delta J_y)^2 \geq N/4$.

Case 4. For symmetric states it is known that $\langle J^2_1 \rangle + \langle J^2_y \rangle + \langle J^2_2 \rangle = N(N + 2)/4$ \[7\]. So no state of the symmetric subspace can violate Eq. (2b). Furthermore, from this and Eq. (2b) one can directly derive $1 - 4\langle J_m \rangle^2/N^2 \leq 4(\Delta J_m)^2/N$ from Ref. \[3\].

Let us come to a surprising consequence of our results, namely the existence of bound entanglement in spin models. As a first model, let us consider four spin-1/2 particles, interacting via the Hamiltonian

$$H = J_1(h_{12} + h_{23} + h_{34} + h_{41}) + J_2(h_{13} + h_{24}),$$

where $h_{ij} = \sigma_i^z \otimes \sigma_j^z + \sigma_i^y \otimes \sigma_j^y + \sigma_i^z \otimes \sigma_j^z$ is a Heisenberg interaction between the qubits $i, j$ \[11\]. Models of this kind are by no means artificial, they are used to describe cuprate and polyoxovanadate clusters \[11\], \[12\].

For the above Hamiltonian, we set $J_1 = 1$, compute the thermal state $\rho = \rho(T, J_2)$ and investigate its separability properties. For different separability criteria

FIG. 2: Entanglement properties of the spin model with the Hamiltonian Eq. (5). For Eq. (2d) and the PPT criterion with respect to different partitions the critical temperatures, below which the state is detected as entangled, are shown. The temperatures for the criterion in Ref. \[13\] coincide with the ones from the PPT criterion. Furthermore, the temperatures are shown below which the CCN criterion \[16\] detects entanglement in some bipartition and below which one of the other permutation criteria \[17\] are successful.
for $k, l = x, y, z$. Choosing a coordinate system $x', y', z'$ via some local unitary transformation leads effectively to some orthogonal transformation $v \mapsto Oy, C \mapsto OCOT$ and $\gamma \mapsto O\gamma O^T$ with an orthogonal $3 \times 3$ matrix $O$.

Looking at the inequalities of Observation 1 one finds that the first two inequalities are invariant under a change of the coordinate system, since the trace of $C$ and $\gamma$, respectively, is invariant under orthogonal transformations. Concerning Eq. (2b), we can reformulate it as $(J^2_x + J^2_y)_{\rho_{12}} - N/2 \leq (N - 1)(\Delta J_{\pi})^2 + (J^2_{\pi}/N)$. Then, the left hand side is again invariant under rotations, and we find a violation of Eq. (2b) in some direction if the minimal eigenvalue of $X := (N - 1)\gamma + C$ is smaller than $Tr(C) - N/2$. Similarly, we find a violation of Eq. (2a) if the largest eigenvalue of $X$ exceeds $(N - 1)Tr(\gamma) - N(N - 2)/4$. Consequently, the orthogonal transformation, which diagonalizes $X$ delivers the optimal measurement directions $x', y', z'$.

Further, it is interesting to compare the regions in the $(J^2_{\pi}/N)$-space allowed for separable states to the $N$-space allowed for product states. Based on the theory of angular momentum, Eq. (2b) is valid for all quantum states. However, for separable states it can be proved easily without this knowledge using the fact that for such states $\langle \sigma_{x}^{(i)} \sigma_{x}^{(j)} \rangle + \langle \sigma_{y}^{(i)} \sigma_{y}^{(j)} \rangle + \langle \sigma_{z}^{(i)} \sigma_{z}^{(j)} \rangle \leq 1$. For Eq. (2a) one first needs that for product states $(\Delta J_{\pi})^2 = N/4 - (1/4) \sum_i (\sigma_{x}^{(i)})^2$ holds, then the statement follows form the normalization of the Bloch vector. Concerning Eq. (2a), we have to show that $2 \mathcal{K} := (N - 1)(\Delta J_{\pi})^2 + N/2 - \langle J^2_{\pi}\rangle \geq 0$. Using the abbreviation $x_i = \langle \sigma_{x}^{(i)} \rangle$, etc. this can be written as $\mathcal{K} = (N - 1)[N/4 - (1/4) \sum_i x_i^2] - (1/4) \sum_{i,j \neq i} y_i y_j + z_i z_j = (N - 1)[N/4 - (1/4) \sum_i x_i^2] - (1/4)(\sum_i y_i^2 + \sum_i z_i^2) + (1/4) \sum_i (y_i^2 + z_i^2)$. 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 $\mathcal{K} \geq 0$. Eq. (2a) can then be proved in the same way.

\[\square\]

[21] Note, however, that the condition $[H, M_i] = 0$ is difficult to guarantee in realistic situations.
[25] Note also that the violation of Eq. (10) does not imply two-qubit entanglement in general. The following state violates Eq. (10), while it does not have two-qubit entanglement.
element: $\rho_{sq} \propto \exp(-H/T)$ for $H = 2J_z^2 - J_x$, $N = 8$, and $T = 0.3$. See also X. Wang and B.C. Sanders, Phys. Rev. A 68, 012101 (2003).