Spin squeezing inequalities and entanglement of $N$ qubit states

J. K. Korbiecz$^1$, J.I. Cirac$^2$, and M. Lewenstein$^{1,3,*}$

$^1$ Institut für Theoretische Physik, Universität Hannover, D-30167 Hannover, Germany
$^2$ Max-Planck Institut für Quantenoptik, Hans-Kopfermann Str. 1, D-85748, Garching, Germany and
$^3$ ICFO—Institut de Ciències Fotòniques, 08034 Barcelona, Spain

We derive spin squeezing inequalities that generalize the concept of the spin squeezing parameter and provide necessary and sufficient conditions for genuine 2-, or 3-qubit entanglement for symmetric states, and sufficient condition for general $N$-qubit states. Our inequalities have a clear physical interpretation as entanglement witnesses, can be easy measured, and are given by complex, but elementary expressions.

Recently, the area of quantum correlated systems of atoms or ions, and in particular mesoscopic ionic and macroscopic atomic ensembles has been developing very rapidly. Spin squeezing of, say few ions to $10^7$ atoms is nowadays routinely achieved in such systems. The standard tool to detect the generated forms of multipartite entanglement provides the, so called, spin squeezing parameter introduced in Ref. [4]. The spin squeezing parameter is particularly appreciated by experimentalists for the following reasons: i) it has a clear physical meaning, ii) it can be relatively easy measured, iii) it is defined by a simple operation expression, iv) it provides a figure of merit for atomic clocks. Moreover, as shown in [4], $\xi^2$ is directly connected to entanglement in atomic ensembles, providing a sufficient entanglement condition. However, one should stress that no further investigations to relate $\xi^2$ to other concepts of quantum information have been carried out so far.

In this Letter we generalize and connect the concept of spin squeezing parameters to the theory of entanglement witnesses, i.e. such observables $W$ that have non-negative averages for all separable states and there exists an entangled state $\varrho$ such that $\text{tr}(\varrho W) < 0$. In order to derive the generalized spin squeezing inequalities, we express state averages of the appropriate entanglement witnesses in terms of the macroscopic spin operators:

$$J_i = \sum_{a=1}^{N} \frac{1}{2} \sigma_a^i, \quad i = 1, 2, 3,$$

where $J_n = n \cdot J$.

In the proposed approach we begin with considering symmetric states of $N$ qubits first, i.e. states $\varrho$ supported on the symmetrized product of individual qubit spaces $\mathcal{H}_n = \text{Sym}(\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2)$ (Sym denotes symmetrization). We then use the fact that for symmetric states of 2, and 3 qubits separability is equivalent to positivity of the, so called, partial transpose of a state $\varrho$ (PPT condition $\Box$). From that we derive the complete families of generalized spin squeezing inequalities, which provide necessary and sufficient conditions for genuine 2-, or 3-qubit entanglement for symmetric states; at the same time they provide a sufficient condition for general states of $N$ qubits. Our results imply that spin squeezing leads to the genuine 2-qubit entanglement (i.e. the corresponding reduced two-qubit density matrices are entangled) $\Box$. For symmetric states the converse is also true: 2-qubit entangled states show a specific type of spin squeezing. In addition, we obtain somewhat simpler necessary conditions for the 3-qubit case, that lead to entanglement not implied by the standard spin squeezing.

The proposed novel inequalities, similarly as the squeezing parameter, i) have a clear physical meaning in terms of generalized squeezing and entanglement conditions, ii) can be relatively easy measured, and iii) are given by complex, but elementary expressions.

The simplest form of entanglement that a multiqubit state $\varrho$ can possess is a 2-qubit entanglement: $\varrho$ is 2-qubit entangled if for some qubits $a$ and $b$ the reduced density matrix

$$\varrho_{ab} = \text{tr}_{1..a..b..N} \varrho$$

is entangled (the hats over indices mean that those indices are omitted). Let us first consider symmetric states. Then all the reductions $\varrho_{ab}$ are of the same form and act in a symmetric subspace of $\mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$ - the space of qubits $a$ and $b$. The PPT criterion $\Box$ implies that $\varrho_{ab}$ is entangled iff there exists a vector $\psi$ such that

$$\text{tr}_{ab}(\varrho_{ab} \psi \langle \psi | T^1) < 0,$$

where transpose is defined w.r.t. the standard basis $|0\rangle, |1\rangle$. As $\psi$ we can take any eigenvector of $\varrho_{ab}$, corresponding to a negative eigenvalue.

From the explicit form of $\varrho_{ab}$ we deduce that $|\psi\rangle$ can be parametrized as follows $\Box$: $|\psi\rangle = \eta |00\rangle + \beta |01\rangle + \beta^* |10\rangle + \gamma |11\rangle$, with $\alpha, \gamma \in \mathbb{R}$. Hence the coefficients of $|\psi\rangle$ form a hermitean matrix: $[\psi_{CD}]_{C,D=0,1,1}$.

We can diagonalize it: $\psi_{CD} = U_{AC} \Delta_{AB} \psi_{BD}$, where $\Delta = \text{diag}(\sin^2 \alpha, \pm \cos^2 \alpha)$, $-\pi \leq \alpha \leq \pi$, $U \in SU(2)$, and then define $U = \sum_{C,D=0,1} U_{CD} |D\rangle \langle C|$ to finally obtain
the following parametrization:
\[
|\psi\rangle = U^* \otimes U|\psi_0\rangle , \quad |\psi_0\rangle = \sin \frac{\theta}{2}|00\rangle + \cos \frac{\theta}{2}|11\rangle ,
\]
(we have fixed the overall phase). Substituting 4 into 3 leads to the condition:
\[
\text{tr}_{ab}(g_{ab} U \otimes U |\psi_0\rangle \langle \psi_0| T_1 U^\dagger U^\dagger) < 0 .
\]
(6)

Note, that $|\psi_0\rangle \langle \psi_0| T_1$ can be decomposed into Pauli matrices:
\[
|\psi_0\rangle \langle \psi_0| T_1 = \frac{1}{2} \sin^2 \frac{\theta}{2} (1 + \sigma^z) \otimes (1 + \sigma^z)
+ \frac{1}{2} \cos^2 \frac{\theta}{2} (1 - \sigma^z) \otimes (1 - \sigma^z)
+ \frac{1}{4} \sin \theta (\sigma^x \otimes \sigma^x + \sigma^y \otimes \sigma^y),
\]
and the adjoint action of $SU(2)$ in 6 induces a $SO(3)$ rotation $R$ of $\sigma^z$: $U \sigma^z U^\dagger = R \sigma^z R^\dagger$, (here and throughout we sum over repeated indices). We will denote the axes of the rotated frame by $k, l, n$.

Using 7 we can express the inequality 6 through the following parametrization:
\[
\theta_{abc} = \text{tr}_{1,\ldots,6} \otimes \otimes |\psi\rangle \langle \psi| T_1
\]
(11)
is 3-party entangled. If we again consider symmetric states first, then PPT criterion is still necessary and sufficient for separability, since Sym($C^2 \otimes C^2 \otimes C^2$) is a subspace of $C^2 \otimes C^3 \otimes C^3$. Thus we can proceed as before.

A vector $|\psi\rangle$, corresponding to any negative eigenvalue of $\theta_{abc}$ must be necessarily a 3-party entangled vector from Sym($C^2 \otimes C^2 \otimes C^2$). The parametrization of such vectors was found in Ref. [13]; there are two families:
\[
|\psi\rangle = A \otimes B \otimes \otimes GHZ (12)
\]
(12)
\[
|\psi\rangle = A \otimes U \otimes U |W\rangle,
\]
(13)
where matrices $A, B \in SL(2, \mathbb{C})$, $U \in SU(2)$, and |GHZ$ = (1/\sqrt{2})|(000) + |111\rangle$, |$W$ = (1/\sqrt{3})|(001) + |010\rangle + |100\rangle). The action of $SL(2, \mathbb{C})$ on the Pauli matrices in the decomposition of $|\psi\rangle \langle \psi| T_1$ now induces restrictions, i.e. orientation and time-orientation preserving, Lorenz transformations:
\[
A^* \sigma^\mu A = \Lambda^\mu_\nu \sigma^\nu , \quad B \sigma^\mu B^\dagger = \Lambda^\mu_\nu \sigma^\nu , \quad \sigma^0 = 1,
\]
(14)
(Greek indices run through $0 \ldots 4$). Hence we obtain the following inequality, analogous to 10:
\[
\text{tr}_{abc}(g_{abc} |\psi\rangle \langle \psi| T_1) = \frac{1}{8} K_{\alpha\beta\gamma} \langle \sigma^\alpha_0 \otimes \sigma^\beta_0 \otimes \sigma^\gamma_0 \rangle < 0 ,
\]
(15)
where
\[
K_{\alpha\beta\gamma}(A, L, L, L) = \Lambda^0_\alpha \lambda^0_\beta \rho^0_\gamma + \Lambda^0_\alpha \lambda^3_\beta \rho^3_\gamma + \Lambda^3_\alpha \lambda^0_\beta \rho^3_\gamma + 2 \lambda^3_\alpha \rho^0_\beta \rho^3_\gamma - \lambda^0_\alpha \lambda^0_\beta \lambda^3_\gamma + 2 \lambda^3_\alpha \lambda^0_\beta \lambda^3_\gamma,
\]
(16)
for the GHZ family [12], or
\[
K_{\alpha\beta\gamma}(A, R, R, R) = \frac{1}{4} \left\{ \Lambda^0_\alpha \Lambda^0_\beta \rho^0_\gamma - \Lambda^3_\alpha \Lambda^3_\beta \rho^3_\gamma + 2 \Lambda^3_\alpha \Lambda^0_\beta \rho^3_\gamma + 4 \Lambda^1_\alpha \Lambda^0_\beta \rho^3_\gamma + 4 \Lambda^1_\alpha \Lambda^1_\beta \rho^3_\gamma - 4 \Lambda^2_\alpha \Lambda^0_\beta \rho^3_\gamma - 4 \Lambda^2_\alpha \Lambda^1_\beta \rho^3_\gamma \right\},
\]
(17)
for the W family [13]. Here $R^\mu_\nu$ is the four-dimensional embedding of the rotation generated by $U$ from 13 and round brackets denote symmetrization.
In order to express the inequality \([15]\) through \(g\)-averages of the spin operators \([11]\), we introduce an artificial time-component \(J^0 = (N/2)\mathbf{1}\). The operators \(J^I = (J^0, J^I)\) do not constitute relativistic generalization of the operators \(J^I\) and we introduce them just for notational reasons. Since \(g_{abc}\) is symmetric, the indices \(\alpha, \beta, \gamma\) in \([15]\) can be symmetrized. Then after summation \([15]\), over all triples of qubits \(\sum_{abc} = \sum_{a=1}^{N-2} \sum_{b=a+1}^{N-1} \sum_{c=b+1}^{N}\), we can use the identity:

\[
3 \sum_{abc} \sigma^a_\alpha \otimes \sigma^b_\beta \otimes \sigma^c_\gamma = 4 \langle J^\alpha J^\beta J^\gamma \rangle - 6 f^{(\alpha \beta \gamma)} \mu J^\mu,
\]

where \(f^{(\alpha \beta \gamma)} \mu = f^{(0 \beta \gamma)} \mu = \delta^{\alpha \beta} \delta^{\gamma \mu} = 1 \sum_i \epsilon^{ijl} \delta^{\alpha \gamma} + \delta^{ij} \delta^{\alpha \mu}\), to finally obtain:

**Criterion for tripartite entanglement.** A symmetric state \(\varrho\) possesses a genuine tripartite entanglement iff there exist two restricted Lorenz transformations \(\Lambda, L\), or a restricted Lorenz transformation \(\Lambda\) and a rotation \(R\), such that:

\[
K_{(\alpha \beta \gamma)} \left( 2 \langle J^\alpha J^\beta J^\gamma \rangle - 3 f^{(\alpha \beta \gamma)} \mu J^\mu \right) + f^{(\alpha \beta \gamma)} \mu J^\mu < 0
\]

holds, with \(K_{(\alpha \beta \gamma)}\) given by \([16]\), or by \([17]\) respectively.

The above criterion serves also as a sufficient condition for tripartite entanglement of a general state \(\varrho\), with the modification that \(K(\Lambda, L, L)\) or \((\Lambda, R, L)\) in \([18]\) have to be substituted with \(1/3 K(\Lambda, L, L) + K(L, L, L) + K(L, L, L)\) or \(1/3 K(\Lambda, R, L) + K(R, L, L) + K(L, R, L)\) respectively to achieve the index symmetrization.

The search for matrices \(\Lambda, L\) can be difficult due to non-compactness of the restricted Lorenz group. It is therefore desirable to develop some simpler conditions as well. For mesoscopic systems with not too large \(N\) we may do so, using some specific witnesses that detect genuine GHZ-type, or genuine W-type entanglement, found in Ref. \([14]\):

\[
\mathcal{W}_{\text{GHZ}} = \frac{1}{4} \mathbf{1} - |GHZ\rangle \langle GHZ| \quad (20)
\]

\[
\mathcal{W}_W = \frac{3}{4} \mathbf{1} - |W\rangle \langle W| \quad (21)
\]

\[
\mathcal{W}_W = \frac{1}{4} \mathbf{1} - |GHZ\rangle \langle GHZ|, \quad (22)
\]

where, in order to be more general, we may now define the vectors \(|GHZ\rangle\) and \(|W\rangle\) in an arbitrary frame \(k, l, n\), rotated w.r.t. the original one. The witnesses \(\mathcal{W}_{\text{GHZ}}\) detects states of GHZ class which are neither of the W class, nor biseparable. Finally, the witnesses \(\mathcal{W}_W\) and \(\mathcal{W}_W\) detect states of GHZ- or W-class, which are not biseparable \([14]\). Proceeding as before and using the same witnesses \([20]-[22]\) for all tripartite reductions \(g_{abc}\) of a general state \(\varrho\), we get necessary conditions for:

**GHZ-type entanglement.** If for a state \(\varrho\) there exist orthogonal directions \(k, l, n\) such that the following inequality is fulfilled:

\[
-\frac{1}{3} \langle J^3_k \rangle + \langle J_l J_k J_l \rangle - \frac{N-2}{24} \langle J^2_n \rangle + \frac{1}{2} \langle J_k \rangle
\]

then the state \(\varrho\) possesses a genuine GHZ-type entanglement.

**W-type entanglement.** If for a state \(\varrho\) there exist orthogonal directions \(k, l, n\) such that one of the following inequalities is fulfilled:

\[
\langle J^2_n \rangle - 2 \langle J_l J_n J_l \rangle - 2 \langle J_k J_n J_k \rangle
\]

\[
- \frac{N-2}{24} \langle J^2_n \rangle - \frac{1}{2} \langle J^3_k \rangle + \langle J_l J_n J_l \rangle - \frac{N-2}{2} \langle J^2_n \rangle + \frac{1}{2} \langle J_k \rangle
\]

then the state \(\varrho\) possesses a genuine 3-qubit (GHZ- or W-type) entanglement.

The above spin squeezing criteria \([10], [11], [23]-[26]\) constitute the main result of this Letter. The inequalities \([24]\) and \([25]\) can be further simplified if we choose the directions \(k, \alpha, \beta\) such that \(\langle J^\alpha \rangle = \langle J^\beta \rangle = 0\). Let us further assume that \(\langle J^\alpha \rangle \geq N/4, \langle J^\beta \rangle \geq N/4\), so that there is no spin-squeezing in the sense of the definition \([2]\). Then from criteria \([24], [25]\) it follows, that if:

\[
- \frac{1}{3} \langle J^3_k \rangle + \langle J_l J_k J_l \rangle + \frac{N(N-1)(N+8)}{24} < 0 \quad (26)
\]

or

\[
- \frac{1}{3} \langle J^3_k \rangle + \langle J_l J_k J_l \rangle + \frac{N(N-1)(N-2)}{8} < 0 \quad (27)
\]

holds, then the state \(\varrho\) possesses a genuine GHZ or 3-qubit entanglement respectively. Thus, in this specific situation, the inequalities \([26]\) and \([27]\) detect a different type of entanglement than that implied by the standard spin squeezing \([3, 4]\).

Generalization of the above procedure to study the entanglement between more qubits is straightforward - one uses inequalities of the type \(\text{tr}(\varrho N) < 0\) with approprate witnesses \(W\). However, for the case of four or more qubits the PPT criterion is no longer sufficient and only necessary conditions of the type \([28]-[31]\) can be obtained.

Let us conclude with a general remark concerning full (i.e. N-qubit) separability of a symmetric state and a connection to the method of Ref. \([12]\). Every symmetric state \(\varrho\) of \(N\)-qubits admits an analog of Glauber-Sudarshan \(F\)-representation \([16, 17]\):

\[
\varrho = \int_{S^2} d\Omega P(\theta, \phi) |\theta, \phi\rangle \langle \theta, \phi| \otimes \cdots \otimes |\theta, \phi\rangle \langle \theta, \phi|,
\]

where \(d\Omega = \sin \theta d\theta d\phi\) is the volume element on the Bloch sphere, and \(|\theta, \phi\rangle = \cos(\frac{\theta}{2}) |0\rangle + e^{i\phi} \sin(\frac{\theta}{2}) |1\rangle\) is a spin
coherent state of a single qubit. Note that every qubit is representable in this form. The representation is not unique, as in the decomposition of $P(\theta, \phi)$ over spherical harmonics $Y_{lm}$, $\varrho$ determines only terms with $l \leq N$, and hence $P(\theta, \phi)$ can be chosen to be a polynomial in the Cartesian coordinates on the sphere. Now the following fact holds [15, 16]:

A symmetric state $\varrho$ is fully separable iff there exists a representation $\mathcal{S}$ where $P(\theta, \phi)d\Omega$ is an element of a probabilistic measure on $S^2$.

Proof. Implication $\Rightarrow$ is obvious as the integral in $\mathcal{S}$ is a norm limit of separable states. To prove the implication $\Rightarrow$, observe that if $\varrho$ is separable, then it can be decomposed as $\varrho = \sum_k p_k |\theta_k, \phi_k\rangle \langle \theta_k, \phi_k| \otimes \cdots \otimes |\theta_k, \phi_k\rangle \langle \theta_k, \phi_k|$, where $p_k \geq 0$, $\sum p_k = 1$, as vectors of the form $|\theta_k, \phi_k\rangle \langle \theta_k, \phi_k| \otimes \cdots \otimes |\theta_k, \phi_k\rangle \langle \theta_k, \phi_k|$ are the only symmetric product vectors. We define then $P(\theta, \phi) = \sum_k p_k (\cos \theta - \cos \theta_k) (\delta(\phi - \phi_k)$; the expansion of $\delta$'s over $Y_{lm}$ can be truncated at $l = N$ □.

We observe that if $W$ is an entanglement witness, then:

$$\text{tr}(\varrho W) = \int d\Omega P(\theta, \phi) w(\theta, \phi)$$

(29)

where $w(\theta, \phi) = \langle (\theta, \phi)^{\otimes N} | W | (\theta, \phi)^{\otimes N} \rangle$ is a positive semidefinite polynomial of the $N$th order in the Cartesian coordinates. Hence, the criteria [9] and [19], with the reversed inequality signs, can be interpreted as necessary and sufficient conditions for $P(\theta, \phi)d\Omega$ to be an element of a probabilistic measure for $N = 2, 3$ respectively.

The above fact establishes an interesting link between separability of symmetric states and the problem of description of classical states of a 1D harmonic oscillator [15, 20]. In the latter problem, classical states are in one-to-one correspondence with probabilistic measures on $\mathbb{R}^2$. We have proved in [15] that, among some specific subclass of states, the classical ones are detected by observables, arising from positive semidefinite (psd) polynomials which are sums of squares of other polynomials.

Summarizing, we have introduced a method of deriving generalized spin squeezing inequalities, that characterize genuine $N$-qubit entanglement. The results of the paper provide connection of spin squeezing to entanglement witnesses, and an alternative physical meaning to spin squeezing as qualitative and quantitative characterization of the $N$-qubit entanglement. The inequalities can be directly measured and provide novel entanglement detection tools for macroscopic atomic ensembles.

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