

Singlet fraction is an entanglement witness in partially polarized ensembles

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We establish a sufficient and tight condition for bipartite entanglement in an arbitrary system of qubits, namely $p_s > (1 - m^2)/2$ where p_s is the singlet fraction and m is the magnetization of the state, by deriving an explicit expression for the lower bound of its concurrence as well as through geometric arguments. This entanglement witness can be used to investigate the possible existence of pairwise quantum spin correlations in partially polarized ensembles of ultracold atoms.

I. INTRODUCTION

The nature of spin correlations has been explored in several recent experiments with cold atoms [1–7]. Such ensembles do not lend themselves to a full tomography. Instead, spin correlations between atom pairs can be studied through macroscopic measurements that probe averaged pairwise interactions between atoms of the ensemble. For example, swap gates and formation of alkali dimers provide access to the singlet fraction in balanced spin ensembles [6–8]. The singlet fraction also plays a key role in the physics of fermions with s-wave interactions. Though there already exists a bound on the singlet fraction for pairwise entanglement in unpolarized ensembles, i.e. a singlet fraction larger than half [9, 10], this has not yet been extended to partially polarized ensembles.

In the case of single bipartite qubit systems, such as polarized photon pairs, direct measurement of the concurrence or quantum tomography is achievable [11, 12]. Despite this, it is desirable to have a simple entanglement witness in order to reduce the number of measurements required to detect entanglement. Indeed, many such witnesses involve the singlet fraction of the qubit pair [13]. However, these witnesses do not hold for all classes of states [14, 15], or can be improved upon by including the degree of polarization of the state [16].

Here we establish a bound on the singlet fraction of a general two-body mixed state that is a sufficient and tight condition for its entanglement, namely

$$p_s > \frac{1 - m^2}{2} \quad (1)$$

where p_s is the singlet fraction and m is the magnetization. This result, which henceforth we refer to as the “singlet bound”, makes no assumptions on the initial state and therefore is a condition for bipartite entanglement of any qubit system. For the sake of consistency, we adopt a notation that suits the discussion of spin ensembles (e.g. spin state of an atom instead of polarization state of a photon), where the qubit system of interest is the reduced density matrix describing the spin state of pairs in the ensemble.

The paper is organized as follows: in Sec. II, we introduce some notation and describe the physical limit on the

singlet fraction of a general two-body mixed state with magnetization, while in Sec. III, we derive a lower bound for the concurrence of this general state from which we can obtain the singlet bound. In Sec. IV we provide an intuitive derivation of the singlet bound based on geometric arguments. Finally in Sec. V, we summarize and discuss implications of the result.

II. DEFINITIONS AND PHYSICAL LIMIT

The spin state of pairs in a spin-1/2 ensemble can be described using the antisymmetric singlet state $|s_0\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ and the symmetric triplet states $|t_0\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$, $|t_1\rangle = |\uparrow\uparrow\rangle$, $|t_{-1}\rangle = |\downarrow\downarrow\rangle$. These form an orthonormal set of basis states with well defined angular momentum quantum numbers $|S, S_z\rangle$. A general mixed state can be written in this basis using the notation

$$\begin{aligned} \rho^{AB} = & p_s |s_0\rangle \langle s_0| + \sum_{i \in \{0, \pm 1\}} (q_i |s_0\rangle \langle t_i| + q_i^* |t_i\rangle \langle s_0|) \\ & + \sum_{i, j \in \{0, \pm 1\}} (p_{ij} |t_i\rangle \langle t_j|) \end{aligned} \quad (2)$$

where the populations are normalized, i.e. $\text{Tr}[\rho^{AB}] = 1$. The total spin operator is $\vec{S} = (\hat{\sigma}^A + \hat{\sigma}^B)/2$ where e.g. $\hat{\sigma}^A = (\sigma_x, \sigma_y, \sigma_z)^A$ are the Pauli spin operators applied on the reduced state A, which is obtained by tracing over state B, i.e. $\rho_A = \text{Tr}_B \rho^{AB}$. Then the magnetization $\vec{m} = (m_x, m_y, m_z)$ is defined as

$$\vec{m} = \langle \vec{S} \rangle = \text{Tr}[\vec{S} \rho^{AB}]. \quad (3)$$

In particular, using the fact that $S_z |s_0\rangle = S_z |t_0\rangle = 0$, we can obtain a general expression for the z component of the magnetization:

$$m_z = \text{Tr}[S_z \rho^{AB}] = p_{11} - p_{-1-1}. \quad (4)$$

Since the populations of Eq. 2 must sum to unity for a normalized probability, the singlet fraction is thus bounded by the relation $p_s \leq 1 - |m_z| - p_{00}$. By definition we have $|m_z| \leq m$ (using the notation $|\vec{m}| = m$),

and so we establish a physical limit on the largest singlet fraction for an arbitrary magnetization:

$$p_s \leq 1 - m. \quad (5)$$

III. CONCURRENCE

When the concurrence associated with a two-body density matrix is positive, i.e. $C(\rho^{AB}) > 0$, the state ρ^{AB} is entangled [17]. The state in Eq. 2 has 15 degrees of freedom. In order to more easily bound its concurrence, we first apply a transformation that decreases its number of degrees of freedom without increasing its entanglement. Using the unitary rotation operator about the z axis $U_z(\theta) = U_z^A(\theta) \otimes U_z^B(\theta)$ where $\theta \in [0, 2\pi)$, we define the “spun state” as

$$\langle \rho^{AB} \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta U_z^\dagger(\theta) \rho^{AB} U_z(\theta) \quad (6)$$

which is the mixed state ρ^{AB} after uniform rotation about the z axis. This transformation eliminates coherences between states in Eq. 2 with different angular momentum quantum number S_z . This can be understood by recalling that S_z is the generator of rotation i.e. $U_z(\theta) = e^{i\theta S_z}$, and also that $U_z^\dagger(\theta) = U_z(-\theta)$. Thus

$$\langle \rho^{AB} \rangle \rightarrow \frac{1}{2} \begin{pmatrix} b + m_z & 0 & 0 & 0 \\ 0 & a + p_s + 2c \cos \phi & a - p_s - i2c \cos \phi & 0 \\ 0 & a - p_s + i2c \cos \phi & a + p_s - 2c \cos \phi & 0 \\ 0 & 0 & 0 & b - m_z \end{pmatrix}. \quad (9)$$

Using the “spin-flipped” state $\langle \tilde{\rho}^{AB} \rangle = (\sigma_y \otimes \sigma_y) \langle \rho^{AB} \rangle^* (\sigma_y \otimes \sigma_y)$, we compute the eigenvalues of the

$$\lambda_{1,2} = \frac{\sqrt{a^2 + p_s^2 - 2c^2 \cos 2\phi \pm \sqrt{(a^2 + p_s^2 - 2c^2 \cos 2\phi)^2 - 4(c^2 - ap_s)^2}}}{\sqrt{2}}$$

$$\lambda_3 = \lambda_4 = \frac{\sqrt{b^2 - m_z^2}}{2}.$$

By majoritizing these eigenvalues, we obtain the concurrence:

the spinning operation in Eq. 6 acts trivially on the populations and the coherence between $|s_0\rangle$ and $|t_0\rangle$ (i.e. the q_0 term), while all other coherences are given a non-trivial θ dependence, namely $e^{in\theta}$ with $n \neq 0$, and hence the spinning causes these terms to vanish. After spinning, the general two-body density matrix is

$$\langle \rho^{AB} \rangle = p_s |s_0\rangle \langle s_0| + q_0 |s_0\rangle \langle t_0| + q_0^* |t_0\rangle \langle s_0| + \sum_{i \in \{0, \pm 1\}} (p_{ii} |t_i\rangle \langle t_i|) \quad (7)$$

and has only 6 degrees of freedom. Crucially, because rotation can be implemented using local operation and classical communication (LOCC), the spun state is at most as entangled as the unspun state i.e. $C(\rho^{AB}) \geq C(\langle \rho^{AB} \rangle)$ [18].

We can now explicitly compute the concurrence of the spun state. First we rewrite the spun state in a more suitable notation using the magnetization m_z ,

$$\langle \rho^{AB} \rangle = p_s |s_0\rangle \langle s_0| + a |t_0\rangle \langle t_0| + ce^{i\phi} |s_0\rangle \langle t_0| + ce^{-i\phi} |t_0\rangle \langle s_0| + \frac{b + m_z}{2} |t_1\rangle \langle t_1| + \frac{b - m_z}{2} |t_{-1}\rangle \langle t_{-1}|, \quad (8)$$

where the normalized populations are $p_s + a + b = 1$ and the coherence is $c = \eta \sqrt{ap_s}$ with $\eta \in [0, 1]$. Then we write this state in the standard basis $\{|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle\}$, which in matrix form yields

matrix $R = \sqrt{\sqrt{\langle \rho^{AB} \rangle} \langle \tilde{\rho}^{AB} \rangle \sqrt{\langle \rho^{AB} \rangle}}$, which are equal to the square root of the eigenvalues of the matrix $\langle \rho^{AB} \rangle \langle \tilde{\rho}^{AB} \rangle$ [17], namely

rence:

$$C(\langle \rho^{AB} \rangle) = \max[0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4] = \max[0, \sqrt{(p_s - a)^2 + 4c^2 \sin^2 \phi} - \sqrt{b^2 - m_z^2}], \quad (10)$$

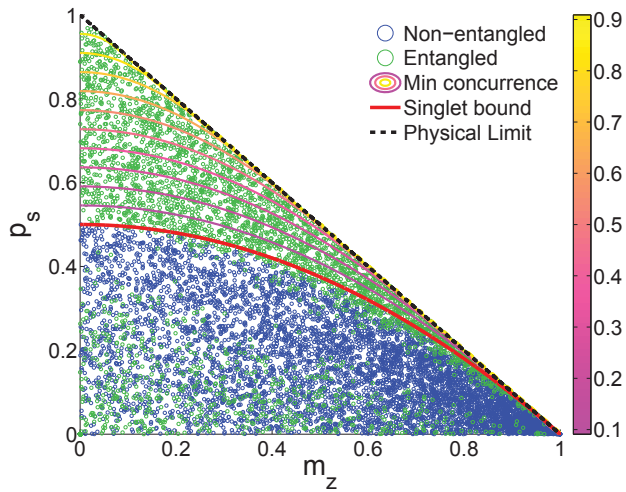


FIG. 1. Each circle in singlet fraction p_s vs. magnetization m_z space is one of 10,000 randomly generated spin mixed states $\langle \rho^{AB} \rangle$ described by Eq. 7. Blue (darker) circles have $C(\langle \rho^{AB} \rangle) = 0$ and are not entangled while green (lighter) circles have $C(\langle \rho^{AB} \rangle) > 0$ and are entangled. Note that there are blue circles immediately beneath the singlet bound while there are none above, effectively demonstrating that the bound is a tight and sufficient condition for entanglement. Contour lines are described by Eq. 13 and give the minimum concurrence of the general state in Eq. 2.

which is positive when

$$p_s > \frac{1}{2} \left(\frac{1 - 2a - m_z^2}{1 - 2a + 2a\eta^2 \sin^2 \phi} \right). \quad (11)$$

Eqn. 11 provides a general bound on the singlet fraction for the entanglement of a magnetized state with triplet population a and coherence c . However in order to ensure entanglement for all choices of $\{a, \eta, \phi\}$, we consider the worst case where $a = 0$, which yields a sufficient condition for entanglement:

$$p_s > \sup_{a, \eta, \phi} \left[\frac{1}{2} \frac{1 - 2a - m_z^2}{1 - 2a + 2a\eta^2 \sin^2 \phi} \right] = \frac{1 - m_z^2}{2}. \quad (12)$$

Note that we can choose our coordinate system such that $m_z^2 = m^2$. Furthermore Eq. 12 is a tight condition for entanglement as there exists a class of non-entangled states (i.e. with zero concurrence) immediately below the bound, which is the class of spun states with $a = 0$ and $p_s = (1 - m_z^2)/2$. To be more precise, if the magnetization is measured only along a specific direction n that is not aligned with the magnetization vector (i.e. the z direction), then the bound is sufficient as $|m_n| < |m|$, but is no longer tight.

We verify that the singlet bound is a tight and sufficient condition for entanglement by numerically generating many random mixed states that span the p_s and m_z space, and computing their concurrence. Each circle in Fig. 1 corresponds to one of 10,000 random spun

mixed states. As expected, the physical limit in Eq. 5 is satisfied. The blue circles have $C(\langle \rho^{AB} \rangle) = 0$ and are not entangled while green circles have $C(\langle \rho^{AB} \rangle) > 0$ and are entangled. Because the spinning transformation can be implemented with LOCC, it is true that $C(\rho^{AB}) \geq C(\langle \rho^{AB} \rangle)$. Thus the absence of non-entangled states above the singlet bound demonstrates that the bound is a sufficient condition for entanglement of ρ^{AB} , while the existence of non-entangled states immediately beneath the bound demonstrates the tightness of the bound. Note that there are entangled states well below the singlet bound as it is not a necessary condition for entanglement.

Furthermore, we can use the fact that the minimum of Eq. 10 occurs when $a = 0$ along with the constraint of a normalized probability, $p_s + b = 1$, to generalize the singlet bound to a tight and sufficient condition for having positive concurrence $C(\rho^{AB})$, namely

$$p_s > \frac{1 - C(\rho^{AB})^2 - m_z^2}{2(1 - C(\rho^{AB}))} \quad (13)$$

where we used the fact that $\min[C(\rho^{AB})] = \min[C(\langle \rho^{AB} \rangle)]$. In other words, Eq. 13 describes the minimum concurrence of a state with p_s and m_z , the contour lines of which are shown in Fig. 1.

We note that this result improves upon the concurrence bound provided in Ref. [16], which yields the sufficient condition $p_s \geq \frac{1}{3}(1 + \sqrt{1 + 3C^2})$ when applied to Eq. 8 with $a = 0$.

IV. VECTORIAL ARGUMENT

Here we provide a more intuitive derivation of the singlet bound based on geometric arguments. The state of a spin-1/2 system can be represented on the Bloch sphere using the relation

$$\rho = I/2 + \vec{v} \cdot \hat{\sigma}/2 \quad (14)$$

where I is the identity operator and \vec{v} is the Bloch vector [19]. Starting from the definition of the magnetization given in Eq. 3, it follows that the magnetization of the two-body state is related to the sum of the individual Bloch vectors: $\vec{m} = \frac{1}{2}\vec{v}_A + \frac{1}{2}\vec{v}_B$, i.e. an equally weighted sum in Bloch space. Squaring this expression yields

$$\begin{aligned} m^2 &= \frac{1}{4}(v_A^2 + v_B^2 + 2\vec{v}_A \cdot \vec{v}_B) \\ &= \frac{1}{4}(v_A^2 + v_B^2 + 2v_A v_B \cos \beta) \end{aligned} \quad (15)$$

where β is the angle between the two Bloch vectors.

First consider the case of a separable two-body state $\rho^{AB} = \rho^A \otimes \rho^B$ where ρ^A and ρ^B are pure (we will later generalize to the case where these states are mixed). We are free to choose the coordinate system, thus we can align ρ^A along the z axis such that $\rho^A = |\uparrow\rangle\langle\uparrow|$ while ρ^B

is arbitrary, so $\rho^B = |\psi\rangle\langle\psi|$ where $|\psi\rangle = c_\uparrow|\uparrow\rangle + c_\downarrow|\downarrow\rangle$. Then the two-body state is

$$\rho^{AB} = \rho^A \otimes \rho^B = \sum_{i,j \in \{\uparrow, \downarrow\}} c_{ij} |\uparrow_A i_B\rangle \langle \uparrow_A j_B| \quad (16)$$

whose singlet fraction is $p_s = \text{Tr}[\rho^{AB} |s_0\rangle\langle s_0|] = c_{\downarrow\downarrow}/2$ since the only non-zero term in the singlet projector is $|\uparrow_A \downarrow_B\rangle \langle \uparrow_A \downarrow_B|/2$ (state ρ^A has no spin \downarrow component). The singlet fraction is uniquely determined by β :

$$p_s = \frac{1}{4}(1 - \cos\beta) = \frac{1}{4}(1 - \vec{v}_A \cdot \vec{v}_B). \quad (17)$$

Since both ρ^A and ρ^B are pure states, then $v_A = v_B = 1$, and so Eq. 15 reduces to

$$m^2 = \frac{1}{2}(1 + \vec{v}_A \cdot \vec{v}_B) = \frac{1}{2}(1 + \cos\beta). \quad (18)$$

Using $\cos\beta = 2m^2 - 1$ from this result along with Eq. 17, we obtain the critical singlet fraction

$$p_s^* = \frac{1 - m^2}{2} \quad (19)$$

which is the boundary of a non-entangled state as derived in Sec. III.

Next consider the case of a separable state $\rho^{AB} = \rho^A \otimes \rho^B$ where ρ^A and ρ^B are mixed. We can still choose the coordinate system such that ρ^A is aligned along z : $\rho^A = p_{\uparrow A}|\uparrow\rangle\langle\uparrow| + p_{\downarrow A}|\downarrow\rangle\langle\downarrow|$. The state ρ^B remains arbitrary therefore $\rho^B = \sum_{ij} c_{ij} |i\rangle\langle i|$ where $i, j \in \{\uparrow, \downarrow\}$. Computing the singlet projector yields

$$\begin{aligned} p_s &= \frac{p_{\uparrow A} c_{\downarrow B}}{2} + \frac{p_{\downarrow A} c_{\uparrow B}}{2} \\ &= \frac{1}{4}(1 - v_A v_B \cos\beta) = \frac{1}{4}(1 - \vec{v}_A \cdot \vec{v}_B). \end{aligned} \quad (20)$$

Using Eq. 15 we arrive at

$$p_s = \frac{1}{2} \left(1 - m^2 + \frac{1}{4}(v_A^2 - 1 + v_B^2 - 1) \right) \leq p_s^*, \quad (21)$$

where the inequality holds because $|v_A| < 1$ and $|v_B| < 1$.

Finally, we generalize this result to all classes of possible non-entangled states by considering a mixture of such states i.e. $\rho^{AB} = \sum_i P_i \rho_i^{AB}$ where P_i is the probability of $\rho_i^{AB} = \rho_i^A \otimes \rho_i^B$. The singlet fraction p_{si} of each ρ_i^{AB} is still bounded by Eq. 21, thus

$$\bar{p}_s = \sum_i P_i p_{si} \leq \frac{1 - \sum_i P_i m_i^2}{2} = \frac{1 - \bar{m}^2}{2} \quad (22)$$

since $\bar{m}^2 = \sum_i P_i m_i^2$. Hence if the two-body state is non-entangled i.e. $\rho^{AB} = \sum_i P_i \rho_i^A \otimes \rho_i^B$, then the inequality in Eq. 22 holds. The contrapositive is also true: If $p_s > (1 - \bar{m}^2)/2$, then ρ^{AB} is entangled.

V. CONCLUSION AND OUTLOOK

In summary, we derived a sufficient and tight condition for entanglement of a general two-body mixed state using the magnetization and singlet fraction of the state, namely $p_s > (1 - m^2)/2$. This is generalized to a similar condition for having positive concurrence $C(\rho^{AB})$ in Eq. 13.

Equivalently, an entanglement witness $W[\rho^{AB}]$ can be constructed:

$$W[\rho^{AB}] = \langle s_0 | \rho^{AB} | s_0 \rangle - \frac{1}{2} + \frac{|\text{Tr}[\vec{S}\rho^{AB}]|^2}{2}. \quad (23)$$

If $W[\rho^{AB}] > 0$, then entanglement is required to explain the spin correlations in the ensemble. If $W[\rho^{AB}] \leq 0$, then there exists a non-entangled state that has the same observed p_s and m . The witness detects bipartite entanglement in an arbitrary system of qubits, where the physical meaning of the magnetization depends on the internal degree of freedom of the system. For example, in the case of polarization entanglement between a photon pair, magnetization is replaced by the degree of polarization.

The witness is derived by first reducing the number of degrees of freedom (without increasing entanglement) of the general two-body density matrix using the ‘‘spinning’’ transformation in Eq. 6, after which we can explicitly compute its concurrence. This approach might be useful to derive witnesses for higher-dimensional qubit systems. For example, the 63 degrees of freedom in a three-body density matrix can be reduced to a block-diagonal matrix with 12 degrees of freedom by spinning along both x and z . However this would require the use of an entanglement measure for higher-than-bipartite systems [20, 21].

We note that there exist ‘‘spin-squeezing’’ type bounds for entanglement of N -qubit states which have the benefit of needing only collective spin and angular momentum measurements, but these types of bounds do not completely characterize all separable states [22–24]. Hence, our entanglement witness is a new tool that can be used to detect pairwise quantum correlations in partially polarized ensembles.

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