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Entanglement measure for rank-2 mixed states

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We provide an easily computable formula for a bipartite mixed-state entanglement measure. Our formula can be applied to readily calculate the entanglement for any rank-2 mixed state of a bipartite system. We use this formula to provide a tight upper bound for the entanglement of formation for rank-2 states of a qubit and a qudit. We also outline situations where our formula could be applied to study the entanglement properties of complex quantum systems.

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Quantum entanglement is now commonly believed to be a type of physical resource whose manipulation is critical for the success of a majority of quantum-information processing tasks. There is also some evidence that the theory of entanglement may provide additional insights into the physics of complex quantum systems. For this reason, the formulation of a good way to measure entanglement has become a guiding problem in quantum-information science.

For bipartite quantum systems, it is relatively straightforward to propose good mixed-state entanglement measures. However, the evaluation of such measures typically involves difficult minimizations over high-dimensional spaces. As a result, the development of an easily computable formula for a good entanglement measure has become an immediate priority.

In this paper we provide an easily computable formula for a good bipartite mixed-state entanglement measure, the Itangle proposed by Rungta *et al.* [1]. In particular, we develop a simple procedure to calculate the mixed-state entanglement for general rank-2 mixed states of an *arbitrary* bipartite quantum system.

The structure of this paper is as follows. We begin by reviewing two entanglement measures, the concurrence and the tangle, for a pair of qubits. The main result of this paper, a formula for the *I* tangle for rank-2 mixed states, is then established. We also prove a corollary of the main result, an upper bound for the entanglement of formation of a rank-2 mixed state of a qubit and a qudit. We conclude by outlining situations where our formula may be applied to study the entanglement for complex quantum systems.

Before we discuss the *I* tangle, we introduce the *concurrence*, a mixed-state entanglement measure for states of a pair of qubits *AB* [2–4]. The definition of the concurrence makes use of a specific transformation on density operators, the *spin-flip* operation, which is defined as follows. Consider an arbitrary mixed state ρ of *AB*. We define the spin-flip of ρ to be

$$\tilde{\rho} \equiv \operatorname{tr}(\rho^{\dagger})I \otimes I - \rho_A^{\dagger} \otimes I - I \otimes \rho_B^{\dagger} + \rho^{\dagger}, \qquad (1)$$

where $\rho_A = \text{tr}_B(\rho)$ and $\rho_B = \text{tr}_A(\rho)$ denote the reduced density operators for subsystems *A* and *B*, respectively. (We have

included the trace and Hermitian adjoint terms so that the spin-flip operation is defined for *arbitrary* operators acting on AB.) The formula for the spin flip is applicable to arbitrary bipartite systems, in which case it is called the *universal state inverter* [1].

The spin-flip operation Eq. (1) on a pair of qubits is an example of an antilinear operation. To be more precise, consider a pure state $\rho = |\psi\rangle\langle\psi|$. The spin-flip operation, when applied to this state, is equivalent to the expression $\tilde{\rho} = |\tilde{\psi}\rangle\langle\tilde{\psi}|$, where

$$|\tilde{\psi}\rangle = \sigma^{y} \otimes \sigma^{y} (|\psi\rangle)^{*},$$
 (2)

and where σ^{y} is expressed in the computational basis as $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and the complex conjugation is taken in the computational basis. The operation in Eq. (2) is clearly an antilinear operator [5]. The definition of the spin flip as an antilinear operator extends, via linearity, to all mixed states, $\tilde{\rho} = \vec{\theta}\rho \vec{\theta}$, where we have added the arrows above the antilinear operator θ representing the spin flip to indicate the direction in which it acts. It is worth noting that the description of the spin flip Eq. (1) in terms of an antilinear operator θ is specific to two qubits.

For pure states $\rho = |\psi\rangle\langle\psi|$, the concurrence *C* of $|\psi\rangle$ is defined to be $C = |\langle\psi|\tilde{\psi}\rangle| = \sqrt{\langle\psi|\tilde{\rho}|\psi\rangle}$. When the state ρ of the two qubits is mixed, the concurrence *C* is defined to be a minimum over all pure-state decompositions $\{p_i, |\psi_i\rangle\}$ of ρ :

$$C(\rho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i |\langle \psi_i | \tilde{\psi}_i \rangle|.$$
(3)

It is convenient to introduce another entanglement measure closely related to the concurrence, the *tangle* τ [6], which is also defined as a minimization over pure-state decompositions:

$$\tau(\rho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i |\langle \psi_i | \tilde{\psi}_i \rangle|^2.$$
(4)

The squared concurrence satisfies the inequality $C^2 \leq \tau$, which follows from the convexity of $|\langle \psi_i | \tilde{\psi}_i \rangle|^2 = C^2(|\psi_i \rangle)$. It turns out that the reverse inequality also holds, so that the tangle is equal to the square of the concurrence, $\tau(\rho)$ = $C^2(\rho)$ [7]. [The reverse inequality may be established by

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noting that there exists a decomposition $\{p_i, |\psi_i\rangle\}$ achieving the minimum in Eq. (3) which has the property that $C(|\psi_i\rangle)$ = $C(|\psi_j\rangle)$ [3]. The inequality follows from substituting this decomposition into the expressions for τ and C^2 .] A simple formula for the concurrence of two qubits is known [3],

$$C(\rho) = \max[0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4], \qquad (5)$$

where the λ_i are the square roots of the singular values, in decreasing order, of the matrix $\rho \tilde{\rho}$.

We now focus our attention on the general case of two d-dimensional quantum systems or *qudits*. For a pair of qudits AB we use a variant of the I concurrence of Rungta *et al.* [1] to measure the entanglement for mixed states of A and B. The I concurrence is defined via Eq. (1) [1],

$$C(\rho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i \sqrt{\langle \psi_i | \widetilde{\rho}_i | \psi_i \rangle}, \tag{6}$$

where $\rho_i = |\psi_i\rangle \langle \psi_i|$. The entanglement measure we use is a generalization of the tangle, the *I tangle*, defined by

$$\tau(\rho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i \langle \psi_i | \widetilde{\rho}_i | \psi_i \rangle.$$
(7)

The *I* concurrence and the *I* tangle are good mixed-state entanglement measures because they satisfy the standard properties usually regarded as essential for a good entanglement measure (see, for example, [8,9]). The inequality $C^2 \leq \tau$ may be established, by convexity, as for two qubits. Because the equal-entanglement decomposition only exists for pairs of qubits, the *I* tangle is not, in general, equal to the square of the *I* concurrence. Based on the results of this paper, and the calculations of the *I* concurrence for isotropic states [10], we feel that the *I* tangle, as defined by a minimization, is the proper generalization of the tangle Eq. (4).

The universal state inverter Eq. (1) may be expressed in terms of another formula which will be most useful in the following. Before we write down this formula, however, we need to introduce some definitions. Let $|i\rangle_A$ and $|j\rangle_B$ denote the computational basis states for subsystems *A* and *B*, with dimensions d_A and d_B , respectively. For an arbitrary pair $\{|i\rangle_A, |i'\rangle_A\}$, $\{|j\rangle_B, |j'\rangle_B\}$ of the computational basis states of *AB* we set up the projectors $P_A^{(ii')} = |i\rangle_A \langle i| + |i'\rangle_A \langle i'|$, $P_B^{(jj')} = |j\rangle_B \langle j| + |j'\rangle_B \langle j'|$, and $Q_\alpha = P_A^{(ii')} \otimes P_B^{(jj')}$, where $\alpha = (i, i', j, j')$. Consider the object $\rho_\alpha = Q_\alpha \rho Q_\alpha$. The operator ρ_α is a positive operator supported on a 2 × 2 subspace of the Hilbert space of *AB* spanned by $\{|ij\rangle, |i'j\rangle, |ij'\rangle, |i'j'\rangle\}$. In this way we can think of ρ_α as a subnormalized state of two qubits. The two-qubit spin flip, when applied to ρ_α , gives

$$\tilde{\rho}_{\alpha} = \vec{\theta}_{\alpha} \rho \, \vec{\theta}_{\alpha} = \sigma^{y} \otimes \sigma^{y} (Q_{\alpha} \rho Q_{\alpha})^{*} \sigma^{y} \otimes \sigma^{y}, \qquad (8)$$

where $\theta_{\alpha} = \theta Q_{\alpha}$ is the antilinear operator representing the spin-flip operation on the 2×2 subspace, and σ^{y} is naturally defined on the two-dimensional subspaces of *A* and *B*, respectively. Using these definitions we can write an alternative formula for the universal state inverter,

$$\tilde{\rho} = \sum_{\alpha} \vec{\theta}_{\alpha} \rho \, \tilde{\theta}_{\alpha}, \tag{9}$$

where the sum over α runs over all of the $[d_A(d_A-1)/2][d_B(d_B-1)/2]$ possible choices of pairs of computational basis states. [The reader may verify that Eq. (9) follows from the expression of the universal state inverter as a tensor product of two superoperators of the form $\mathcal{P}\circ\mathcal{T}$. See [1] for further details.]

It is convenient, at this point, to introduce two quantities that will simplify the statement of our main result. Let ρ be a density operator for a pair of qudits having no more than two nonzero eigenvalues. We may write ρ in terms of its eigenvectors,

$$\rho = p |v_1\rangle \langle v_1| + (1-p) |v_2\rangle \langle v_2|. \tag{10}$$

Using these eigenvectors we construct the tensor

$$T_{ijkl} = \operatorname{tr}(\gamma_{ij}\tilde{\gamma}_{kl}), \qquad (11)$$

where $\gamma_{ij} = |v_i\rangle\langle v_j|$. We also construct the real symmetric 3 \times 3 matrix M_{ij} whose independent entries are given by

$$M_{11} = \frac{1}{4}T_{1221} + \frac{1}{2}T_{1122} + \frac{1}{4}T_{2112},$$

$$M_{12} = \frac{i}{4}T_{1221} - \frac{i}{4}T_{2112},$$

$$M_{13} = \frac{1}{4}T_{1121} - \frac{1}{4}T_{2122} + \frac{1}{4}T_{1112} - \frac{1}{4}T_{1222},$$

$$M_{22} = -\frac{1}{4}T_{1221} + \frac{1}{2}T_{1122} - \frac{1}{4}T_{2112},$$

$$M_{23} = \frac{i}{4}T_{1121} - \frac{i}{4}T_{1112} + \frac{i}{4}T_{2122} - \frac{i}{4}T_{1222},$$

$$M_{33} = \frac{1}{4}T_{1111} - \frac{1}{2}T_{1122} + \frac{1}{4}T_{2222}.$$
(12)

(The entries of *M* will be shown to be real in the following.)

We now have all the necessary ingredients required for the statement of our main result.

Theorem 1. Let ρ be any density operator for a pair AB of qudits, of dimensions d_A and d_B , respectively, having no more than two nonzero eigenvalues. The I tangle τ between A and B is given by the expression

$$\tau(\rho) = \operatorname{tr}(\rho\tilde{\rho}) + 2\lambda_{\min}[1 - \operatorname{tr}(\rho^2)], \qquad (13)$$

where λ_{\min} is the smallest eigenvalue of the matrix *M* defined by Eq. (12).

It is worth noting that the formula Eq. (13) for the *I* tangle is easy to compute for all rank-2 mixed states of a pair of qudits.

Proof. The method we use to prove this theorem is similar to that employed by Hill and Wootters [2].

Consider an arbitrary pure state $|\psi\rangle$ which can be written as a linear combination of the two eigenvectors of ρ , $|\psi\rangle$ $=c_1|v_1\rangle+c_2|v_2\rangle$. The *I* tangle of $|\psi\rangle$ is given by the expression

$$\tau(\psi) = \langle \psi | \tilde{\sigma} | \psi \rangle = \sum_{\alpha} \langle \psi | \tilde{\theta}_{\alpha} | \psi \rangle \langle \psi | \tilde{\theta}_{\alpha} | \psi \rangle, \qquad (14)$$

where $\sigma = |\psi\rangle\langle\psi|$, and we have used Eq. (9) to rewrite the spin flip in terms of the antilinear operators θ_{α} . Each of the terms in the sum over α may be written as a trace,

$$\tau(\psi) = \sum_{\alpha} \operatorname{tr}(\omega^* \zeta^{\alpha} \omega \zeta^{\alpha^*}), \qquad (15)$$

where $\omega_{ij} = c_i c_j^*$ is the density matrix of $|\psi\rangle$ expressed in the $\{|v_1\rangle, |v_2\rangle\}$ basis, and $\zeta_{ii}^{\alpha} = \langle v_i | \vec{\theta}_{\alpha} | v_i \rangle$.

The function on the right-hand side (RHS) of Eq. (15) can be extended via linearity to a function f of all 2×2 density matrices ω expressed in terms of the $\{|v_1\rangle, |v_2\rangle\}$ basis, i.e., $f(\omega) = \sum_{\alpha} \operatorname{tr}(\omega^* \zeta^{\alpha} \omega \zeta^{\alpha^*})$. The function f has the property that it is equal to the I tangle for all pure states ψ , $f(\psi) = \tau(\psi)$.

Any 2×2 density operator ω may be expressed in terms of the Pauli matrices via the operator expansion, $\omega = 1/2(I + \mathbf{r} \cdot \boldsymbol{\sigma})$, where $r_i = \text{tr}(\omega \sigma^i)$. Substituting this expansion into the expression for *f* gives the quadratic form

$$f(\omega) = \frac{1}{4} \text{tr}(Y) + \sum_{j} r_{j} L_{j} + \sum_{j,k} r_{j} r_{k} M_{jk}, \qquad (16)$$

where $\Upsilon = \sum_{\alpha} \zeta^{\alpha^*} \zeta^{\alpha}$,

$$L_j = \operatorname{tr}(\sigma^j Y), \tag{17}$$

and

$$M_{jk} = \sum_{\alpha} \operatorname{tr}(\sigma^{j^*} \zeta^{\alpha} \sigma^k \zeta^{\alpha^*}).$$
(18)

Each of the terms in the sum over α in Eq. (18) is a real symmetric matrix, so that *M* is a real symmetric matrix. It may be straightforwardly verified that the entries of *M* are given by Eq. (12).

For the rank-2 density operator ρ , the state space of the system *AB* can be considered to be the space of all convex combinations of superpositions of $|v_1\rangle$ and $|v_2\rangle$. If a particular state $|\psi\rangle$ of *AB* is pure, its corresponding 2×2 density operator in the $\{|v_1\rangle, |v_2\rangle\}$ basis, $\omega = 1/2(I + \mathbf{r} \cdot \boldsymbol{\sigma})$, satisfies the condition $|\mathbf{r}|^2 = 1$. In this way, we can think of the entire state space as the Bloch sphere where the poles are the eigenvectors $|v_1\rangle$ and $|v_2\rangle$. A particular decomposition of ρ may be viewed as the weighted sum of points on the surface of the Bloch sphere, where ρ lies at the center of mass of the weighted sum. The function *f* is defined on the entire state space $|\mathbf{r}|^2 \leq 1$.

When the bipartite system *AB* is a pair of qubits, there is only one term in the sum Eq. (9), and *f* reduces to the quadratic form that Hill and Wootters [2] study. In this case, the eigenvalues of *M* are given by $\pm 1/2 |\det \zeta|$ and $1/4tr(\zeta^*\zeta)$, which means that *f* is convex along two directions and concave along a third. In general, the matrix *M* will have three positive eigenvalues, so that *f* is typically convex.

For the purposes of this proof it is essential that a quadratic form g be constructed which agrees with f on pure states ψ which has the additional property that it is convex

along two directions and linear along a third. A function g which has these properties may be constructed from f as follows:

$$g(\omega) \equiv f(\omega) - \lambda_{\min}(|\mathbf{r}|^2 - 1), \qquad (19)$$

where λ_{\min} is the smallest eigenvalue of the matrix *M*. This function is a quadratic form,

$$g(\omega) = K + \sum_{j} r_j L_j + \sum_{j,k} r_j r_k N_{jk}, \qquad (20)$$

where $N=M-\lambda_{\min}I$, and $K=1/4\operatorname{tr}(Y)+\lambda_{\min}$. The matrix N that defines the quadratic form g has two positive eigenvalues and one zero eigenvalue so that g is convex along two directions and linear along the third. The quadratic form g has the additional property that it is equal to f for pure states ψ , $(|\mathbf{r}|^2=1)$.

At this point we recall a theorem due to Uhlmann [11,12], which concerns functions of density matrices expressed as minimisations over all pure-state decompositions.

Theorem 2. Let G be a positive continuous real-valued function defined on pure states. The function \mathcal{G} , defined for all mixed states ρ , given by

$$\mathcal{G}(\rho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i G(\psi_i), \qquad (21)$$

where the minimization runs over all pure-state decompositions of ρ , $\{p_i, |\psi\rangle\}$, is the largest convex function which agrees with G on pure states $\rho = \psi$.

The *I* tangle is expressed as a minimization over all purestate decompositions of a density operator, so if we could find the largest convex function that agrees with $f=\tau$ on pure states ψ it is guaranteed to be equal to the *I* tangle for all mixed states. We claim that *g* is precisely this function.

Assume that there is a convex function g' which agrees with f on pure states but which is larger than g for some density operator ρ . Consider the line running through ρ along which g grows linearly. (The direction along which g grows linearly is given by the eigenvector of N with eigenvalue 0.) Let the points on the surface of the Bloch sphere at either end of this line be the pure states ϕ and ψ , respectively, so that $\rho = q\phi + (1-q)\psi$ for some q, $0 \le q \le 1$. Convexity of g' implies that

$$g'(\rho) \le qg'(\phi) + (1-q)g'(\psi) = qf(\phi) + (1-q)f(\psi) = g(\rho),$$
(22)

which is a contradiction. This implies that g is the largest convex function that takes the values $\tau(\psi)$ on the set of all pure states. Therefore, Theorem 2 shows that g is equal to the *I* tangle.

The expression for the *I* tangle τ may be simplified by noting that, for rank 2 ρ , $1-|\mathbf{r}|^2=2[1-\text{tr}(\rho^2)]$. Note, also, that $f(\rho)=\text{tr}(\rho\tilde{\rho})$. Hence we can write $\tau(\rho)=\text{tr}(\rho\tilde{\rho})$ $+2\lambda_{\min}[1-\text{tr}(\rho^2)]$.

The decomposition that achieves the minimum for the *I* tangle Eq. (13) consists of two terms. In contradistinction to the case of two qubits, the minimizing decomposition will, in general, consist of terms with differing values of τ . This is because the surfaces of constant *g* will typically be curved,

so that the trick of Hill and Wootters cannot be applied (see [2] for the construction of the minimizing decomposition when the surfaces of constant *g* are elliptic cylinders). The construction of the minimizing decomposition follows from observing that the function *g* has the property that it grows linearly in one direction. Consider the line parallel to the eigenvector of *N*, whose associated eigenvalue is zero, which passes through the density operator ρ . The density operator ρ may be written as a convex sum of the two pure states $|\phi_1\rangle$ and $\phi_2\rangle$ which lie at either end of the line, $\rho = q_1 |\phi_1\rangle \langle \phi_1| + q_2 |\phi_2\rangle \langle \phi_2|$. Because the *I* tangle is convex, we obtain the inequality

$$\tau(\rho) \leq q_1 \tau(\phi_1) + q_2 \tau(\phi_2). \tag{23}$$

However, $\tau = g$ varies linearly in this direction, so that the inequality in Eq. (23) is actually an equality.

When one of the subsystems of the bipartite system *AB* is a qubit it is possible to obtain a relation between the *I* tangle τ and the entanglement of formation \mathcal{F} . For pure states ψ of *AB* the entanglement of formation is given in terms of the *I* tangle via

$$\mathcal{F}(\psi) = \mathcal{E}(\tau(\psi)), \qquad (24)$$

where $\mathcal{E}(x) = H(1/2+1/2\sqrt{1-x})$, and *H* is the binary entropy function $H(x) = -x \log x - (1-x)\log(1-x)$, where the logarithm is taken to base 2. The function \mathcal{E} is concave and monotone increasing. If we consider the minimizing decomposition $\{q_i, |\phi_i\rangle\}$ we constructed in the previous paragraph, we obtain the chain of inequalities

$$\mathcal{F}(\rho) \leq q_1 \mathcal{E}(\tau(\phi_1)) + q_2 \mathcal{E}(\tau(\phi_2)) \leq \mathcal{E}(\tau(\rho)), \quad (25)$$

where the first inequality follows from the definition of the entanglement of formation, and the second from the fact $\mathcal{E}(g)$ is concave along the line passing through the pure states $|\phi_i\rangle$.

This statement is the content of the following corollary.

Corollary 1. For rank-2 mixed states ρ of a qubit *A* and a qudit *B*, the entanglement of formation \mathcal{F} of ρ satisfies the inequality

$$\mathcal{F}(\rho) \leq H\left(\frac{1}{2} + \frac{1}{2}\sqrt{1 - \tau(\rho)}\right). \tag{26}$$

Numerical experiments indicate that the expressions on the LHS and RHS of Eq. (26) usually differ only by about 10^{-4} , so that the inequality is typically very close to an equality; it is not, however, an equality.

Our formula for the *I* tangle may be immediately applied to study the entanglement for a wide class of complex quantum systems. For example, consider a pure state $|\psi\rangle$ of an (n+1)-partite quantum system $AB_1B_2\cdots B_n$, where *A* is a qubit and B_j are arbitrary quantum systems. Let ρ be the state found by tracing out the qubit *A*. The *I*-tangle formula Eq. (13) may be used to study the mixed-state entanglement between any bipartition of the *n* parties $B_1B_2\cdots B_n$. This type of configuration can arise in many situations such as a qubit interacting with *n* modes of an electromagnetic field, and most lattice models in condensed matter physics. In particular, it may be possible to use Eq. (13) to provide insight into the scaling of entanglement at a quantum phase transition, along the lines of [13,14].

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