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GLOBAL ENTANGLEMENT IN MULTIPARTICLE SYSTEMS

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ABSTRACT

We define a polynomial measure of multiparticle entanglement which is scalable, *i.e.*, which applies to any number of spin-$\frac{1}{2}$ particles. By evaluating it for three particle states, for eigenstates of the one dimensional Heisenberg antiferromagnet and on quantum error correcting code subspaces, we illustrate the extent to which it quantifies global entanglement. We also apply it to track the evolution of entanglement during a quantum computation.

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Although entanglement has been recognized as a remarkable feature of quantum mechanics since Schrödinger introduced the word [1] in response to Einstein, Podolsky and Rosen's famous paper [2], it remains only incompletely understood. In fact, for more than two particles—even of only spin-$\frac{1}{2}$—there is no complete classification of entanglement. To be more precise, a *measure of entanglement* is a function on the space of states of a multiparticle system which is invariant under local unitary operators, *i.e.*, unitary transformations on individual particles. Thus a complete classification of entanglement for a multiparticle system is a characterization of all such functions. Under the most general local operations assisted by classical communication (LOCC [3]), entanglement can change. A measure of entanglement which decreases under LOCC is called an *entanglement monotone* [4].

On two particle pure states, for example, all measures of entanglement are functions of the eigenvalues of the reduced density matrix (obtained by tracing the density matrix for the whole system over the degrees of freedom of one of the particles), and sums of the k smallest eigenvalues are entanglement monotones [5]. The same information—in somewhat less familiar, but more algebraically convenient form—is contained in the coefficients of the characteristic polynomial of the reduced density matrix. These coefficients are polynomials in the components of the state vector and their complex conjugates. They generate the ring of polynomial functions invariant under the action of local unitary transformations; thus they completely classify two particle pure state entanglement.

As the number of particles n increases, however, the number of independent invariants—measures of entanglement—grows exponentially. Complete classification rapidly becomes impractical. Our goal in this Letter is more modest: we seek a measure of entanglement which is *scalable*, *i.e.*, which is defined for any number of particles; which is easily calculated; and which provides physically relevant information. We concentrate on the case of spin-$\frac{1}{2}$ particles (*qubits*) and begin by defining a family (parameterized by n) of functions on $(\mathbb{C}^2)^{\otimes n}$. We show that each function is a measure of entanglement, vanishing exactly on product states. Next we evaluate this measure for several example states which illustrate its properties, most importantly that it measures *global* entanglement. This is perhaps best exemplified by its values on eigenstates of the antiferromagnetic Hamiltonian, for which we show that it is maximal only on the ground state. In a less traditional context, quantum computation relies heavily on multiparticle entangled states, particularly for error correction. We show that quantum error correcting code states also maximize our measure of entanglement. Finally, we illustrate its use in a dynamical setting, tracking the evolution of entanglement during a specific quantum computation.

The Hilbert space $(\mathbb{C}^2)^{\otimes n}$ of n qubits has a basis labelled by the 2^n n-bit strings: $|b_1 \ldots b_n\rangle$, $b_j \in \{0, 1\}$. For $b \in \{0, 1\}$, define

$$\imath_j(b)|b_1 \ldots b_n\rangle = \delta_{bb_j}|b_1 \ldots \widehat{b_j} \ldots b_n\rangle,$$

where $\widehat{\ }$ denotes absence. We extend $\imath_j$ by linearity to be a map $\mathbb{C}^2 \otimes (\mathbb{C}^2)^{\otimes n} \to (\mathbb{C}^2)^{\otimes n-1}$. For $u, v \in (\mathbb{C}^2)^{\otimes n-1}$ we can write $u = \sum u_x|x\rangle$ and $v = \sum v_y|y\rangle$, where $0 \le x, y < 2^{n-1}$

are $(n-1)$-bit strings. Next, let

$$D(u,v) = \sum_{x<y} |u_x v_y - u_y v_x|^2,$$

the norm-squared of the wedge product of u and v. Finally, for $\psi \in (\mathbb{C}^2)^{\otimes n}$, define

$$Q(\psi) = \frac{4}{n} \sum_{j=1}^{n} D\big(\imath_j(0)\psi, \imath_j(1)\psi\big).$$

As we will see shortly, the $4/n$ factor provides a convenient normalization for Q.

PROPOSITION 1. *For each $n \in \mathbb{Z}_{\geq 2}$, $Q : (\mathbb{C}^2)^{\otimes n} \to \mathbb{R}$ is a measure of entanglement.*

Proof. For $u, v \in (\mathbb{C}^2)^{\otimes n-1}$, $D(u,v)$ is invariant under $\mathrm{U}(2^{n-1})$. A transformation of the j^{th} qubit in $\psi \in (\mathbb{C}^2)^{\otimes n}$ multiplies the j^{th} summand in Q by the norm squared of its determinant. Thus each summand is invariant under $\mathrm{TSL}(2) \times \mathrm{U}(2^{n-1})$, where T denotes the unit scalars. The intersection of these groups for all the summands is $\mathrm{U}(2)^n$, *i.e.*, the local unitary transformations. ∎

The most basic property that a measure of entanglement can have is to identify completely unentangled, *i.e.*, product states. Q has this property:

PROPOSITION 2. *$Q(\psi) = 0$ iff ψ is a product state.*

Proof. Two vectors $u, v \in (\mathbb{C}^2)^{\otimes n-1}$ are linearly dependent iff $D(u,v) = 0$. Thus $Q(\psi) = 0$ implies the existence of $\alpha_j \in \mathbb{C}$ such that $\imath_j(1)\psi = \alpha_j \imath_j(0)\psi$ for all $1 \leq j \leq n$. In particular,

$$\begin{aligned}\psi &= |0\rangle \otimes \imath_1(0)\psi + |1\rangle \otimes \imath_1(1)\psi \\ &= (|0\rangle + \alpha_1|1\rangle) \otimes \imath_1(0)\psi \\ &= (g \otimes I) \cdot (|0\rangle \otimes \psi')\end{aligned}$$

for some $g \in \mathrm{SU}(2)$, $\psi' \in (\mathbb{C}^2)^{\otimes n-1}$. By Proposition 1, Q is invariant under the local unitary transformation $g \otimes I$, so

$$\begin{aligned}0 = Q(\psi) &= Q(|0\rangle \otimes \psi') \\ &= 0 + \sum_{j=2}^{n} D\big(\imath_j(0)[|0\rangle \otimes \psi'], \imath_j(1)[|0\rangle \otimes \psi']\big) \\ &= Q(\psi').\end{aligned}$$

Then, by induction, ψ is a product state.

Conversely, if ψ is a product state, then for all $1 \leq j \leq n$, $\imath_j(0)\psi$ is parallel to $\imath_j(1)\psi$. Thus $Q(\psi) = 0$. ∎

Having demonstrated that Q vanishes on product states, we should now calculate it for some entangled states. First consider the EPR-Bohm [2,6] state $(|01\rangle - |10\rangle)/\sqrt{2}$, or equivalently, $\gamma_2 = (|00\rangle + |11\rangle)/\sqrt{2}$. It is straightforward to calculate:

$$Q(\gamma_2) = 2 \cdot \frac{4}{2}\Big[\det \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\Big]^2 = 1.$$

Next, the three qubit GHZ-Mermin [7,8] state is $\gamma_3 = (|000\rangle + |111\rangle)/\sqrt{2}$. Calculating the invariant, we again find:

$$Q(\gamma_3) = 3 \cdot \frac{4}{3}\Big[\det \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\Big]^2 = 1.$$

Finally, it is now clear that for the n qubit state $\gamma_n = (|0\ldots0\rangle + |1\ldots1\rangle)/\sqrt{2}$, $Q(\gamma_n) = 1$. These examples demonstrate that the $4/n$ factor provides a natural normalization for Q.

PROPOSITION 3. *With this normalization,* $0 \le Q \le 1$.

Proof. Since $D(u, v)$ is the norm-squared of the wedge product of the two vectors u and v, it is bounded above by $\|u\|^2\|v\|^2$, which takes its maximal value of $\frac{1}{4}$ when $\|u\|^2 = \|v\|^2 = \frac{1}{2}$ for vectors $\psi = |0\rangle \otimes \imath_1(0)\psi + |1\rangle \otimes \imath_1(1)\psi$ with $\|\psi\|^2 = 1$. Since there are n summands in Q, it is bounded above by $n \cdot \frac{4}{n} \cdot \frac{1}{4} = 1$. ∎

Proposition 2 and the calculations above show that these bounds are saturated on, respectively, product states and the entangled states γ_n. Of course, Q does take other values: Under the action of $\mathrm{U}(2) \times \mathrm{U}(2) \times \mathrm{U}(2)$ the Hilbert space for three qubits, $\mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2$, decomposes into multiple orbits [9–15]. Representative states are $|000\rangle$ (product states), $|0\rangle \otimes \gamma_2 = |0\rangle(|00\rangle + |11\rangle)/\sqrt{2}$ (and cyclic permutations), $(|100\rangle + |010\rangle + |001\rangle)/\sqrt{3}$, and γ_3. By Proposition 2, $Q(|000\rangle) = 0$. By Proposition 2 and the calculation above, $Q(|0\rangle \otimes \gamma_2) = \frac{4}{3} \cdot \frac{1}{2} = \frac{2}{3}$. A straightforward calculation gives $Q\big((|100\rangle + |010\rangle + |001\rangle)/\sqrt{3}\big) = \frac{8}{9}$. And we have already calculated $Q(\gamma_3) = 1$. Thus for three qubits our measure of entanglement behaves in the way we would want, decreasing through states we would consider successively less globally entangled (and taking different values on each of these states, unlike the 'tangle' [16], for example, which vanishes on all but γ_3). In fact, on three qubits Q is an entanglement monotone and numerical evidence indicates that this is true in general [17].

The traditional context in which globally entangled multiparticle states occur is lattice spin systems. Consider, for example, the one dimensional spin-$\frac{1}{2}$ Heisenberg antiferromagnet [18,19] on a lattice of size n, with periodic boundary conditions, defined by the Hamiltonian

$$H_n = \sum_{j=1}^{n} X_j X_{j+1} + Y_j Y_{j+1} + Z_j Z_{j+1},$$

where the subscripts are to be interpreted mod n, and X, Y, Z denote the Pauli matrices σ_x, σ_y, σ_z, respectively. H_n commutes with $S_z = \sum Z_j$, so the eigenstates of H_n can be labelled by their total spin S_z, *i.e.*, each eigenstate of H_n is a superposition of basis vectors $|b_1 \ldots b_n\rangle$ with $|\{j \mid b_j = 1\}| = s$ for some fixed $0 \le s \le n$. When $s = 1$, the translation invariance of H_n implies that the eigenstates are plane waves

$$\psi_n^{(k)} = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} e^{ikj} |0 \ldots 010 \ldots 0\rangle,$$

where the j^{th} summand has a single 1 at the j^{th} bit and the wave number $k = 2\pi m/n$ for some integer $0 \le m \le n-1$. For $n = 3$ these plane waves are equivalent under local unitary transformations to the state $(|100\rangle + |010\rangle + |001\rangle)/\sqrt{3}$, for which we calculated $Q = \frac{8}{9}$ above. In fact, for arbitrary n the entanglement of these plane waves is simply

$$Q\big(\psi_n^{(k)}\big) = \frac{4}{n} \cdot n \cdot (n-1) \frac{1}{n^2} = \frac{4(n-1)}{n^2}.$$

For $s > 1$ the eigenstates of H_n can be computed using the Bethe *Ansatz*; the ground state has $s = n/2$ (for even n) [20]. Using the translation invariance of these eigenstates we can evaluate Q easily. The result is

$$Q(S_z = s \text{ eigenstate of } H_n) = \frac{4}{n} \cdot n \cdot \binom{n-1}{s} \binom{n-1}{s-1} \binom{n}{s}^{-2} = \frac{4s(n-s)}{n^2}.$$

Notice that for the ground state this entanglement measure is maximal, $Q = 1$. This result contrasts with O'Connor and Wootters' calculations of the 'concurrence' C in these states [21]: they find that C is not maximal on the ground state, but rather for $s/n \approx 0.3$ as $n \to \infty$. This difference is due to the fact that C is really a measure of two particle entanglement, even when generalized to multiparticle states, while Q is a global measure of multiparticle entanglement.

Highly entangled multiparticle states also occur in the relatively new context of quantum error correcting codes. In fact, the code subspace for an additive code can be described as the space of ground states of the Hamiltonian formed by the sum of the stabilizers [22]. For example, the code subspace for a 5 qubit code **[5,1,3]** encoding 1 qubit against single bit errors [23,24] is the space of ground states of the translation invariant Hamiltonian on a one dimensional lattice of five qubits:

$$H_{[5,1,3]} = \sum_{j=1}^{5} X_j Z_{j+1} Z_{j+2} X_{j+3},$$

where the subscripts are to be interpreted mod 5. The space of ground states is two dimensional—which is why it can encode 1 qubit. A basis is

$$\begin{aligned}
|0\rangle &\mapsto [|00000\rangle - (|11000\rangle + \text{cyc.}) + (|10100\rangle + \text{cyc.}) - (|11110\rangle + \text{cyc.})]/4 \\
|1\rangle &\mapsto [|11111\rangle - (|00111\rangle + \text{cyc.}) + (|01011\rangle + \text{cyc.}) - (|00001\rangle + \text{cyc.})]/4,
\end{aligned}$$

where “cyc.” indicates cyclic permutations. From these equations it is straightforward to calculate that $Q = 1$ for all states in this code space. Here the difference from the concurrence is even more dramatic: C vanishes on the code subspace since tracing over all but two qubits leaves a reduced density matrix proportional to the identity [25].

Shor’s original 9 qubit code protecting 1 qubit against single qubit errors [26] can also be described as the ground state subspace of a lattice Hamiltonian—for a lattice triangulating $\mathbb{R}P^2$ [27]. In this case a basis for the code space is

$$
\begin{aligned}
|0\rangle &\mapsto (|000\rangle + |111\rangle)^{\otimes 3}/3 \\
|1\rangle &\mapsto (|000\rangle - |111\rangle)^{\otimes 3}/3.
\end{aligned}
$$

Calculating Q for the states in this subspace we find that again it is maximal, despite the fact that these states decompose into products of three qubit factors. So Q does not distinguish all sub-global entanglements; this is a consequence of using a single invariant. Finer resolution requires a more complete set of invariants, and in general, higher degree polynomials [9,10,12,15,28].

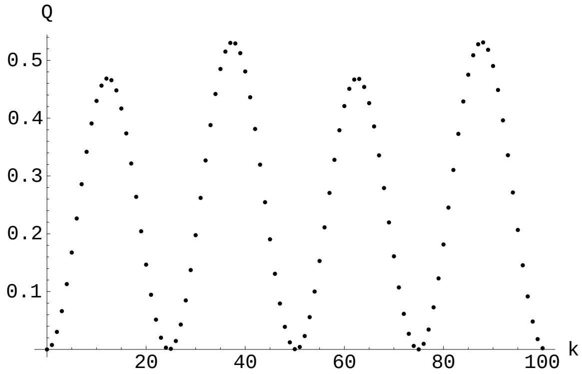

Figure 1. Entanglement in Grover’s algorithm for 10 qubits as a function of number of iterations.

Nevertheless, as we have seen, Q provides useful information about global entanglement in certain contexts. Furthermore, in dynamical problems, Q quantifies the evolution of entanglement. Consider Grover’s algorithm [29], for example: Given $a_j \in \{0,1\}$, $1 \le j \le n$, define

$$
U_a|b_1 \ldots b_n\rangle = (-1)^{\Pi\delta_{a_j b_j}}|b_1 \ldots b_n\rangle
$$

and then extend U_a by linearity to a map $(\mathbb{C}^2)^{\otimes n} \to (\mathbb{C}^2)^{\otimes n}$. The goal of Grover’s algorithm is to convert an initial state of n qubits, say $|0\ldots0\rangle$, to a state with probability bounded above $\frac{1}{2}$ of being in the state $|a_1 \ldots a_n\rangle$, using U_a the fewest times possible. Grover showed that it can be done with $O(\sqrt{2^n})$ uses of U_a by preparing the state

$$
\frac{1}{\sqrt{2^n}}\sum_{x=0}^{2^n-1}|x\rangle = H^{\otimes n}|0\ldots0\rangle \quad \text{where} \quad H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix},
$$

and then iterating the transformation $H^{\otimes n}U_0H^{\otimes n}U_a$ on this state [29]. The initial state is a product state, as is the target state $|a_1 \ldots a_n\rangle$, but intermediate states $\psi(k)$ are entangled for $k > 0$ iterations. We can evaluate Q on these states to quantify this entanglement:

$$
Q\bigl(\psi(k)\bigr) = 4\Bigl(\frac{N}{2} - 1\Bigr)\frac{\cos^2\theta_k}{N-1}\Bigl(\sin\theta_k - \frac{\cos\theta_k}{\sqrt{N-1}}\Bigr)^2,
$$

where $\theta_k = (2k+1)\csc^{-1}(\sqrt{N})$ and $N = 2^n$. The results are plotted in Figure 1 for $n = 10$: the entanglement oscillates, first returning to close to 0 at

$$k = \left[\!\left[\frac{1}{2}\Big(\frac{\pi}{2\csc^{-1}(\sqrt{N})} - 1\Big)\right]\!\right] \sim \left[\!\left[\frac{\pi}{4}\sqrt{N}\right]\!\right] \quad \text{as} \quad N \to \infty,$$

where $[\![\cdot]\!]$ denotes 'closest integer to'; this is when the probability of measuring $|a_1 \ldots a_n\rangle$ is first close to 1.

Three qubit states, eigenstates of lattice Hamiltonians, quantum error correcting code subspaces, and the intermediate states in Grover's algorithm all illustrate how a measure of multiparticle entanglement such as Q provides insight into global properties of quantum multiparticle systems. While Q has the satisfactory properties of Propositions 2 and 3, is an entanglement monotone on three qubits, and is a straightforwardly computable polynomial, it is in no sense a unique measure of multiparticle entanglement. A more complete (but still partial) characterization can be obtained by also using some of the other measures which have been proposed, like the concurrence [21], the closely related n-tangle [30], the Schmidt rank [31], the negativity [32], *etc.* Each emphasizes a specific feature of multiparticle entanglement and describes a different physical property. We anticipate that multiparticle entanglement measures—whose current development is largely motivated by quantum computation—will contribute to the understanding of the physics of quantum multiparticle systems more generally [33–35].

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