Delocalization and Entanglement: A Method of Developing Analytical Multipartite Measures for Mixed W-like States

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We present a method of developing analytical measures of $k$-partite delocalization in arbitrary $n$-body W-like states, otherwise known as mixed states in the single excitation subspace. These measures are distance measures that calculate the distance of a state to its closest reference state with $k - 1$ entanglement. We find that the reference state is determined by the purity of the state undergoing measurement. Measures of up to 6-body entanglement for a 6-body system are derived in full, while an algorithm for general $k$-partite measures is given.

The role of entanglement has extended far beyond fundamental quantum mechanics to fields as diverse as quantum computing [1], astrophysics [2] and even energy transfer in photosynthetic systems [3-6]. Qualifying and quantifying the presence of entanglement has proven an arduous task, often increasing exponentially with the number of parties. In the multipartite setting, notions such as “maximal entanglement”, and separability are no longer black and white; inequivalent classes of entanglement such as the GHZ [7] and W-states [8] arise, while states form a tiered structure of separability.

The difficulty of detecting entanglement is further compounded when considering open systems, i.e. systems that undergo decoherence [9, 10]. For a review, see Horodecki et al. [11], Mintert et al. [12], or Plenio and Virmani [13].

In this letter we develop a method for determining $k$-partite entanglement ($k \leq n$) in $n$-mode open systems with only one excitation. Such mode entanglement can also be viewed as the degree of delocalization of the excitation; indeed in this letter we will use the two concepts interchangeably. This method allows us to measure $k$-partite delocalization by quantifying the $k$-partite entanglement. In quantum information, a state with a single excitation shared across $n \geq 3$ modes is known as a W-type state. W-states are vital in quantum information theory as they are robust against decoherence [9], and may provide a valuable resource for scalable quantum information processing. Therefore, quantifying the entanglement of such states is essential. W-states can be produced in experiments involving atomic ensembles [14], as well as single photon entanglement [15].

While the removal of other excitation subspaces, as well as the ground state, greatly reduces the amount of information to be processed, it should be noted that states subject to these measures must be formed and preserved within the single excitation subspace. Under any local operations that preserve the state within this subspace, the measures described here can be considered to accurately quantify multipartite entanglement.

A famous example of distance measures in entanglement is the relative entropy [16]. This measure compares the entropy of a state to its closest separable state. In contrast, our distance measures make use of the tiered structure of separability in multipartite entanglement and, in order to quantify $k$-partite entanglement, compare a state to its nearest ($k - 1$)-partite entangled state.

Some of the criteria employed are analogous to those within other approaches in the literature; Papp et al. [15] considered entanglement detection as a function of the degree of photon contamination (in our case as a function of purity), while Blasone et al. [17] looked at creating distance measures for $k$-partite entangled pure states by measuring the distance from the closest ($k - 1$)-partite entangled state.

In the single excitation subspace, a convenient equivalence between coherence and entanglement arises. A measure of bipartite entanglement, the tangle [18], is related to coherence between modes $a$ and $b$ by $\tau_{ab} = |\rho_{ab}|^2$. Adding all the possible tangles gives the total tangle, or total bipartite entanglement in the system [4]

$$E_2 (\rho) = \sum_{a=1,b\neq a}^{N} \tau_{ab}. \quad (1)$$

This measure can be rewritten as a function of the purity of the state, and the second order statistical moment [3]

$$E_2 (\rho) = \text{Tr} (\rho^2) - M_2 (\rho). \quad (2)$$

This statistical measure $M_2 (\rho)$ is also known as the Inverse Participation Ratio, a measure of delocalization in pure states [19]. Unlike the purity measure, it is basis dependent, and should be applied to the basis under investigation. In general a statistical moment of order $k$
is written as $M_k (\rho) = \sum_{j=1}^{N} (\rho_{jj})^k$.

Measures of multipartite delocalization in pure W-like states have already been developed [20]. These measures make use of the statistical moments of the state populations to detect and quantify $k$-partite entanglement in $n$-body systems. The equations for bipartite up to quintupartite entanglement are given below.

\[
\begin{align*}
\tau_2 (\rho) &= 1 - M_2 (\rho), \\
\tau_3 (\rho) &= 1 - 3M_2 (\rho) + 2M_3 (\rho), \\
\tau_4 (\rho) &= 1 - 6M_2 (\rho) + 8M_3 (\rho) + 3M_2 (\rho)^2 - 6M_4 (\rho), \\
\tau_5 (\rho) &= 1 - 10M_2 (\rho) + 20M_3 (\rho) + 15M_2 (\rho)^2 - 30M_4 (\rho) - 20M_2 (\rho)M_3 (\rho) + 24M_5 (\rho)
\end{align*}
\]

(3a) (3b) (3c) (3d)

It is evident that equations 2 and 3a are equivalent in the case of a pure state. Our objective is to derive mixed state versions of equations 3b-3d that reduce to the pure state equations when $\text{Tr} (\rho^2) = 1$. We can begin by reinterpreting equation 2 as a distance measure of the state $\rho$ from its nearest separable state $\sigma$ such that

\[
E_2 (\rho) = 1 - M_2 (\rho) - (1 - M_2 (\sigma)).
\]

(4)

In this case, $\sigma$ is just $\rho$ projected into the eigenvalue basis. Given that there are no off-diagonal elements in $\sigma$, it has no entanglement, and also happens to have the same purity as $\rho$. When a matrix like $\sigma$ is diagonal, its purity $\text{Tr} (\sigma^2)$ and $M_2 (\sigma)$ are equivalent, and thus so are equations 2 and 4. In other words, $\sigma$ minimizes the distance between the entangled and separable regimes.

We can now expand upon the idea of distance measures within the context of tripartite entanglement.

Just like in the bipartite measure, we will apply a measure (in this case equation 4) to our state $\rho$, as well as some reference state $\sigma$, of equal purity:

\[
E_3 \equiv \tau_3 (\rho) - \tau_3 (\sigma_3).
\]

(5)

The requirement that our state $\sigma$ should have the same purity as $\rho$ makes sense. Not only is it a natural extension of our bipartite measure but also purity is a measure of entropy. As states become more mixed they become less distinguishable; for a given level of entropy a reference point is needed to distinguish our states. As can be seen in figure the sets of all states and all reference states are both convex and distinct; meaning that, for a given level of purity, only one reference state $\sigma$ can play the role of closest state to $\rho$. Unlike the bipartite measure however, the state $\sigma$ will not be a separable state, but rather is defined as the closest state with bipartite entanglement. This ensures we can distinguish our state from others that are bipartite entangled but not tripartite entangled. The problem now falls to finding the closest bipartite state.

The higher the level of bipartite entanglement, the higher the likelihood that there are higher orders of entanglement. We can see this by imagining infinite-body pure states with varying levels of entanglement. A state with at most 2-body entanglement can have a maximum value of $E_2 (\rho) = 1/2$, a state with at most 3-body entanglement $E_2 (\rho) = 2/3$, and so on as the value of $E_2 (\rho)$ approaches 1 as $k$ approaches infinity.

As our states become mixed, their maximal value for $E_2 (\rho)$ decreases as a function of the purity. In order to minimize the distance between your state of interest $\rho$ and the reference state $\sigma$, the bipartite entanglement...
of $\sigma$ must be maximized; meaning that, according to equation [2], one needs to minimize $M_2(\sigma)$ for a given level of purity. In general, $\sigma$ is comprised of probability-weighted pure states $\sigma = p_1\sigma_1 + p_2\sigma_2 + \ldots + p_n\sigma_n$. However, when adding any two density matrices with population overlap, $M_2(\sigma)$ will not be minimized. For a detailed proof, see the supplementary material.

Therefore, for a 3-body system, one can envision these states to take on the form (or some permutation thereof):

$$\sigma = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & (1-p) \end{pmatrix}$$  \hfill (6)

where the probability $p$ is defined as a function of the purity of the state $\rho$

$$p = \frac{1}{2} \left( 1 + \sqrt{2(\text{Tr}(\rho^2)) - 1} \right),$$  \hfill (7)

and is a solution to the quadratic equation $p^2 + (1-p)^2 = \text{Tr}(\rho^2)$. The value $p$ can run from $1/3$ (when $\text{Tr}(\rho^2) = \text{Tr}(\sigma^2) = 5/9$) up to 1 (when $\text{Tr}(\rho^2) = \text{Tr}(\sigma^2) = 1$). Below a purity of $5/9$ one can no longer distinguish from biseparable states. In the event that a state lies within the biseparable region, its closest biseparable state is set to itself, in order to avoid having negative values.

A clear pattern has emerged: In order to measure $k$-partite delocalization in some $n$-body system, one must generate ($k-1$)-partite entangled states and assess the closest states to the $k$-partite entangled region, such that $E_k(\rho) = \tau_k (\rho) - \tau_k (\sigma)$. In general [21] $\tau_k$ can be calculated from

$$\tau_k = \sum_{i=0}^{N-k+1} \rho_{i_0 i_0} \sum_{i_1=i_0+1}^{N-k+2} \rho_{i_1 i_1} \ldots \sum_{i_{k-1}=i_{k-2}+1}^{N} \rho_{i_{k-1} i_{k-1}}.$$  \hfill (8)

The biggest challenge in deriving these measures is finding the correct reference states for a given system and measure. In order to maximize their $k-1$ entanglement, the number of constituent states in the final mixed state must be minimized. These reference states appear to fall in to three main categories, depending on the size of the system and the level of delocalization being measured.

If $k-1 \geq n/2$ only two states are needed; one with $k-1$-partite entanglement and one with $(n-k+1)$-partite entanglement. Their probabilities are determined just like in our previous example with equation [2]. The second is when $k-1 < n$ and $k-1$ divides $q$ times into $n$.

$$p_1 = 1/q \left( \sqrt{(q^2 - q) \text{Tr}(\rho^2) - q + 1} + 1 \right) \quad \text{and} \quad p_2 = p_3 \ldots = p_q = 1/q(1-p_1).$$

The final category is when $k-1$ divides $q$ times with some remainder $r$. While their probabilities are more difficult to calculate, they are determined in a similar fashion: as a multivariable quadratic equation $p_1^2 + p_2^2 + \ldots + p_q^2 = \text{Tr}(\rho^2)$, with $p_1^2 \geq p_2^2 \geq \ldots \geq p_q^2$.

In the event of being unable to do so, a sufficiently large number of randomly generated reference states will create a distinct region, along the border of which a curve can be fitted and used in lieu of the exact reference states.

As a demonstration of the effectiveness of these measures, we plot in figure 2 the evolution of multi-partite entanglement within a 6-body system, undergoing a dephasing evolution. The initial state chosen is a pure W-state, i.e maximally entangled. The details of the Hamiltonian and master equation employed are included in the supplementary material. The reference states for each measure were fully determined. For $E_3$ we derived the reference state $W_3 = p_1|W_{12}\rangle \langle W_{12}| + p_2|W_{34}\rangle \langle W_{34}| + p_3|W_{56}\rangle \langle W_{56}|$, where

$$|W_{12}\rangle = \frac{1}{\sqrt{2}} (|100000\rangle + |010000\rangle) \equiv \frac{1}{\sqrt{2}} (|11\rangle + |2\rangle),$$

$$|W_{34}\rangle = \frac{1}{\sqrt{2}} (|3\rangle + |4\rangle)$$

$$|W_{56}\rangle = \frac{1}{\sqrt{2}} (|5\rangle + |6\rangle).$$  \hfill (9)

FIG. 2. Early dephased evolution of multipartite entanglement in a 6-body system over the first 50 time steps. The inset shows the long term evolution of multipartite entanglement. All measures have been normalized.
The probabilities for $\sigma_3$ were calculated as

$$p_1 = \frac{1}{3} \left( \sqrt{6} (\text{Tr} (\rho^2)) - 2 + 1 \right)$$
$$p_2 = \frac{1}{2} (1 - p_1)$$
$$p_3 = \frac{1}{2} (1 - p_1).$$

For $E_4 \equiv \tau_4 (\rho) - \tau_4 (\sigma_4)$, our reference state is $\sigma_4 = p_1 |W_{123}\rangle \langle W_{123}| + p_2 |W_{456}\rangle \langle W_{456}|$, and

$$|W_{123}\rangle = \frac{1}{\sqrt{3}} (|1\rangle + |2\rangle + |3\rangle)$$
$$|W_{456}\rangle = \frac{1}{\sqrt{3}} (|4\rangle + |5\rangle + |6\rangle).$$

(10)

For $E_5 \equiv \tau_5 (\rho) - \tau_5 (\sigma_5)$, our reference state is $\sigma_5 = p_1 |W_{1234}\rangle \langle W_{1234}| + p_2 |W_{56}\rangle \langle W_{56}|$, and

$$|W_{1234}\rangle = \frac{1}{\sqrt{4}} (|1\rangle + |2\rangle + |3\rangle + |4\rangle)$$
$$|W_{56}\rangle = \frac{1}{\sqrt{2}} (|5\rangle + |6\rangle).$$

(11)

Finally for $E_6 \equiv \tau_6 (\rho) - \tau_6 (\sigma_6)$, our reference state is $\sigma_6 = p_1 |W_{12345}\rangle \langle W_{12345}| + p_2 |W_6\rangle \langle W_6|$, and

$$|W_{12345}\rangle = \frac{1}{\sqrt{5}} (|1\rangle + |2\rangle + |3\rangle + |4\rangle + |5\rangle)$$
$$|W_6\rangle = |6\rangle.$$

(12)

As there are only two constituent states in the reference states of measures $E_4$ to $E_6$, the probabilities are the same as equation (7). In general the procedure is to maximize the $k - 1$-partite entanglement in each constituent state, and weight those states accordingly with ranked probabilities, such that $p_1 \geq p_2 \geq \ldots \geq p_m$.

The initial state chosen for figure 2 is a non-stationary state of the system Hamiltonian. Thus, under short term evolution we observe the entanglement decay smoothly from a fully entangled state down to near-zero, with higher orders of entanglement disappearing in order. The long term evolution of the state shows an increase in multipartite entanglement as the system enters a steady state and the majority of the excitation lies in one of the eigenstates of the system.

In this letter we have demonstrated, by using only the purity and statistical moments, that one can analytically distinguish mixed states with different, quantifiable levels of entanglement in the single excitation subspace. We have taken advantage of the concept of tiered separability in deriving analytical distance measures of multipartite delocalization. By construction, these distance measures decrease under loss of information, meaning their convexity need not be proven. The key idea of our approach is to calculate the distance from a state to the next closest ($k - 1$)-body entangled state with the same level of purity. Rather than minimizing the distance over a set of randomly generated reference states, the reference states are carefully selected. This allows for instant detection of entanglement, for any level of separability, at any level of decoherence.

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This supplementary information provides proof that two overlapping density matrices do not minimize the statistical moment $M_2(\sigma)$, and contains further detail on deriving reference states. Following our proof we provide the Hamiltonian and quantum master equation employed for our model system undergoing decoherence.

**PROOF OF REFERENCE STATES**

In this proof we clearly derive the general method employed in deriving the reference states needed for our multipartite measures. In order to do so, we must prove that the constituent pure states of these mixed reference states must not overlap. First let us assume that the reference state $\sigma$ is made up of statistically weighted pure states such that $\sigma = p_1\sigma_1 + p_2\sigma_2 + \ldots + p_n\sigma_n$. Given that $\sigma$ must be maximally $k-1$-partite entangled for its level of purity, it stands to reason that at least one of the constituent states is also maximally $k-1$ entangled. We must also ensure that the statistical moment $M_2(\sigma)$ is minimized, in order to maximize the amount of entanglement. Now let us look at what happens if we add two density matrices $\sigma_1$ and $\sigma_2$ that have population overlap. Assume $\sigma_1$ is delocalized across $k-1$ modes and that $\sigma_2$ is delocalized across $m$ modes where $2 \leq m \leq k-1$. Each density matrix is statistically weighted, by $p_1$ and $p_2$ respectively. Their contribution to $M_2(\sigma)$ will appear as follows:

$$M_2(p_1\sigma_1 + p_2\sigma_2) = \frac{k-2}{(k-1)^2}p_1^2 + \frac{m-1}{m^2}p_2^2 + \left(\frac{p_1}{k-1} + \frac{p_2}{m}\right)^2$$

Expanding this out gives us

$$M_2(p_1\sigma_1 + p_2\sigma_2) = \frac{p_1^2}{k-1} + \frac{p_2^2}{m} + \frac{2p_1p_2}{m(k-1)}$$

This result has an extra cross term $\frac{2p_1p_2}{m(k-1)}$ compared to just the two statistical moments $M_2(p_1\sigma_1)$ and $M_2(p_2\sigma_2)$ added together. Now let us apply an extra restriction: let the size of the system, $n$, be smaller than $k-1 + m$, but equal to $k-2+ m$. What happens if we remove the overlapping population from $\sigma_2$ and place it elsewhere in $\sigma_2$, effectively reducing the size of $\sigma_2$ to $m-1$ modes? Here we find that again, the case with population overlap ($\sigma_2$ with $m$ modes) has a larger value of $M_2(p_1\sigma_1 + p_2\sigma_2)$ than the case where $\sigma_2$ has $m-1$ modes, under the condition

$$p_2 \leq \frac{2(m-1)}{k-1} p_1.$$  \hfill (3)

Given that $p_1 \geq p_2$ and that $m < k$ this will be true for a given range of probabilities. For example, in the measures $E_4, E_5$ and $E_6$ defined in the letter, $p_2 = 1 - p_1$. Thus this will always hold true as $\frac{k-1}{2n+k-3} < p_1$. Likewise for $E_3$, $m = k$ and $p_1 \geq p_2 = p_3$.

Now that we have proven that we cannot have any overlapping matrices, this gives the added advantage that the purity of $\sigma$ can also be written in terms of the probabilities of the constituent matrices: $p_1^2 + p_2^2 + \ldots + p_n^2 = \text{Tr}(\sigma^2) = \text{Tr}(\rho^2)$. Each constituent matrix will be fully delocalized according to its size constraints. For example, in the first category of reference states in a system of size $n$, where $k-1 \geq n/2$, only two states are needed; one with $k-1$-partite entanglement and one with $(n-k+1)$-partite entanglement. When $n = k$ this second matrix will be a pure, separable state with a single mode occupied. The probabilities for such a system will be the solutions to the quadratic equation $p_1^2 + (1 - p_1)^2 = \text{Tr}(\rho^2)$, such that $p_1 = \frac{1}{2}\left(1 + \sqrt{2(\text{Tr}(\rho^2)) - 1}\right)$.

Let’s now look at the second category of reference states, where $k-1$ divides $q$ times into system size $n$. Given that each constituent state has the same delocalization ($k-1$) as $\sigma_1$, we will introduce $\sigma_2$ to $\sigma_q$ with equal probability. Therefore the probabilities will again come from a solution to a quadratic equation:

$$p_1^2 + (q-1)\left(\frac{1-p_1}{q-1}\right)^2 = \text{Tr}(\rho^2)$$ \hfill (4)

where we find $p_1 = 1/q\left(\sqrt{q^2-q}\text{Tr}(\rho^2) - q + 1\right)$ and $p_2 = p_3 \ldots = p_q = 1/q(1 - p_1)$.

The final category is when $k-1$ divides $q$ times with some remainder $r$. $q$ states with $k-1$ mode delocalization are required as well as one state with $r$ mode delocalization.
While their probabilities are more difficult to calculate, they are determined in a similar fashion: as a multivariable quadratic equation $p_1^2 + p_2^2 + \ldots + p_{q+1}^2 = \text{Tr}(\rho^2)$, with $p_1^2 \geq p_2^2 \ldots \geq p_{q+1}^2$.

HAMILTONIAN AND MASTER EQUATION

We include the Hamiltonian employed in our simulation that describes a ring of 6 sites with nearest-neighbor coupling. The energy units are cm$^{-1}$.

$$H = \begin{pmatrix}
12500 & 300 & 0 & 0 & 0 & 300 \\
300 & 12000 & 300 & 0 & 0 & 0 \\
0 & 300 & 12500 & 300 & 0 & 0 \\
0 & 0 & 300 & 12000 & 300 & 0 \\
0 & 0 & 0 & 300 & 12500 & 300 \\
300 & 0 & 0 & 0 & 300 & 12000 \\
\end{pmatrix} \quad (5)$$

we use the Redfield equation within the secular approximation [1]. The density matrix of the system obeys now the following master equation:

$$\frac{\partial \rho(t)}{\partial t} = -i[H, \rho(t)] + D(\rho(t)). \quad (6)$$

The first term on the right hand side describes purely coherent evolution and the second induces dephasing and relaxation between excitonic states of the system through the dissipator operator $D(\rho(t))$. The dissipator reads

$$D(\rho(t)) = \sum_\omega \sum_{m,n} \gamma(\omega) \left[ A_n(\omega) \rho(t) A_n^\dagger(\omega) - \frac{1}{2} \{ A_n^\dagger(\omega) A_n(\omega), \rho(t) \} \right], \quad (7)$$

where $A_n(\omega) = \sum_{\epsilon_k - \epsilon_{k'}} a_n^\dagger(\epsilon_k) a_n(\epsilon_{k'}) |\phi_k\rangle \langle \phi_{k'}|$ are the Lindblad operators, with $a_n$ the site coefficients of exciton $|\psi\rangle$ such that $|\psi\rangle = \sum_n a_n |n\rangle$. We assume that site fluctuations are independent. The rates $\gamma(\omega)$ are given by $\gamma_{mn}(\omega) = \gamma(\omega) = 2\pi J(|\omega|) N(-\omega)$. $J(\omega)$ is the spectral density characterizing the system-phonon coupling, which we assume to be ohmic with Drude cutoff, i.e. $J(\omega) = 2E_r \omega_c \omega / \pi (\omega_c^2 + \omega^2)$, where $E_r$ is the reorganization energy, $\omega_c$ is the cutoff frequency and $N(\omega)$ is the thermal occupation number. In this simulation we chose a value of 300 cm$^{-1}$ for $E_r$ equal to the level of coupling within the system. The temperature chosen was 77 K.

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