Critique of generalised purity as an entanglement measure: Explicit failure in simple separable Bose–Hubbard models

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**Abstract**

The SU(2) and SU(3) Lie algebras lend themselves naturally to studies of two- and three-well Bose–Einstein condensates, with the group operators being expressed in terms of bosonic annihilation and creation operators at each site. The success of these representations has led to the purities associated with these algebras to be promoted as a measure of entanglement in these systems. In this work, we show that these purities do not provide an unambiguous measure of entanglement between wells, but instead give results which depend on the quantum statistical states of the atomic ensembles in each well. Using the example of totally uncoupled wells where the atoms in one have never interacted with the atoms in the other, we quantify these purities for different states and show that completely separable states can give values which have been claimed to indicate the presence of entanglement. We also consider claims that the generalised purities measure particle rather than mode entanglement, with emphasis on the case of indistinguishable bosons, as found in these systems.

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1. Introduction

The SU(2) and SU(3) group operators used in the treatment of angular momentum and two- and three-well condensates originate from Schwinger’s oscillator model of angular momentum [1]. In the case of a two-well condensate, and making the two-mode approximation, the relevance of Schwinger’s model is apparent when we use the bosonic annihilation operators for each mode, \( a_1 \) and \( a_2 \), to construct three operators which obey SU(2) commutation relations [2,3],

\[ J_x = \frac{1}{2}(a_1^\dagger a_2 - a_2^\dagger a_1), \]
\[ J_y = \frac{i}{2}(a_1^\dagger a_2 + a_2^\dagger a_1), \]
\[ J_z = \frac{1}{2}(a_1^\dagger a_1 - a_2^\dagger a_2). \]

We note here that we have used the operators as defined in Ref. [3], in order to be consistent with the definition of the SU(2) purity found in that article. The most natural set of states which exhibit spontaneously broken symmetry is then the coherent atomic states introduced by Arecchi et al. [4], constructed from the Dicke states [5], which are themselves eigenstates of \( J_x \). These coherent atomic states exhibit a generalised SU(2) purity of one, which is the maximum value.

In the case of a symmetric three-well condensate in the three-mode approximation [6], it is natural to use operators based on the SU(3) group generators,

\[ Q_1 = \frac{1}{3}(a_1^\dagger a_1 - a_2^\dagger a_2), \]
\[ Q_2 = \frac{1}{3}(a_1^\dagger a_1 + a_2^\dagger a_2 - 2a_3^\dagger a_3), \]
\[ J_k = i(a_j^\dagger a_j - a_k^\dagger a_k), \]
\[ P_k = a_j^\dagger a_j + a_k^\dagger a_k, \]

where \( k = 1, 2, 3 \) and \( j = (k+1)\text{mod}3 + 1 \). Note that \( a_j \) is the bosonic annihilation operator for the mode contained in the third well. As with the two-mode system, atomic coherent states of the SU(3) group may be defined [7], which are again the minimum uncertainty states of the relevant phase space and will therefore have an SU(3) purity of one.

Having defined the appropriate operators for each of these groups, we turn our attention to statements made that a generalised purity of less than one signifies entanglement in these bosonic systems. The Lie algebra purities were introduced as a subsystem-independent generalisation of entanglement [8]. The authors presented a notion of generalised entanglement (GE), which was claimed to incorporate previously introduced entanglement settings in a unifying framework. They wrote “This is achieved by realizing that entanglement is an observer-dependent concept, whose properties are determined by the expectations of a distinguished subspace of observables of the system of interest, without reference to a preferred subsystem decomposition. Distinguished observables may represent a limited means of manipulating and measuring the system. Standard
entanglement is recovered when these means are limited to local observables acting on subsystems”. The view of entanglement that we will use here follows Schrödinger [9], who wrote “When two systems, of which we know the states by their respective representatives, enter into temporary physical interaction due to known forces between them, and when after a time of mutual influence the systems separate again, then they can no longer be described in the same way as before, viz. by endowing each of them with a representative of its own. I would not call that one but rather the characteristic trait of quantum mechanics, the one that enforces its entire departure from classical lines of thought. By the interaction the two representatives [the quantum states] have become entangled”. It can easily be seen that there are two main requirements here, these being (i) the interaction, and (ii) the separation.

We will proceed by giving examples of particular quantum states in two- and three-well systems which are separated but have not interacted, and calculate the purities for these. Given that the Schwinger model was originally introduced for uncoupled oscillators, we are justified in defining initial quantum states in each well. We will not address whether or not it is possible to manufacture such states in the laboratory, but will use the fact that, according to Schrödinger’s definition, none of them can possibly be entangled, as they have never interacted and are completely separable. We will thus show that a generalised purity of less than unity is not a reliable signal of entanglement for indistinguishable particles.

2. Generalised purity for the two-well model

The generalised purity of the SU(2) algebra is defined as [3]

\[ P_{SU(2)}(|\psi\rangle) = \frac{\langle J_x \rangle^2 + \langle J_y \rangle^2 + \langle J_z \rangle^2}{\langle \tilde{F}^2 \rangle}, \]

where \( \tilde{F}^2 = J_x^2 + J_y^2 + J_z^2 \) and the expectation values are those for the state \( |\psi\rangle \). It is a reasonably simple matter to evaluate this expression for a number of different quantum states. We will consider three different states for a system where the atoms in each of the two wells have never interacted with those in the other, the density matrix is fully separable, and thus entanglement in the standard sense cannot be present. These will be (i) an independent Glauber–Sudarshan coherent state in each well; (ii) an independent Fock state of fixed atom number in each well; and (iii) an independent coherently displaced squeezed state in each well [10].

2.1. Coherent states

We write a state with a coherent state in each well as \( |\psi\rangle = |\alpha_1, \alpha_2\rangle \), so that we have \( \hat{a}_1 \hat{a}_2|\alpha_1, \alpha_2\rangle = \alpha_1 \alpha_2|\alpha_1, \alpha_2\rangle \). It is then a trivial matter to find the expectation values,

\[ \langle J_x \rangle = \frac{1}{2} (\langle \alpha_1 \rangle^2 - \langle \alpha_2 \rangle^2), \]
\[ \langle J_y \rangle = \frac{1}{2} (\alpha_1 \langle \alpha_2 \rangle - \alpha_2 \langle \alpha_1 \rangle), \]
\[ \langle J_z \rangle = \frac{1}{2} (\alpha_1 \langle \alpha_2 \rangle + \alpha_2 \langle \alpha_1 \rangle). \]

We can also calculate

\[ \langle J_x^2 \rangle = \frac{1}{4} (\langle \alpha_1 \rangle^4 + \langle \alpha_2 \rangle^4 + \langle \alpha_1 \rangle^2 + \langle \alpha_2 \rangle^2 - 2\langle \alpha_1 \rangle^2 \langle \alpha_2 \rangle^2), \]
\[ \langle J_y^2 \rangle = \frac{1}{4} (2\langle \alpha_1 \rangle^2 \langle \alpha_2 \rangle^2 + \langle \alpha_1 \rangle^2 + \langle \alpha_2 \rangle^2 - \alpha_1^2 \alpha_2^2 - \alpha_2^2 \alpha_1^2), \]
\[ \langle J_z^2 \rangle = \frac{1}{4} (2\langle \alpha_1 \rangle^2 \langle \alpha_2 \rangle^2 + \langle \alpha_1 \rangle^2 + \langle \alpha_2 \rangle^2 + \alpha_1 \alpha_2^2 + \alpha_2 \alpha_1^2). \]

so that

\[ \langle \tilde{F}^2 \rangle = \frac{1}{4} \left( \langle \alpha_1 \rangle^4 + \langle \alpha_2 \rangle^4 + 2\langle \alpha_1 \rangle^2 \langle \alpha_2 \rangle^2 + 3\langle \alpha_1 \rangle^2 + 3\langle \alpha_2 \rangle^2 \right), \]

which is easily seen to equal \( \frac{N_I}{2} \left( \frac{N_I}{2} + 1 \right) \) given in Ref. [2], with \( N_I \) being the expectation value of the total number of atoms.

It is now a trivial matter to calculate

\[ \langle J_x \rangle^2 + \langle J_y \rangle^2 + \langle J_z \rangle^2 = \frac{1}{4} (\langle \alpha_1 \rangle^2 + \langle \alpha_2 \rangle^2)^2, \]

so that the generalised purity for the Glauber–Sudarshan coherent states is

\[ P_{SU(2)}(|\alpha_1, \alpha_2\rangle) = \frac{(\langle \alpha_1 \rangle^2 + \langle \alpha_2 \rangle^2)^2}{(\langle \alpha_1 \rangle^2 + \langle \alpha_2 \rangle^2)^2 + 3(\langle \alpha_1 \rangle^2 + \langle \alpha_2 \rangle^2)}. \]

This expression is obviously always less than unity, and has an upper limit of unity in the limit of infinite coherent excitation.

2.2. Fock states

We now consider a system with an independent Fock state in each well, so that \( |\psi\rangle = |n_1, n_2\rangle \). It is immediately obvious that there is only one possible non-zero expectation value \( \langle J_0 \rangle \), which is

\[ \langle J_0 \rangle = \frac{1}{2} (n_1 - n_2), \]

and we find the sum of the expectation values of the squares as

\[ \langle \tilde{F}^2 \rangle = \frac{1}{4} \left[ (n_1 + n_2)^2 + 2(n_1 + n_2) \right]. \]

This then gives the SU(2) purity as

\[ P_{SU(2)}(|n_1, n_2\rangle) = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2 + 2(n_1 + n_2)}. \]

which can vary from zero when \( n_1 = n_2 \) to a value which approaches unity when one of the wells has a much higher occupation than the other.

We can use this example of two independent Fock states as a prime example of exactly why “generalised entanglement” is not a good measure for these systems. Considering the simplest possible case, with one atom in each well (labelled by L and R), in the notation of first quantisation the state is defined as

\[ |1, 1\rangle = \frac{1}{\sqrt{2}} (|L\rangle - |R\rangle + |R\rangle - |L\rangle), \]

where the symmetrisation is imposed by the fact that we are dealing with bosons. Written in this form, the overall state appears entangled but when we use the formalism of second quantisation, the situation is quite different, as shown by Benatti et al. [11,12]. In fact, all situations with Fock states of indistinguishable particles in each well can be shown to be separable with respect to the natural partition of the overall state, which is in terms of the atoms in each well. Benatti et al. [12] discuss how the tensor product structure which is natural for addressing issues of separability in systems of distinguishable particles is not appropriate for indistinguishable particles. These should instead be investigated within the formalism of second quantisation through introduction of the canonical bosonic creation and annihilation operators. In this context, entanglement corresponds to the existence of non-classical correlations among commuting observables which are measured in non-overlapping spatial regions, labelled \( V_1 \) and \( V_2 \). In the two-well model we consider here, these regions are
the two separate wells and the operators are \( \hat{a}_1 \) and \( \hat{a}_2 \), along with their creation equivalents. They then define two-point functions of the form \( \omega(P_x, P_y) \), where the \( P_x \) are polynomials in the creation and annihilation operators acting in the regions \( V_1 \) and \( V_2 \). An observable is then separable in terms of \( \omega \) if it can be decomposed into a convex linear combination of a product of expectation values of two commuting subalgebras \( (AB) \) of the entire algebra of the operators,

\[
\omega(AB) = \sum_i \lambda_i \omega_i^2(A) \omega_i^2(B),
\]

with \( \lambda_i > 0 \) and \( \sum \lambda_i = 1 \). Otherwise it is entangled with respect to the algebras \( (AB) \). In the context of this article, it should be obvious that we are dealing with separable states in terms of the algebras pertinent to the different wells.

### 2.3. Coherently displaced squeezed states

For notational convenience we will write our squeezed states as \( |s_1, s_2\rangle \), where \( s_j = \alpha_j r_j \), with \( \alpha_j \) the coherent displacement and \( r_j \) the squeezing parameter \([10]\). Note that, in the interests of simplicity, we will consider \( r_1 \) and \( r_2 \) to be real. Using the fact that such a state is produced by the action of first squeezing and then displacing the vacuum,

\[
|s_1, s_2\rangle = D(\alpha_1)S(r_1)D(\alpha_2)S(r_2)|0, 0\rangle,
\]

we may calculate all the required expectation values. We find

\[
\begin{align*}
\langle J_x \rangle &= \frac{1}{2}(\alpha_1^2 + \sinh^2 r_1 - \alpha_2^2 - \sinh^2 r_2), \\
\langle J_y \rangle &= \frac{1}{2}(\alpha_1 \alpha_2 - \alpha_1 \alpha_2), \\
\langle J_z \rangle &= \frac{1}{2}(\alpha_1 \alpha_2 + \alpha_1 \alpha_2),
\end{align*}
\]

so that

\[
\langle J_x \rangle^2 + \langle J_y \rangle^2 + \langle J_z \rangle^2 = \frac{1}{4} \left[ (\alpha_1^2 + \alpha_2^2)^2 + 2(\alpha_1^2 - \alpha_2^2)(\sinh^2 r_1 - \sinh^2 r_2) + (\sinh^2 r_1 - \sinh^2 r_2)^2 \right].
\]

which we can see is the same expression as for a coherent state when \( r_j = 0 \). We now turn to the terms in the denominator, finding

\[
\begin{align*}
\langle J_x^2 \rangle &= \frac{1}{4} \left[ (\alpha_1^2 - \alpha_2^2)^2 + \alpha_1^2(\cosh r_1 - \sinh r_1)^2 + \alpha_2^2(\cosh r_2 - \sinh r_2)^2 + (\sinh^2 r_1 - \sinh^2 r_2)^2 \right], \\
\langle J_y^2 \rangle &= \frac{1}{4} \left[ (\alpha_1^2 + \alpha_2^2)^2 + \alpha_1^2(\sinh r_2 + \cosh r_2)^2 + \alpha_2^2(\sinh r_1 + \cosh r_1)^2 \right], \\
\langle J_z^2 \rangle &= \frac{1}{4} \left[ 4(\alpha_1^2 \alpha_2^2 + \alpha_1^2 \sinh r_2 - \cosh r_2)^2 + \alpha_2^2(\sinh r_1 - \cosh r_1)^2 \right] + (\sinh r_1 \cosh r_2 + \sinh r_2 \cosh r_1)^2.
\end{align*}
\]

so that

\[
\begin{align*}
\langle J^2 \rangle &= \frac{1}{4} \left[ (\alpha_1^2 + \alpha_2^2)^2 + \alpha_1^2(\cosh r_1 - \sinh r_1)^2 + (\sinh^2 r_2 + \cosh^2 r_2) \right] \\
&+ 2 \left( \sinh^2 r_1 + \sinh^2 r_2 \right) \left( \cosh^2 r_1 + \cosh^2 r_2 \right), \\
&+ \alpha_2^2 \left( \cosh r_2 - \sinh r_2 \right)^2 + 2 \left( \sinh^2 r_1 + \cosh^2 r_1 \right) \\
&+ 2 \left( \sinh^2 r_1 + \sinh^2 r_2 \right) \left( \cosh^2 r_1 + \cosh^2 r_2 \right).
\end{align*}
\]

The expression for \( P_{SU(2)}(s_1, s_2) \) is therefore rather complicated and large, but we can evaluate it readily for some special cases. Firstly, when \( r_1 = r_2 = 0 \), so that we have two independent Glauber–Sudarshan coherent states, we find the same result as that given above in Eq. (8), as required. For two squeezed states with zero coherent excitation, we find

\[
P_{SU(2)}(|r_1, r_2\rangle) = \frac{\sinh^2 r_1 - \sinh^2 r_2}{2 \left( \sinh^2 r_1 + \sinh^2 r_2 \right) \left( \cosh^2 r_1 + \cosh^2 r_2 \right)},
\]

which is zero if \( r_1 = r_2 \) and tends towards one half for \( r_1 \gg r_2 \).

### 3. Generalised purity for the three-well model

We will now consider the generalised purity associated with the SU(3) algebra which is defined by Vischidi et al. \([6]\) as

\[
P_{SU(3)}(|\psi\rangle) = \frac{9}{N^2} \left( \frac{\langle \psi | Q_1 | \psi \rangle^2}{3} + \frac{\langle \psi | Q_2 | \psi \rangle^2}{4} + \sum_{j=1}^{3} \frac{\langle \psi | P_j | \psi \rangle^2}{12} + \frac{1}{3} \sum_{j=1}^{3} \langle \psi | J_j | \psi \rangle^2 \right),
\]

where \( P_j, Q_j \) and \( Q_1 \) are as defined in the Introduction, Eq. (2), and \( N = \sum a_i^2 \). It has been stated in various publications that states with \( P_{SU(3)}(|\psi\rangle) = 1 \) are separable, with any decrease from this maximum value indicating entanglement among the particles \([6,13,14]\). We will now evaluate this purity for the three-mode analogues of the separable states considered in Section 2.

#### 3.1. Independent coherent states

We consider independent occupations of each well by Glauber–Sudarshan coherent states, \( |\psi\rangle = |\alpha_1, \alpha_2, \alpha_3\rangle \), and calculate

\[
\begin{align*}
\langle Q_1 \rangle^2 &= \frac{1}{4} \left( |\alpha_1|^2 - |\alpha_2|^2 \right)^2, \\
\langle Q_2 \rangle^2 &= \frac{1}{4} \left( |\alpha_1|^2 + |\alpha_2|^2 - 2 |\alpha_3|^2 \right)^2, \\
\langle P_1 \rangle^2 &= (|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2)^2, \\
\langle P_2 \rangle^2 &= (|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2)^2, \\
\langle P_3 \rangle^2 &= (|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2)^2, \\
\langle J_1 \rangle^2 &= -|\alpha_1|^2 |\alpha_3|^2, \\
\langle J_2 \rangle^2 &= -|\alpha_2|^2 |\alpha_3|^2, \\
\langle J_3 \rangle^2 &= -|\alpha_3|^4,
\end{align*}
\]

as well as

\[
\begin{align*}
\langle N^2 \rangle &= \left( |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 \right)^2 + |\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 \]
\quad = \langle N \rangle^2 + \langle N \rangle.
\end{align*}
\]
It is the a simple matter to combine these expressions as in Eq. (20) to find
\[ P_{(3)}(\alpha_1, \alpha_2, \alpha_3) = \frac{(|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2)^2}{(|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2) + (|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2)} \]
\[ = \frac{(N)^2}{(N)^2 + (N)} \]

It is readily seen that this value will always be smaller than one, approaching one in the limit of extremely large \( N \).

3.2. Independent Fock states

We now turn our attention to three independent Fock states, \( |n_1, n_2, n_3\rangle \). We find
\[ Q_1 = \frac{1}{2}(n_1-n_2), \]
\[ Q_2 = \frac{1}{2}(n_1 + n_2 - 2n_3), \]
\[ J_k = P_k = 0. \]

After a little simple algebra, we find
\[ P_{(3)}(|n_1, n_2, n_3\rangle) = 1 - \frac{3(n_1n_2 + n_3n_3)}{(n_1 + n_2 + n_3)^2}. \]

It is readily seen that this will be equal to zero when \( n_1 = n_2 = n_3 \) and can take on a range of values when one well is much more highly occupied than the others.

3.3. Independent squeezed states

In the case of three independent coherently displaced squeezed states, with \( \alpha \) the coherent displacements and \( r \) the squeezing parameters, we find
\[ (Q_1)^2 = \frac{1}{4} \left( |\alpha|^2 + \sinh^2 r_1 - |\alpha|^2 - \sinh^2 r_2 \right)^2, \]
\[ \text{and} \]
\[ (Q_2)^2 = \frac{1}{4} \left[ |\alpha|^2 + \sinh^2 r_1 + |\alpha|^2 + \sinh^2 r_2 - 2\left( |\alpha|^2 + \sinh^2 r_3 \right) \right]^2, \]
with the \( P_k \) and \( J_k \) being the same as for coherent states, see Eq. (21). This gives the numerator as
\[ N = \left( |\alpha|^2 + |\alpha|^2 + |\alpha|^2 + \sinh^2 r_2 + |\alpha|^2 + \sinh^2 r_3 \right)^2 \]
\[ - 3 \left[ |\alpha|^2 \left( \sinh^2 r_2 + \sinh^2 r_3 \right) + |\alpha|^2 \left( \sinh^2 r_1 + \sinh^2 r_3 \right) + |\alpha|^2 \left( \sinh^2 r_1 + \sinh^2 r_2 \right) \right]. \]

The denominator is found as
\[ \langle N^2 \rangle = \left( |\alpha|^2 + |\alpha|^2 + |\alpha|^2 + |\alpha|^2 + \sinh^2 r_2 + |\alpha|^2 + |\alpha|^2 \right)^2 \]
\[ + \left( |\alpha|^2 + |\alpha|^2 \sinh^2 r_1 + |\alpha|^2 \sinh^2 r_2 + |\alpha|^2 \sinh^2 r_3 \right)^2 \]
\[ + 2 \sum_{j=1}^{3} \sinh^2 r_j \cosh^2 r_j. \]

Again we see that the full expression for \( P_{SU(3)} \) is complicated, but easy to evaluate in some special cases. For example, when \( r_j = 0 \), we find the same value as for coherent states, given in Eq. (23). When the \( \alpha_i \) are all set to zero, we find
\[ P_{SU(3)}(|r_1, r_2, r_3\rangle) = \frac{N_i^2}{N_i^2 + 2\sum_j \sinh^2 r_j \cosh^2 r_j}, \]
where \( N_i = \sinh^2 r_1 + \sinh^2 r_2 + \sinh^2 r_3 \). It is readily seen that, whatever combination of \( \alpha \) and \( r \) we choose, the purity will be less than one, despite the fact that the states have been constructed so as to be completely separable.

4. Discussion and conclusions

While we follow what we see as the spirit of Schrödinger’s view of entanglement and consider the standard definition of entanglement as applied to bosonic systems, Ref. [13] introduces the concept of generalised entanglement, stating “it may also be that for some problems, correlations between particles, rather than modes, are relevant, taking us beyond the distinguishable-subsystems framework of standard entanglement theory”. The claim may therefore be made that the systems we examine in this work, which demonstrate Lie algebra purities of less than unity, exhibit “particle entanglement” rather than mode entanglement. This seems to leave two options: either some of the particles in one well are somehow entangled with some of the particles in the other, or this generalised entanglement is a property of the particles in one well. As the operators used to define the purity operate on atoms in both wells, this leaves open the question as to how an indistinguishable boson from one well can be entangled with one in the other well with which it has never interacted. If we confine ourselves to single wells, there also seems to be a contradiction in that condensed bosons all share the same, non-separable, wavefunction and density matrix, so what the purity measures can therefore also not be measuring entanglement in any meaningful physical sense.

We believe that the differences in the definitions of what can be considered entangled come about because of the use of first quantisation, where, as seen above, two separable but indistinguishable bosons are seen as being entangled. We believe that the formalism of second quantisation is necessary to meaningfully discuss entanglement when the constituent particles of the overall system are indistinguishable, with the entanglement that seems to exist in first quantisation merely being a formal consequence of symmetrisation of the wavefunction. In fact, if we rely on the states as written in first quantisation, and use the fact that any states of indistinguishable bosons can be expanded in bases of number states, the necessary symmetrisation would lead us to write almost every possible system as being “particle entangled” with any other system of similar indistinguishable particles, irrespective of any interactions which may have taken place, and irrespective of whether second quantisation showed them to be separable or not. For indistinguishable particles, this can make the idea of generalised entanglement defined in this way so broad as to become essentially meaningless.

In conclusion, we have shown that the generalised SU(2) and SU(3) purities are not a useful entanglement measure for multi-mode continuous variable bosonic systems by considering the cases of two- and three-well Bose–Hubbard models and demonstrating that fully separable states can be constructed which give a value of less than one. This suggests strongly that great care should be used with this measure if it is desired to use it as a signature of quantum entanglement for bosonic systems, and that by itself it is not sufficient. What it does measure is the “distance” of a quantum state from one of the SU(N) coherent states, which is not necessarily related to entanglement, but may be useful when considering other properties of a system, such as critical points and phase transitions. While it is obviously a useful mathematical and abstract generalisation of standard
entanglement measures, in the cases we have discussed in this article it is very difficult to give any physical content to this generalisation.

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