Entanglement and Composite Bosons

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Abstract

We build upon work by C. K. Law [Phys. Rev. A \textbf{71}, 034306 (2005)] to show in general that the entanglement between two fermions largely determines the extent to which the pair behaves like an elementary boson. Specifically, we derive upper and lower bounds on a quantity $\chi_{N+1}/\chi_N$ that governs the bosonic character of a pair of fermions when $N$ such pairs approximately share the same wavefunction. Our bounds depend on the purity of the single-particle density matrix, an indicator of entanglement, and demonstrate that if the entanglement is sufficiently strong, the quantity $\chi_{N+1}/\chi_N$ approaches its ideal bosonic value.
Under what circumstances can a pair of fermions be treated as an elementary boson? Many authors have done detailed studies of this question, as it applies, for example, to atomic Bose-Einstein condensates [1, 2], excitons [2–4], and Cooper pairs in superconductors [5]. In a 2005 paper, C. K. Law presented evidence that the question can be answered in general in terms of entanglement: two fermions can be treated as an elementary boson if they are sufficiently entangled [6]. Consider, for example, a single hydrogen atom in a harmonic trap. Within the atom, the proton and electron are strongly entangled with respect to their position variables; for example, wherever the proton might be found—it could be anywhere in the trap—the electron is sure to be nearby. Law suggests that this entanglement is the essential property underlying the (approximate) bosonic behavior of the composite particle, allowing, for example, a collection of many hydrogen atoms to form a Bose-Einstein condensate [7].

Specifically, his hypothesis can be expressed as follows: For a single composite particle in a pure state, let $P$ be the purity of the reduced state of either of the two component fermions—$P$ is small when the entanglement between the two particles is large (see below for the definition)—and let $N$ be the number of composite particles that approximately share the given quantum state. Then the composite particles can be treated as bosons as long as $NP \ll 1$. That is, according to this hypothesis, the quantity $1/P$ roughly quantifies the number of particles one can put into the same pure state, before the composite nature of the particles begins to interfere appreciably with their ideal bosonic behavior.

Law's argument in support of this hypothesis assumes a two-particle wavefunction within a certain class, characterized by a specific form of the eigenvalues of the reduced density matrix of either particle, and he notes that it would be desirable to extend the argument to more general wavefunctions. Such a generalization is the aim of the present paper. With no restrictions on the form of the two-particle wavefunction, we use the purity to place upper and lower bounds on Law’s measure of bosonic character, and we show that these bounds are the tightest possible of the given form. In this way we obtain a more general connection between entanglement and bosonic character.

Before proceeding to our general argument, it may be instructive to consider the special case of the hydrogen atom. Let $\Psi(\vec{R}, \vec{r})$ be the wavefunction of a single hydrogen atom in a harmonic trap, with $\vec{R}$ and $\vec{r}$ being the position coordinates of the proton and electron, respectively. For simplicity we assume that the proton is sufficiently massive compared to
the electron that we can write this wavefunction as

\[ \Psi(\vec{R}, \vec{r}) = \psi(\vec{R}) \phi(\vec{r} - \vec{R}), \]  

(1)

where \( \psi \) is the ground-state harmonic oscillator wavefunction

\[ \psi(\vec{R}) = \frac{1}{\pi^{3/4} b^{3/2}} \exp(-R^2/2b^2), \]  

(2)

and \( \phi \) is the ground-state wavefunction of the electron in a hydrogen atom:

\[ \phi(\vec{r}) = \frac{1}{\pi^{1/2} a_0^{3/2}} \exp(-r/a_0). \]  

(3)

Here \( a_0 \) is the Bohr radius and \( b \) is a length parameter characterizing the size of the trap.

The purity \( P \) of the reduced state of either of the two particles is defined by

\[ P = \text{Tr} \rho^2, \]  

(4)

where \( \rho \) is the density matrix of the particle in question. (Because the pair is in a pure state, the purities of the two particles are guaranteed to be equal.) Note that \( P \) takes values between zero and one. For the hydrogen atom, the purity of the proton is given by

\[ P = \int |\psi(\vec{R})|^2 |\psi(\vec{R} + \vec{q})|^2 |\sigma(\vec{q})|^2 d\vec{R} d\vec{q}, \]  

(5)

where the proton’s density matrix \( \rho \) is

\[ \rho(\vec{R}, \vec{R}') = \int \Psi(\vec{R}, \vec{r}) \Psi^*(\vec{R}', \vec{r}) d\vec{r}. \]  

(6)

Inserting Eq. (1) into the definition of \( P \), we find that

\[ P = \int |\psi(\vec{R})|^2 |\psi(\vec{R}' - \vec{R})|^2 d\vec{R} d\vec{R}'. \]  

(7)

But the range of \( \sigma \) is comparable to the Bohr radius and much smaller than the dimension of the trap. So we can reasonably replace \( |\psi(\vec{R} + \vec{q})|^2 \) in Eq. (8) with \( |\psi(\vec{R})|^2 \) and write

\[ P = \int |\psi(\vec{R})|^4 d\vec{R} \int |\sigma(\vec{q})|^2 d\vec{q}. \]  

(10)
The integrals can be done, and one finds that
\[ P = \frac{33}{4\sqrt{2\pi}} \left( \frac{a_0}{b} \right)^3. \] (11)

Thus the purity depends, not surprisingly, on the ratio of the volume of an atom to the volume of the trap, and Law’s condition \( NP \ll 1 \) essentially says that the space available to each atom must be large compared to its size. This condition is in rough agreement with the condition that the number of atoms be small compared to the maximum occupation number as computed in Ref. [2].

We now turn to the general argument.

Consider a composite particle formed from two distinguishable, fundamental fermions \( A \) and \( B \) with wavefunction \( \Psi(x_A, x_B) \). (Here the \( x \)'s could be vectors in any number of dimensions.) Writing this wavefunction in its Schmidt decomposition yields
\[ \Psi(x_A, x_B) = \sum_p \lambda_p^{1/2} \phi_p^{(A)}(x_A) \phi_p^{(B)}(x_B). \] (12)

Here \( \phi_p^{(A)} \) and \( \phi_p^{(B)} \) are the Schmidt modes, constituting orthonormal bases for the states of particles \( A \) and \( B \), and the \( \lambda_p \)'s, which are the eigenvalues of each of the single-particle density matrices, are nonnegative real numbers satisfying \( \sum_p \lambda_p = 1 \). In terms of the \( \lambda_p \)'s, the purity can be written as
\[ P = \sum_p \lambda_p^2. \] (13)

Again, a small value of the purity indicates a large entanglement.

In terms of creation operators, the state \( \Psi(x_A, x_B) \) can be written as
\[ \Psi(x_A, x_B) = \sum_p \lambda_p^{1/2} a_p^\dagger b_p^\dagger |0\rangle, \] (14)

where \( a_p^\dagger \) creates an \( A \) particle in the state \( \phi_p^{(A)}(x_A) \), \( b_p^\dagger \) creates a \( B \) particle in the state \( \phi_p^{(B)}(x_B) \), and \( |0\rangle \) is the vacuum state. The composite particle creation operator \( c^\dagger \), which creates a pair of \( A \) and \( B \) particles in the state \( \Psi(x_A, x_B) \), is defined to be
\[ c^\dagger = \sum_p \lambda_p^{1/2} a_p^\dagger b_p^\dagger. \] (15)

Our analysis, like Law’s, aims to determine to what extent the operators \( c^\dagger \) and \( c \) act like bosonic creation and annihilation operators when applied to a state consisting of \( N \) composite particles.
Consider the state obtained by antisymmetrizing the product state
\[ \Psi\left(x_A^{(1)}, x_B^{(1)}\right) \cdots \Psi\left(x_A^{(N)}, x_B^{(N)}\right). \]
In terms of the creation operator \( c^\dagger \), we can write the properly antisymmetrized state as
\[ |N\rangle = \frac{1}{\sqrt{N!}} \chi_N^{-1/2} (c^\dagger)^N |0\rangle. \]  
(16)

Here \( \chi_N \) is a normalization constant necessary because \( c^\dagger \) is not a perfect bosonic creation operator. The quantity \( \chi_N \) is given by
\[ \chi_N = \frac{1}{N!} \langle 0 | c^N (c^\dagger)^N | 0 \rangle = \sum_{p_1 \ldots p_N \text{ all different}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N}. \]  
(17)

(This expression gives \( \chi_N = 0 \) if the number \( N \) exceeds the number of Schmidt modes with nonzero Schmidt coefficient. In that case \( (c^\dagger)^N |0\rangle = 0 \) and we cannot define the state \( |N\rangle \).) For an ideal boson, we would have \( \chi_N = 1 \).

Note that \( c^\dagger |N\rangle \) is not necessarily equal to \( \sqrt{N+1} |N+1\rangle \). Rather, it follows from the definition (16) that
\[ c^\dagger |N\rangle = \alpha_{N+1} \sqrt{N+1} |N+1\rangle, \]  
(18)

where
\[ \alpha_N = \sqrt{\frac{\chi_N}{\chi_{N-1}}}. \]  
(19)

Similarly, instead of \( c |N\rangle = \sqrt{N} |N-1\rangle \), we have
\[ c |N\rangle = \alpha_N \sqrt{N} |N-1\rangle + |\epsilon_N\rangle, \]  
(20)

where \( |\epsilon_N\rangle \) is orthogonal to \( |N-1\rangle \). For perfect bosons, we would have \( \langle \epsilon_N | \epsilon_N \rangle = 0 \), but the actual value is
\[ \langle \epsilon_N | \epsilon_N \rangle = 1 - \frac{\chi_{N+1}}{\chi_N} - N \left( \frac{\chi_N}{\chi_{N-1}} - \frac{\chi_{N+1}}{\chi_N} \right). \]  
(21)

In the Appendix, we show that the ratio \( \chi_{N+1}/\chi_N \) which appears in Eqs. (19) and (21) is strictly non-increasing as \( N \) increases (more precisely, we show that \( \chi_N^2 - \chi_{N+1} \chi_{N-1} \) is non-negative), so that the quantity in parentheses in Eq. (21) is non-negative. It follows that both \( \alpha_N \) and \( \langle \epsilon_N | \epsilon_N \rangle \) will be within a small amount \( \delta \) of their bosonic values when \( \chi_{N+1}/\chi_N \geq 1 - \delta \). One can also show that
\[ \langle N | [c, c^\dagger] | N \rangle = 2 \left( \frac{\chi_{N+1}}{\chi_N} \right) - 1, \]  
(22)
which is within $2\delta$ of its ideal bosonic value, 1, under the same condition. We therefore follow Law in using the ratio $\chi_{N+1}/\chi_N$—we call it the “$\chi_N$-ratio”—as our indicator of bosonic character [6, 9].

One might wonder why we confine our attention to quantities involving only the state $|N\rangle$ and nearby states, rather than insisting that the operator $c$ act like a bosonic operator on the whole subspace spanned by $\{|0\rangle, \ldots, |N\rangle\}$. The reason is that we are interested in a state that approximates $|N\rangle$, and we wish to quantify the degree to which the system behaves like a collection of bosons when a composite particle is added to or removed from this state. Hence our focus on $\chi_{N+1}/\chi_N$ as the quantifier of bosonic character rather than $\chi_N$ itself. We note that because the $\chi_N$-ratio is non-increasing with $N$, a lower bound on $\chi_{N+1}/\chi_N$ will also be a lower bound on $\chi_{N'+1}/\chi_{N'}$ for all $N' < N$. However, as one can see in Ref. [8], this fact is not sufficient to guarantee that $\chi_N$ itself is close to unity whenever $\chi_{N+1}/\chi_N$ is.

In the remainder of the paper we prove two inequalities relating the $\chi_N$-ratio to the purity.

The first is a lower bound: $\chi_{N+1}/\chi_N \geq 1 - NP$. To show this, we consider the quantity $\chi_{N+1} - \chi_N(1 - NP)$ and show that it must be non-negative.

\[
\chi_{N+1} - \chi_N(1 - NP) = \sum_{p_1 \ldots p_{N+1}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_{N+1}} - \left(1 - N \sum_p \lambda_p^2\right) \sum_{p_1 \ldots p_N} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N}
\]

\[
= \sum_{p_1 \ldots p_{N+1}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_{N+1}} - \sum_{p_1 \ldots p_N} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N} \lambda_{p_{N+1}} + N \sum_{p_1 \ldots p_N} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N} \lambda_{p_{N+1}}^2
\]

\[
= -N \sum_{p_1 \ldots p_{N}} \lambda_{p_1}^2 \lambda_{p_2} \ldots \lambda_{p_N}.
\]

Note that the first two sums of the last line have many terms in common, which therefore cancel out. The only terms remaining from those sums are the terms in the second sum for which the value of $p_{N+1}$ is equal to the value of one of the indices $p_k$ with $k = 1, \ldots, N$. Each of these $N$ possibilities yields the same result; so we can combine those first two sums into the expression

\[
- N \sum_{p_1 \ldots p_{N}} \lambda_{p_1}^2 \lambda_{p_2} \ldots \lambda_{p_N}.
\]
We therefore have
\[ \chi_{N+1} - \chi_N(1-NP) = -N \sum_{p_1 \ldots p_N \text{ all different}; p_{N+1} \text{ free}} \lambda_{p_1}^2 \lambda_{p_2} \ldots \lambda_{p_N} \lambda_{p_{N+1}} + N \sum_{p_1 \ldots p_N \text{ all different}; p_{N+1} \text{ free}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N} \lambda_{p_{N+1}}^2. \] (25)

Again the two sums have many terms in common. Cancelling these terms leaves
\[ \chi_{N+1} - \chi_N(1-NP) = N(N-1) \sum_{p_1 \ldots p_N \text{ all different}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N} \right] \left( \lambda_{p_1}^2 + \lambda_{p_2}^2 - 2\lambda_{p_1} \lambda_{p_2} \right). \] (26)

Now, Eq. (26) can be rewritten as
\[ \chi_{N+1} - \chi_N(1-NP) = \frac{N(N-1)}{2} \sum_{p_1 \ldots p_N \text{ all different}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N} \right] \left( \lambda_{p_1}^2 + \lambda_{p_2}^2 - 2\lambda_{p_1} \lambda_{p_2} \right) - \sum_{p_1 \ldots p_N \text{ all different}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N} \lambda_{p_{N+1}}^2 \geq 0, \] (27)
thus yielding the bound
\[ \frac{\chi_{N+1}}{\chi_N} \geq 1 - NP. \] (28)

This bound shows that a sufficiently small purity entails nearly bosonic character as quantified by $\chi_{N+1}/\chi_N$. We now derive a bound in the other direction, showing that a nearly bosonic value of $\chi_{N+1}/\chi_N$ implies a small purity. For this purpose we start with
\[ (1-P)\chi_N - \chi_{N+1} = \left( 1 - \sum_p \lambda_p^2 \right) \sum_{p_1 \ldots p_N \text{ all different}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_N} - \sum_{p_1 \ldots p_{N+1} \text{ all different}} \lambda_{p_1} \lambda_{p_2} \ldots \lambda_{p_{N+1}} \right] \left( \lambda_{p_1}^2 + \lambda_{p_2}^2 - 2\lambda_{p_1} \lambda_{p_2} \right) \] (29)
By combining sums as before (inserting the identity 1 = \(\sum_{p_{N+1}} \lambda_{p_{N+1}}\) when needed), we get

\[(1 - P)\chi_N - \chi_{N+1} = (N-1) \sum_{p_1 \cdots p_{N+1}} \lambda_{p_1}^2 \lambda_{p_2} \cdots \lambda_{p_{N+1}} + N(N-1) \sum_{p_1 \cdots p_N} \lambda_{p_1}^2 \lambda_{p_2}^2 \cdots \lambda_{p_{N}} \geq 0.\]  

(30)

Combining this result with our earlier inequality (Eq. (28)), we have

\[1 - NP \leq \frac{\chi_{N+1}}{\chi_N} \leq 1 - P.\]  

(31)

We have thus put upper and lower bounds on the \(\chi_N\)-ratio of a composite particle made of two distinguishable fermions, in terms of the entanglement of the pair. We have not specified anything about the form of the wavefunction of the composite particle; so the link between the \(\chi_N\)-ratio and entanglement is established in general.

The lower bound in Eq. (31) is in fact as strong a bound as one could hope to derive in terms of purity, in that the bound is achievable: if there are \(M\) nonzero Schmidt modes and \(\lambda_p = 1/M\), then, by Eq. (27), \(\chi_{N+1}/\chi_N = 1 - NP\) as long as \(N\) is less than \(M\). This lower bound is also achieved by wavefunctions in the class Law considers—this class includes double Gaussian wavefunctions—in the limit \(NP \ll 1\). Because Eq. (30) is never zero unless \(N = 1\) (in which case it is always zero), our upper bound is not, for general \(N\), achievable. Nevertheless, it is the best possible upper bound of the form \(\chi_{N+1}/\chi_N \leq 1 - bP\), whether or not \(b\) depends on \(N\). This is because for any value of \(b\) greater than 1, there exists a distribution of Schmidt coefficients that makes \(1 - bP\) negative—it suffices to make one of the coefficients \(\lambda_k\) very large—whereas \(\chi_{N+1}/\chi_N\) is certainly non-negative. We note also that there can be no upper bound of the form \(1 - bP^r\) with \(r\) less than 1, because such a bound would contradict our lower bound when \(P\) is small.

We have considered in this paper only a single wavefunction \(\Psi(x_A, x_B)\) of the composite particle. One would also like to investigate whether, for several orthogonal wavefunctions \(\Psi_j(x_A, x_B)\), the corresponding creation operators \(c_j^\dagger\) approximately satisfy the bosonic relation \([c_j, c_k] = 0\) for \(j \neq k\). (The relation \([c_j, c_k] = 0\) will automatically be satisfied because of the anticommutation of the underlying fermionic operators.) If the relevant deviation from this commutation relation similarly diminishes to zero as the entanglement of each wavefunction increases, one will then have further evidence for the proposition that entanglement is crucial for determining whether a pair of fermions can be treated as a boson.
Taking this idea to its logical conclusion, Law notes that two particles can be highly entangled even if they are far apart. Could we treat such a pair of fermions as a composite boson? The above analysis suggests that we can do so. However, we would have to regard the pair as a very fragile boson in the absence of an interaction that would preserve the pair’s entanglement in the face of external disturbances. On this view, the role of interaction in creating a composite boson is not fundamentally to keep the two particles close to each other, but to keep them entangled.

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APPENDIX: PROOF THAT $\chi_N^2 - \chi_{N+1}\chi_{N-1} \geq 0$

Let us use the symbol $\sum'$ to indicate a sum over all the indices appearing in the summand, with the restriction that they must all take distinct values. We have, then,

$$\chi_N^2 - \chi_{N+1}\chi_{N-1} = \sum' \lambda_{r_1} \cdots \lambda_{r_N} \sum' \lambda_{p_1} \cdots \lambda_{p_{N-1}} - \sum' \lambda_{r_1} \cdots \lambda_{r_{N+1}} \sum' \lambda_{p_1} \cdots \lambda_{p_{N-1}}. \quad (32)$$

We now treat separately the sum over $p_N$ in the first term and the sum over $r_{N+1}$ in the second term, obtaining

$$\chi_N^2 - \chi_{N+1}\chi_{N-1} = \sum' \lambda_{r_1} \cdots \lambda_{r_N} \left[ \sum' \lambda_{p_1} \cdots \lambda_{p_{N-1}} - \sum' \lambda_{p_1} \cdots \lambda_{p_{N-1}} (\lambda_{p_1} + \cdots + \lambda_{p_{N-1}}) \right]$$

$$- \left[ \sum' \lambda_{r_1} \cdots \lambda_{r_N} - \sum' \lambda_{r_1} \cdots \lambda_{r_{N-1}} (\lambda_{r_1} + \cdots + \lambda_{r_{N-1}}) \right] \sum' \lambda_{p_1} \cdots \lambda_{p_{N-1}} \quad (33)$$

$$= \sum' \lambda_{r_1} \cdots \lambda_{r_N} \sum' \lambda_{p_1} \cdots \lambda_{p_{N-1}} \left[ \lambda_{r_1} + \cdots + \lambda_{r_{N-1}} - (\lambda_{p_1} + \cdots + \lambda_{p_{N-1}}) \right].$$

We now separate the sum over the $p$’s into two parts: (i) the part in which $p_1, \ldots, p_{N-1}$ have the same restrictions as $r_1, \ldots, r_{N-1}$, and (ii) the part in which one of the $p$’s has the same value as $r_N$. So the expression becomes

$$\sum \lambda_{r_N} \sum' \lambda_{r_{N-1}} \sum' \lambda_{p_1} \cdots \lambda_{p_{N-1}} \left[ \lambda_{r_N} + (\lambda_{r_1} + \cdots + \lambda_{r_{N-1}}) - (\lambda_{p_1} + \cdots + \lambda_{p_{N-1}}) \right]$$

$$+ (N - 1) \sum \lambda_{r_N} \sum' \lambda_{r_{N-1}} \sum' \lambda_{p_1} \cdots \lambda_{p_{N-2}} \left[ (\lambda_{r_1} + \cdots + \lambda_{r_{N-1}}) - (\lambda_{p_1} + \cdots + \lambda_{p_{N-2}}) \right].$$

In the first line, everything in the square bracket vanishes except for $\lambda_{r_N}$, because of the symmetry between the $r$’s and the $p$’s. Thus the first line is non-negative. Meanwhile the
expression in the second line that appears within the sum over $r_N$ has the same form as the last line of Eq. (33), except with one fewer $r$ index and one fewer $p$ index. Therefore the same maneuver can be repeated again and again, until at last we are left with an expression that is manifestly non-negative, because there are no more of the negative $p$ terms. It follows that

$$\chi_N^2 - \chi_{N+1}\chi_{N-1} \geq 0. \quad (34)$$

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