Entanglement and Composite Bosons

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We build upon work by C. K. Law [Phys. Rev. A **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 χ_{N+1}/χ_N that governs the bosonic character of a pair of fermions when N such pairs approximately share the same wave function. 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 χ_{N+1}/χ_N approaches its ideal bosonic value.

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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, 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. The bosonic character is quantified, in Law's paper, by the ratio χ_{N+1}/χ_N, where χ_N is a normalization factor for the state with N composite particles. The quantity χ_{N+1}/χ_N captures the deviation from the ideal bosonic case when another composite particle is added to the N-particle state. For ideal bosons, we would have $\chi_N = 1$ for all N.

Law's argument in support of his hypothesis assumes a two-particle wave function 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 wave functions. Such a generalization is the aim of the present Letter. With no restrictions on the form of the two-particle wave function, we use the purity to place upper and lower bounds on χ_{N+1}/χ_N, 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 wave function 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 wave function as

$$\Psi(\vec{R}, \vec{r}) = \psi(\vec{R})\phi(\vec{r} - \vec{R}), \tag{1}$$

where ψ is the ground-state harmonic oscillator wave function $\psi(\vec{R}) = (1/\pi^{3/4}b^{3/2})\exp(-R^2/2b^2)$ and ϕ is the ground-state wave function of the electron in a hydrogen atom: $\phi(\vec{r}) = (1/\pi^{1/2}a_0^{3/2})\exp(-r/a_0)$. 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 $P = \mathrm{Tr}\rho^2$, where ρ 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

$$P = \int \rho(\vec{R}, \vec{R}')\rho(\vec{R}', \vec{R})d\vec{R}d\vec{R}', \tag{2}$$

where the proton's density matrix ρ is $\rho(\vec{R}, \vec{R}') = \int \Psi(\vec{R}, \vec{r})\Psi^*(\vec{R}', \vec{r})d\vec{r}$. We assume that $\psi(\vec{R}')$ can be approximated by $\psi(\vec{R})$ when $|\vec{R}' - \vec{R}|$ is of the order of the

Bohr radius. With this assumption, upon inserting Eq. (1) into the definition (2) of P, we get

$$P = \int |\psi(\vec{R})|^4 d\vec{R} \int |\sigma(\vec{q})|^2 d\vec{q}, \tag{3}$$

where $\sigma(\vec{q}) = \int \phi(\vec{r})\phi^*(\vec{r} - \vec{q}) d\vec{r}$. The integrations can be done, and one finds that

$$P = \frac{33}{4\sqrt{2\pi}}\left(\frac{a_0}{b}\right)^3. \tag{4}$$

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 wave function $\Psi(x_A, x_B)$. (The x's could be vectors in any number of dimensions.) Writing this wave function in its Schmidt decomposition yields

$$\Psi(x_A, x_B) = \sum_p \lambda_p^{1/2} \phi_p^{(A)}(x_A)\phi_p^{(B)}(x_B). \tag{5}$$

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 λ_p's, which are the eigenvalues of each of the single-particle density matrices, are non-negative real numbers satisfying $\sum_p \lambda_p = 1$. In terms of the λ_p's, the purity can be written as $P = \sum_p \lambda_p^2$. 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

$$\Psi(x_A, x_B) = \sum_p \lambda_p^{1/2} a_p^\dagger b_p^\dagger |0\rangle, \tag{6}$$

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 $c^\dagger = \sum_p \lambda_p^{1/2} a_p^\dagger b_p^\dagger$. 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 $\Psi(x_A^{(1)}, x_B^{(1)}) \cdots \Psi(x_A^{(N)}, x_B^{(N)})$. In terms of the creation operator $c^\dagger$, we can write the properly antisymmetrized state as

$$|N\rangle = \frac{1}{\sqrt{N!}} \chi_N^{-1/2} (c^\dagger)^N |0\rangle. \tag{7}$$

Here χ_N is a normalization constant necessary because $c^\dagger$ is not a perfect bosonic creation operator. The quantity χ_N is given by [6,8]

$$\chi_N = \frac{1}{N!}\langle 0| c^N (c^\dagger)^N |0\rangle = \sum\nolimits' \lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}, \tag{8}$$

where we use the symbol $\sum'$ to indicate that the sum is over all the indices appearing in the summand, with the restriction that all the indices must take distinct values. (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 $|N\rangle$.) Again, for ideal bosons, 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 (7) that

$$c^\dagger|N\rangle = \alpha_{N+1}\sqrt{N+1}|N+1\rangle, \tag{9}$$

where

$$\alpha_N = \sqrt{\frac{\chi_N}{\chi_{N-1}}}. \tag{10}$$

Similarly, instead of $c|N\rangle = \sqrt{N}|N-1\rangle$, we have

$$c|N\rangle = \alpha_N\sqrt{N}|N-1\rangle + |\epsilon_N\rangle, \tag{11}$$

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 [6,8]

$$\langle\epsilon_N|\epsilon_N\rangle = 1 - \frac{\chi_{N+1}}{\chi_N} - N\left(\frac{\chi_N}{\chi_{N-1}} - \frac{\chi_{N+1}}{\chi_N}\right). \tag{12}$$

It is possible to show that the ratio χ_{N+1}/χ_N which appears in Eqs. (10) and (12) is strictly nonincreasing as N increases (more precisely, the quantity $\chi_N^2 - \chi_{N+1}\chi_{N-1}$ is non-negative) [9], so that the quantity in parentheses in Eq. (12) is non-negative. It follows that both α_N and $\langle\epsilon_N|\epsilon_N\rangle$ will be within a small amount δ of their bosonic values when $\chi_{N+1}/\chi_N \geq 1 - \delta$. One can also show [6,8] that $\langle N|[c, c^\dagger]|N\rangle = 2(\chi_{N+1}/\chi_N) - 1$, which is within 2δ of its ideal bosonic value, 1, under the same condition. We therefore follow Law in using the ratio χ_{N+1}/χ_N—we call it the "χ_N ratio"—as our indicator of bosonic character [6,10].

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 χ_{N+1}/χ_N as the quantifier of bosonic character rather than χ_N itself. We note that because the χ_N ratio is nonincreasing with N, a lower bound on χ_{N+1}/χ_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 χ_N itself is close to unity whenever χ_{N+1}/χ_N is.

In the remainder of the Letter we prove two inequalities relating the χ_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.

$$\chi_{N+1} - \chi_N(1 - NP) = \sum{}' \lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_{N+1}} - \Big(1 - N\sum \lambda_p^2\Big)\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}$$
$$= \sum{}' \lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_{N+1}} - \Big(\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}\Big)\sum \lambda_{p_{N+1}} + N\Big(\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}\Big)\sum\lambda_{p_{N+1}}^2. \quad (13)$$

(Again, the prime indicates that all indices have distinct values.) 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

$$-N\sum{}'\lambda_{p_1}^2\lambda_{p_2}\ldots\lambda_{p_N}. \quad (14)$$

We therefore have

$$\chi_{N+1} - \chi_N(1 - NP) = -N\Big(\sum{}'\lambda_{p_1}^2\lambda_{p_2}\ldots\lambda_{p_N}\Big)\sum\lambda_{p_{N+1}} + N\Big(\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}\Big)\sum\lambda_{p_{N+1}}^2. \quad (15)$$

Again the two sums have many terms in common. Canceling these terms leaves

$$\chi_{N+1} - \chi_N(1 - NP) = N(N-1)\sum{}'\lambda_{p_1}^3\lambda_{p_2}\ldots\lambda_{p_N} - N(N-1)\sum{}'\lambda_{p_1}^2\lambda_{p_2}^2\ldots\lambda_{p_N}$$
$$= N(N-1)\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}(\lambda_{p_1}^2 - \lambda_{p_1}\lambda_{p_2}). \quad (16)$$

Now, Eq. (16) can be rewritten as

$$\chi_{N+1} - \chi_N(1-NP) = \frac{N(N-1)}{2}\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}(\lambda_{p_1}^2 + \lambda_{p_2}^2 - 2\lambda_{p_1}\lambda_{p_2}) = \frac{N(N-1)}{2}\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}(\lambda_{p_1} - \lambda_{p_2})^2 \geq 0, \quad (17)$$

thus yielding the bound

$$\frac{\chi_{N+1}}{\chi_N} \geq 1 - NP. \quad (18)$$

This bound shows that a sufficiently small purity entails nearly bosonic character as quantified by χ_{N+1}/χ_N. We now derive a bound in the other direction, showing that a nearly bosonic value of χ_{N+1}/χ_N implies a small purity. For this purpose we start with

$$(1 - P)\chi_N - \chi_{N+1} = \Big(1 - \sum\lambda_p^2\Big)\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N} - \sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_{N+1}}$$
$$= \Big(\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}\Big)\sum\lambda_{p_{N+1}} - \Big(\sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_N}\Big)\sum\lambda_{p_{N+1}}^2 - \sum{}'\lambda_{p_1}\lambda_{p_2}\ldots\lambda_{p_{N+1}}. \quad (19)$$

By combining sums as before (inserting the identity $1 = \sum\lambda_{p_{N+1}}$ when needed), we get

$$(1 - P)\chi_N - \chi_{N+1} = (N-1)\sum{}'\lambda_{p_1}^2\lambda_{p_2}\ldots\lambda_{p_{N+1}} + N(N-1)\sum{}'\lambda_{p_1}^2\lambda_{p_2}^2\ldots\lambda_{p_N} \geq 0. \quad (20)$$

Combining this result with our earlier inequality [Eq. (18)], we have

$$1 - NP \leq \frac{\chi_{N+1}}{\chi_N} \leq 1 - P. \quad (21)$$

We have thus put upper and lower bounds on the χ_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 wave function of the composite particle; so the link between the χ_N ratio and entanglement is established in general.

The lower bound in Eq. (21) 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. (17), $\chi_{N+1}/\chi_N = 1 - NP$ as long as N is less than M. This lower bound is also achieved by wave functions in the class Law considers—this class includes double Gaussian wave functions—in the limit $NP \ll 1$. Because Eq. (20) 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 one, there exists a distribution of Schmidt coefficients that makes $1 - bP$ negative—it suffices to make one of the coefficients λ_k very large—whereas χ_{N+1}/χ_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 one, because such a bound would contradict our lower bound when P is small.

We have considered in this Letter only a single wave function $\Psi(x_A, x_B)$ of the composite particle. One would also like to investigate whether, for several orthogonal wave functions $\Psi_j(x_A, x_B)$, the corresponding creation operators $c_j^\dagger$ approximately satisfy the bosonic relation $[c_j, c_k^\dagger] = 0$ 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 wave function 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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