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Quantum correlations in two-boson wave functions

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We present the Schmidt decomposition for arbitrary wave functions of two indistinguishable bosons, extending the recent studies of *entanglement* or *quantum correlations* for two fermion systems [J. Schliemann *et al.*, Phys. Rev. B **63**, 085311 (2001) and quant-ph/0012094]. We point out that the von Neumann entropy of the reduced single-particle density matrix remains to be a good entanglement measure for two identical particles.

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Recently, quantum information and computing has emerged as an active research field. Of the more fundamental issues in quantum information science, characterization of inseparable *quantum correlations*, or *entanglement*, has received considerable attention [1]. As is well accepted by now, the power of quantum computing lies mostly at the inseparable nature of multipartite quantum states. In fact, it is often said that entanglement is a quantum information processing resource (currency) which all known quantum information protocols need to consume. Historically, quantum entanglement was first raised by Schrödinger [2] in responses to electron paramagnetic resonance (EPR's) local realism [3]. Despite more than 70 years of successful applications of quantum theory, however, we still do not understand the full content of this quantum inseparability. At the simplest level of multipartite pure states, a complete knowledge for classifying and measuring entanglement exists only if two distinguishable particles are involved. For mixtures or states of more than two particles, our current understanding of inseparable correlations remains limited [4].

For quantum computing applications, generation of entanglement is the prelude of any useful protocol [1]. One commonly adopted mechanism relies on a direct interaction of the constituent quantum particles [5]. For indistinguishable particles, e.g., qubits represented by bosonic or fermionic atoms, photons, or electrons as often envisioned in scalable quantum computer architecture [6], a direct short-range interaction may cause significant overlap of individual particle wave functions, thus compromising the ability of keeping track of which particle is which qubit. This calls for understanding inseparable quantum correlations for identical particles including exchange symmetry.

The aim of this paper is to investigate entanglement measures for systems of two identical bosons. We extend the recent results on two fermion systems by J. Schliemann *et al.* [7,8], and present a unified entanglement measure in terms of the von Neumann entropy of the reduced single-particle density matrix. This paper is organized as follows: we first present the well-known result for two distinguishable particles. We then summarize the recent results of two fermions [7,8] and show that the von Neumann entropy of the reduced single-particle state remains a good entanglement measure. Finally we provide a simple proof of the Schmidt decomposition of two boson wave functions and obtain its von Neumann entropy measure of entanglement in terms of the reduced single-particle density matrix. We conclude that in all three cases two distinguishable particles, two fermions or bosons, the reduced single-particle density matrix, fully characterizes their inseparable quantum correlations.

Physically, we arrive at the following conclusion: for two identical particles, simply being in usually inseparable quantum states does no necessarily imply their use for quantum information science. In agreement with the authors of Ref. [8], we will use *quantum correlations*, rather than *entanglement*, to characterize useful inseparable correlations of two identical particles that are beyond what is normally required by the permutation symmetry.

Two distinguishable particles. For two distinguishable particles A and B, any joint pure state wave function can be expressed as

$$|\Psi\rangle=\sum_{i,j=1}^{N,M} C_{ij}a_i^\dagger b_j^\dagger|0\rangle, \tag{1}$$

where C is a complex matrix $(N\times M)$. $a_i^\dagger$ (a_i) and $b_j^\dagger$ (b_j) are, respectively, the single-particle creation (annihilation) operators for A and B in orthogonormal single states $|i\rangle_A$ (of dimension N) and $|j\rangle_B$ (of dimension M). In the position representation, one simply has $a_i^\dagger|0\rangle\to\psi_i(\vec{r}_A)$ and $b_j^\dagger|0\rangle\to\phi_j(\vec{r}_B)$. The normalization condition gives $\mathrm{Tr}(C^\dagger C)=\mathrm{Tr}(CC^\dagger)=1$.

The Schmidt decomposition of Eq. (1) can now be constructed [9,10]. Using the theorem of singular value decomposition (SVD) for a complex matrix [11], we write $C=U^TDV$ with unitary matrices U $(N\times N)$ and V $(M\times M)$, and a diagonal matrix D [of dimension $\min(N, M)$]. Transforming the single particle basis according to

$$a_k'^\dagger=\sum_{i=1}^{N} U_{ik}^* a_i^\dagger,$$

$$b_k'^\dagger=\sum_{j=1}^{M} V_{jk}^* b_j^\dagger,$$

the state vector (1) becomes diagonal

$$|\Psi\rangle=\sum_{k=1}^{\min(N,M)} D_k a_k'^\dagger b_k'^\dagger|0\rangle. \tag{2}$$

Therefore, it is said to be *entangled* if more than one diagonal elements of D (D_k) is nonzero, i.e., if the rank of matrix C is larger than one. A good entanglement measure in this case is the von Neumann entropy of the reduced one-particle density matrix. The two-particle density matrix is $\rho = |\Psi\rangle\langle\Psi|$, and the reduced density matrix is defined according to $\rho^A \equiv \mathrm{tr}_B(\rho)$ and $\rho^B \equiv \mathrm{tr}_A(\rho)$, whose elements can be evaluated according to

$$\rho^A_{\nu\mu} = \langle\Psi|a^\dagger_\mu a_\nu|\Psi\rangle = (CC^\dagger)^*_{\mu\nu},$$

$$\rho^B_{\nu\mu} = \langle\Psi|b^\dagger_\mu b_\nu|\Psi\rangle = (C^\dagger C)_{\mu\nu}. \tag{3}$$

We immediately note that both *Schmidt coefficients* $|D_k|^2$ and the rank of matrix C are independent of unitary single-particle transformations on $|\Psi\rangle$. Furthermore, the von Neumann entropy measure for entanglement

$$S = -\mathrm{Tr}_A[\rho_A \ln(\rho_A)] = -\mathrm{Tr}_B[\rho_B \ln(\rho_B)] = -\sum_{k=1}^{\min(N,M)} |D_k^2| \ln |D_k^2| \tag{4}$$

is also representation independent. Because $0 \leqslant |D_k^2| \leqslant 1$ and $\Sigma_k |D_k^2| = 1$, S is zero for nonentangled states and takes a maximum value $\ln[\min(N,M)]$ for the maximum entangled state.

Two-fermions. A general two fermion state can be expressed as

$$|\Psi_F\rangle = \sum_{i,j=1}^{N} \omega_{ij} f_i^\dagger f_j^\dagger |0\rangle, \tag{5}$$

where ω is a complex and antisymmetric matrix ($N\times N$) $\omega_{ij} = -\omega_{ji}$. $f_i^\dagger$ (f_i) is the creation (annihilation) operator of a fermion in single-particle state $|i\rangle$, and in position representation $f_i^\dagger f_j^\dagger |0\rangle \to [\psi_i(\vec{r}_A)\psi_j(\vec{r}_B) - \psi_i(\vec{r}_B)\psi_j(\vec{r}_A)]/\sqrt{2}$. The normalization condition is $\mathrm{Tr}(\omega^\dagger\omega) = 1/2$.

As was first shown in Ref. [7], and extended in Ref. [8], a Schmidt decomposition also exists in this case (5). A unitary transformation of $f_i = \Sigma_j U_{ij} f'_j$ to new fermionic operators $f'^\dagger_j$ and f'_j, transforms ω in a nonsimilar way. The state (5) becomes

$$|\Psi_F\rangle = \sum_{i,j=1}^{N} (U^\dagger \omega U^*)_{ij} f'^\dagger_i f'^\dagger_j |0\rangle. \tag{6}$$

There exists a matrix U such that ω takes a block diagonal form [7,8,11], containing 2×2 blocks of the type

$$\begin{bmatrix} 0 & z_k \\ -z_k & 0 \end{bmatrix}, \tag{7}$$

with eigenvalues z_k. Consequently the state (5) becomes "diagonal" [8]

$$|\Psi_F\rangle = 2\sum_{k=1}^{\leqslant \frac{N}{2}} z_k f'^\dagger_{2k-1} f'^\dagger_{2k} |0\rangle. \tag{8}$$

Several earlier studies on two-electron correlations in atomic systems also used this Slater-Schmidt expansion [13,14]. In Ref. [13], Grobe *et al.* called it the "canonical representation" (see also [10]), and a correlation measure was defined to be $K = 1/\mathrm{Tr}(\rho^{f2})$. Approximately, K measures the number of Slater orbitals needed for the expansion of a two-electron wave function. $K=1$, therefore, corresponds to no quantum correlation.

Schliemann *et al.* [7,8] propose to use the Slater rank, the number of nonzero z_i's, as the criterion for quantum correlations. If the Slater rank is larger than one, the two-fermion state $|\Psi_F\rangle$ contains additional quantum correlation beyond the antisymmetric permutation requirement. Immediately, one sees that there is no quantum correlations for two fermions in two or three states $N=2,3$. The simplest case where additional inseparable quantum correlations can exist occurs for $N=4$. Several entanglement measures were proposed and studied in Refs. [7,8] for this case.

Compared to states for two distinguishable particles, we note the analog of the von Neumann entropy remains a good correlation measure for two fermions [15]. The two-fermion density matrix is $\rho_F = |\Psi_F\rangle\langle\Psi_F|$. Because the two fermions are identical particles, there is now only one single-particle density matrix, ρ^f (normalized to one), which can be computed according to

$$\rho^f_{\nu\mu} = \frac{\mathrm{Tr}(\rho_F f^\dagger_\mu f_\nu)}{\mathrm{Tr}\left(\rho_F \sum_\mu f^\dagger_\mu f_\mu\right)} = \frac{1}{2}\langle\Psi_F|f^\dagger_\mu f_\nu|\Psi_F\rangle = 2(\omega^\dagger\omega)_{\mu\nu}. \tag{9}$$

The normalization condition is thus reduced to simply $\Sigma_{k=1}^{\leqslant N/2} |z_k|^2 = 1/4$. The corresponding von Neumann entropy is then

$$S_f = -\mathrm{Tr}[\rho^f \ln(\rho^f)] = -\ln 2 - 4\sum_{k=1}^{\leqslant \frac{N}{2}} |z_k|^2 \ln(|z_k|^2). \tag{10}$$

It provides a smooth measure from the noncorrelated state $S_f = \ln 2$ to the maximum correlated state with $S_f = \ln(N_E)$. N_E is the largest even number not larger than N, i.e., $N_E = N$ for even N and $N_E = N-1$ for odd N. We note that both the Slater rank and the von Neumann entropy S_f are independent of unitary transformations on the single particle basis.

Two bosons. We now study wave functions for two indistinguishable bosons:

$$|\Psi_B\rangle = \sum_{i,j=1}^{N} \beta_{ij} b_i^\dagger b_j^\dagger |0\rangle. \tag{11}$$

In this case, β a complex symmetric matrix ($N\times N$) $\beta_{ij}=\beta_{ji}$. $b_i^\dagger$ (b_i) are the boson creation (annihilation) operators for single-particle state $|i\rangle$, and in position representation $b_i^\dagger b_{j\neq i}^\dagger|0\rangle\rightarrow[\psi_i(\vec{r}_A)\psi_j(\vec{r}_B)+\psi_i(\vec{r}_B)\psi_j(\vec{r}_A)]/\sqrt{2}$ and $b_i^\dagger b_i^\dagger|0\rangle\rightarrow\psi_i(\vec{r}_A)\psi_i(\vec{r}_B)$. The normalization gives $\mathrm{Tr}(\beta^\dagger\beta)=1/2$. Under a unitary transformation of b's to new bosonic operators b''s according to $b_i=\Sigma_j U_{ij}b_j'$, the matrix β undergoes a nonsimilarity transformation $\beta=U^\dagger\beta U^*$. The new state vector becomes

$$|\psi_B\rangle=\sum_{i,j=1}^{N}(U^\dagger\beta U^*)_{ij}b_i'^\dagger b_j'^\dagger|0\rangle. \tag{12}$$

We now prove that the Schmidt decomposition also exists in this case. According to SVD [11], a complex symmetric matrix needs only one unitary matrix U, such that $\beta=UBU^T$, and B being a diagonal matrix (with complex diagonal elements B_k). The proof is rather simple. SDV gives $\beta=UBV^T$, while β being symmetric gives $\beta=\beta^T=VBU^T$. Since SDV is unique, we obtain $U=V$ [12]. In fact, the matrix U may be chosen to be the one that diagonalizes β. Thus, the state vector of two bosons can be represented in a diagonal form

$$|\Psi_B\rangle=\sqrt{2}\sum_{k=1}^{N}B_k b_k'^\dagger b_k'^\dagger|0\rangle. \tag{13}$$

We note that such a Schmidt expansion was suggested earlier in Refs. [13,14]. The inseparable correlations criterion is again related to the number of nonzero diagonal elements B_k, i.e., the rank of matrix β. In general, quantum correlations can arise as long as $N\geqslant 2$.

Again, there is only one single-particle density matrix

$$\rho_{\nu\mu}^b=\frac{\langle\Psi_B|b_\mu^\dagger b_\nu|\Psi_B\rangle}{\left\langle\Psi_B\left|\sum_\mu b_\mu^\dagger b_\mu\right|\Psi_B\right\rangle}=2(\beta^\dagger\beta)_{\mu\nu}. \tag{14}$$

Similar to the fermionic case, the von Neumann entropy

$$S_b=-\mathrm{Tr}[\rho^b\ln\rho^b]=-\sum_{k=1}^{N}(2|B_k|^2)\ln(2|B_k|^2), \tag{15}$$

measures quantum correlations between the noncorrelated state $S_b=0$ and the maximum correlated state $S_b=\ln(N)$.

Finally, we note as discussed in Refs. [7,8], within a given rank, the determinant of the corresponding nonzero submatrix can also be used to measure quantum correlations. This was first shown in the simplest case of $N=4$ for two fermions [7] by introducing a *dual* space (dual matrix for ω). One can show in general the submatrix determinant takes the maximum value when S_f or S_b is the maximum. We provide the simple case of two bosons below. Let us assume the rank of β matrix r_b is equal to N. We denote $|B_k|^2=\xi_k$ and construct a functional $\mathcal{F}=\Pi_{k=1}^N\xi_k-\lambda(\Sigma_{k=1}^N\xi_k-1/2)$. The second term is due to the requirement for a proper normalization of the matrix $\beta^\dagger\beta$. We find the condition for a maximum by taking partial derivatives $\partial_{\xi_i}\mathcal{F}=0$. The resulting equations then become $\Pi_{i\neq j}\xi_i=\lambda$. Therefore, the extreme occurs at $\xi_1=\xi_2=,\ldots,=\xi_N=1/2N$. We may then express the determinant of β as

$$\mathcal{F}=\xi_1(\xi_2,\xi_3,\ldots,\xi_N)\prod_{j=2}^{N}\xi_j. \tag{16}$$

Its second-order derivative at $\xi_i=1/2N$ is then

$$\partial_{ij}^2\mathcal{F}=(\delta_{ij}-2)\left(\frac{1}{2N}\right)^{N-1}, \tag{17}$$

which forms a strictly negative matrix. Therefore the submatrix determinant does take its maximum at this extreme point of S_b, a point that corresponds to the maximally correlated state within the same rank. Extending the proof to $r_b<N$ is straightforward.

Finally, we note that for two bosons, our proposed entanglement measure in terms of the single-particle density matrix shares same spirit with the so-called condensate fragmentation phenomena in systems of many bosons [16]. Therefore, it may also provide a useful starting point for the investigation of quantum correlations beyond two particle systems. One obvious consequence for many-boson systems is that fragmented condensates contain nonzero inseparable quantum correlations or entanglement.

From a technical point of view, we note Schmidt decompositions for two-particle pure states can be constructed starting from unitary transformations that diagonalize the respective reduced single-particle density matrices. We hope this unified approach will stimulate further discussions into quantum information science of indistinguishable particles. In the next paper, we will address the question of such inseparable quantum correlations for two bosons in quantum mixture states.

In conclusion, we have presented the Schmidt decomposition for pure states of two indistinguishable bosons. We find the rank of the Fock space wave-function matrix may be used to determine if additional quantum correlations (or entanglement) beyond the usual permutation symmetry exists. We have suggested the von Neumann entropy for the reduced single-particle density matrix as a smooth entanglement measure for both two-fermion and two-boson wave functions, just as in the case of two distinguishable particles. There remains one point of concern in this von Neumann entropy measure in that it did not seem to reflect the information content of quantum correlations. For instance, the uncorrelated two-fermion state gives $S_f=\ln 2$, rather than 0 as in the classical case. This points to the need for studies of quantum information coding and processing with correlated identical particle states.

Note added in proof.—Recently, an e-print [17] on the same topic of entanglement in a two-identical-particle system appeared. It provided a different proof of Eq. (12) in analogy with the original approach used for two fermions [8]. The reduced single particle density matrix was not invoked in [17]. Although both results are essentially the same in terms of mathematics, we seem to arrive at different conclusions. In particular, an interesting construction is provided in Ref. [17] which transforms a symmetric state $|B_k|(e^{i\phi_k}b'^{\dagger}_{k1}b'^{\dagger}_{k1}+e^{-i\phi_k}b'^{\dagger}_{k2}b'^{\dagger}_{k2})|0\rangle$ of a degenerate pair of nonzero diagonal elements $B_k=|B_k|e^{i\phi_k}$ into state $b^{\dagger}_{k1}b^{\dagger}_{k2}|0\rangle$. Since both states are of rank 2, we consider them as containing quantum correlations. This is further evidenced by the fact that both can be used for quantum teleportation [18]. On the other hand, Ref. [17] considers them as separable according to their definition 1.

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