Quantum entanglement of identical particles

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(Received 20 May 2002; revised manuscript received 1 August 2002; published 6 February 2003)

We consider entanglement in a system with a fixed number of identical particles. Since any operation should be symmetrized over all the identical particles and there is the precondition that the spatial wave functions overlap, the meaning of identical-particle entanglement is fundamentally different from that of distinguishable particles. The identical-particle counterpart of the Schmidt basis is shown to be the single-particle basis in which the one-particle reduced density matrix is diagonal. But it does not play a special role in the issue of entanglement, which depends on the single-particle basis chosen. The nonfactorization due to (anti)symmetrization is naturally excluded by using the (anti)symmetrized basis or, equivalently, the particle number representation. The natural degrees of freedom in quantifying the identical-particle entanglement in a chosen single-particle basis are occupation numbers of different single-particle basis states. The entanglement between effectively distinguishable spins is shown to be a special case of the occupation-number entanglement.

DOI: 10.1103/PhysRevA.67.024301 PACS number(s): 03.67.−a, 03.65.−w, 73.21.−b

How does one characterize entanglement in a fixed number of identical particles? Obviously, a correct characterization must exclude the nonfactorization due to (anti)symmetrization. Here, we clarify that it can be done by using the (anti)symmetrized basis, which is equivalent to the particle number representation. This leads to the use of occupation numbers of different single-particle basis states as the (distinguishable) degrees of freedom in quantifying identical-particle entanglement *even when the number of particles is conserved*. The occupation numbers of different modes have already been used in quantum computing [1]. The use of modes was made in a previous study of identical-particle entanglement, based on formally mapping the Fock space to the state space of qubits or harmonic oscillators [2], but it was under the unphysical presumption of full access to the Fock space. We shall elaborate that the concept of entanglement in a system of identical particles is fundamentally different from that of distinguishable particles, for which entanglement is invariant under local unitary transformations. There is no local operation that acts only on one of the identical particles. The single-particle basis transformation is made on each particle and chooses a different set of particles in representing the many-particle system. Thus, the entanglement property of a system of identical particles depends on the *single-particle* basis used. The particle number basis state *for a fixed number of particles* is just the normalized (anti)symmetrized basis in the configuration space, i.e., Slater determinants or permanents. Therefore the occupation-number entanglement in a fixed number of particles is nothing but the situation that the state is a superposition of different Slater determinants or permanents. Another consequence is that the two-identical-particle counterpart of the Schmidt decomposition, which we call Yang decomposition since the corresponding transformation of an antisymmetric matrix was first obtained by Yang long ago [4], does not play a similar role in characterizing the entanglement. On the other hand, we show that like the Schmidt basis, the Yang basis is the single-particle basis in which the one-particle reduced density matrix is diagonal. It is a common wisdom to treat the entanglement between spins of identical particles, when they are effectively distinguished in terms of another degree of freedom, in the way of distinguishable particles. We show that it is in fact a special case of the occupation-number entanglement with a constraint on the accessible subspace of the Fock space.

In terms of the product basis $|k_1,\ldots,k_N\rangle \equiv |k_1\rangle\otimes\cdots\otimes|k_N\rangle$, the N-particle state is

$$|\psi\rangle=\sum_{k_1,\ldots,k_N} q(k_1,\ldots,k_N)|k_1,\ldots,k_N\rangle, \tag{1}$$

where summations are made over $k_1,\ldots,k_N$ independently, the coefficients $q(k_1,\ldots,k_N)$ are (anti)symmetric.

It is often convenient to use the unnormalized (anti)symmetrized basis, $|k_1,\ldots,k_N\rangle^{(\pm)}=\Sigma_P^{N!}(-1)^P|k_1,\ldots,k_N\rangle$, where P denotes permutations, "+" is for bosons while "−" is for fermions. Suppose that in $k_1,\ldots,k_N$, there are n_α k_i's which are α, then there are only $N!/\Pi_{\alpha=0}^{\infty}n_\alpha!$ different permutations. Hence, $|k_1,\ldots,k_N\rangle^{(\pm)}=\Sigma'_P(-1)^P\Pi_\alpha n_\alpha|k_1,\ldots,k_N\rangle$, where the summation is only over all different permutations. The N-particle state is then

$$|\psi\rangle=\sum_{(k_1,\ldots,k_N)} g(k_1,\ldots,k_N)|k_1,\ldots,k_N\rangle^{(\pm)}, \tag{2}$$

where $(k_1,\ldots,k_N)$, disregarding the order of $k_1,\ldots,k_N$, is *a single index*. Up to the sign depending on the order of $k_1,\ldots,k_N$ in $q(k_1,\ldots,k_N)$, q is equal to g, i.e., each set of (anti)symmetrized terms in Eq. (1) corresponds to one term in Eq. (2). Equation (2) can be rewritten in terms of the normalized (anti)symmetrized basis

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$|k_1,\ldots,k_N\rangle^{(s)}=\sqrt{1/N!\Pi_\alpha n_\alpha!}|k_1,\ldots,k_N\rangle^{(\pm)}$, as $|\psi\rangle=\Sigma_{(k_1,\ldots,k_N)}h(k_1,\ldots,k_N)|k_1,\ldots,k_N\rangle^{(s)}$.

For a fixed number of particles, the normalized (anti)symmetrized basis can be rewritten in terms of the occupation numbers of different single-particle basis states. This is the particle number representation, in which

$$|\psi\rangle=\sum_{n_1,\ldots,n_\infty}f(n_1,\ldots,n_\infty)|n_1,\ldots,n_\infty\rangle, \tag{3}$$

where n_j is the occupation number of mode j, $|n_1,\ldots,n_\infty\rangle\equiv(a_1^\dagger)^{n_1},\ldots,(a_\infty^\dagger)^{n_\infty}|0\rangle$, the summations are subject to the constraint $\Sigma_\alpha n_\alpha=N$, hence in the complete summation, of course most of the f's are zero.

In Refs. [5–9], an arbitrary N-particle state, in an arbitrary single-particle basis, is inappropriately written as $\Sigma_{i_1\cdots i_N}w_{i_1\cdots i_N}a_{i_1}^\dagger\cdots a_{i_N}^\dagger|0\rangle$, where $w_{i_1\cdots i_N}$ is (anti)symmetric, and each subscript of the creation operators runs over all the modes. One should note that the creation or annihilation operators are associated with *(anti)symmetrized basis*. For example, $a_i^\dagger a_j^\dagger|0\rangle=\pm a_j^\dagger a_i^\dagger|0\rangle=|1_i\rangle|1_j\rangle=1/\sqrt{2}(|i\rangle|j\rangle\pm|i\rangle|j\rangle)$, where $i\neq j$. Therefore $a_{i_1}^\dagger\cdots a_{i_N}^\dagger|0\rangle$ in these papers may be corrected to $|i_1\cdots i_N\rangle$. On the other hand, if one uses the particle number basis states, *no* (anti)symmetrization needs to made [10].

Single-particle basis transformation for identical particles is *not* the counterpart of the local unitary transformation in a system of distinguishable particles. It acts on each identical particle in the same way. For distinguishable particles, local unitary transformations do not change the entanglement. In contrast, for identical particles, the entanglement depends on which single-particle basis is chosen. Consequently, unlike the Schmidt decomposition of distinguishable particles, the Yang decomposition does not play a special role in identical-particle entanglement [11].

As a simple example, consider a two-particle state $a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger|0\rangle=1/\sqrt{2}(|\mathbf{k}_1\rangle|\mathbf{k}_2\rangle\pm|\mathbf{k}_2\rangle|\mathbf{k}_1\rangle)$, assuming $\mathbf{k}_1\neq\mathbf{k}_2$. In terms of momentum basis, this is only a basis state in particle number representation. Written in terms of the product basis, the nonfactorization is only due to (anti)symmetrization. Therefore, there is no entanglement. However, in terms of the position basis, it becomes $\Sigma_{\mathbf{r}_1,\mathbf{r}_2}e^{i(\mathbf{k}_1\cdot\mathbf{r}_1+\mathbf{k}_2\cdot\mathbf{r}_2)}a_{\mathbf{r}_1}^\dagger a_{\mathbf{r}_2}^\dagger|0\rangle$, which is entangled.

Since a single-particle basis transformation is made on every particle, *both the reduced density matrix and its von Neumann entropy depend on the single-particle basis*. This invalidates the claim that partial entropy is still a measure of entanglement for two identical particles [8]. The n-particle reduced density matrix for a N-particle system is $\langle k_1',\ldots,k_n'|\rho^{(n)}|k_1,\ldots,k_n\rangle=\mathrm{Tr}(a_{k_1'}\cdots a_{k_n'}\rho a_{k_n}^\dagger\cdots a_{k_1}^\dagger)$, with $\mathrm{Tr}\rho^{(n)}=N(N-1)\cdots(N-n+1)$. One can find

$$\langle k_1'\cdots k_n'|\rho^{(n)}|k_1\cdots k_n\rangle$$
$$=\frac{1}{(N-n)!}\sum_{k_{n+1}\cdots k_N}{}^{(\pm)}\langle k_1'\cdots k_n'k_{n+1}\cdots k_N|\rho|$$
$$\times k_1\cdots k_nk_{n+1}\cdots k_N\rangle^{(\pm)}. \tag{4}$$

For a two-boson product state $a_{\mathbf{k}_1}^\dagger a_{\mathbf{k}_2}^\dagger|0\rangle$, the one-particle reduced density matrix is given by $\langle\mathbf{k}_1|\rho^{(1)}|\mathbf{k}_1\rangle=\langle\mathbf{k}_2|\rho^{(1)}|\mathbf{k}_2\rangle=1$ and $\langle\mathbf{k}_1|\rho^{(1)}|\mathbf{k}_2\rangle=\langle\mathbf{k}_2|\rho^{(1)}|\mathbf{k}_1\rangle=0$, hence the one-particle partial entropy is $\log 2>0$, contradicting the previous claim.

The dependence of entanglement on the single-particle basis is consistent with the point of view that individual particles are excitation of quantum fields, and that each different single-particle basis, in fact, defines a different set of particles representing the many-body state. In fact, in many-body physics, it is a routine to make various transformations, which usually changes the nature of entanglement [13].

With (anti)symmetrization already made on the basis, the correlation embedded in the coefficients naturally gives the information on entanglement. A Slater determinant or permanent is just a (anti)symmetrized basis state, hence is nonentangled with respect to the given single-particle basis. Furthermore, one can regard a superposition of the Slater determinant or permanent as entangled in the given single-particle basis. Any operation, even a one-body one, of which the single-particle basis transformation is an example, acts on all the particles. A transformation from a superposition of Slater determinant or permanent to a single Slater determinant or permanent, in another single-particle basis, must involve operations on all particles and actually chooses a different set of particles in representing the state. In a sense, there is a builtin nonseparability, based on both the symmetrization of any operation *and the spatial wave function overlap*. Consistently, without spatial wave function overlap or under the condition of the so-called remoteness [12], the symmetrization does not have any physical effect.

Hence, the entanglement is between different single-particle basis states. Whether a certain single-particle basis state is entangled with other single-particle basis states can be decided by whether the former is mixed with the latter in the single-particle basis transformation which transforms the superposition into a single Slater determinant or permanent. This can be seen most clearly by using the second quantization. For example, in a two-particle state $1/\sqrt{m}a_{\mathbf{k}_1}^\dagger(a_{\mathbf{k}_2}^\dagger+\cdots+a_{\mathbf{k}_{m+1}}^\dagger)|0\rangle$, where $\mathbf{k}_i$'s are different from each other, $m>1$, the $|\mathbf{k}_1\rangle$ state is obviously separated from the others. One can obtain the one-particle partial entropy as $\log 2+\frac{1}{2}\log m>\log 2$.

Since the distinguishable label is the set of occupation numbers of different single-particle basis states, clearly they can be used to quantify entanglement, in the way of entanglement between distinguishable objects. From Eq. (3), one obtains the density matrix as

$$\langle n_1',\ldots,n_\infty'|\rho|n_1,\ldots,n_\infty\rangle$$
$$=f^*(n_1',\ldots,n_\infty')f(n_1,\ldots,n_\infty),$$

from which one can obtain the reduced density matrices *of occupation numbers*. For example, the reduced density matrix of mode 1 is defined as

$$\langle n_1'|\rho_1(1)|n_1\rangle = \Sigma_{n_2,\ldots,n_\infty}\langle n_1',n_2,\ldots,n_\infty|\rho \times|n_1,n_2,\ldots,n_\infty\rangle.$$

Similarly, the reduced density matrix of the set of modes $1,\ldots,l$ is

$$\langle n_1',\ldots,n_l'|\rho_l(1,\ldots,l)|n_1,\ldots,n_l\rangle = \sum_{n_{l+1},\ldots,n_\infty}\langle n_1',\ldots,n_l',n_{l+1},n_\infty|\rho| \times n_1,\ldots,n_l,n_{l+1},n_\infty\rangle, \quad (5)$$

the nonvanishing elements of which satisfy $\Sigma_{i=1}^{l}n_i' = \Sigma_{i=1}^{l}n_i$ as constrained by the particle number conservation. From these Fock-space reduced density matrices, we can, for example, calculate bipartite entanglement between the occupation numbers of l modes and the occupation numbers of the other modes.

It is important to note that the use of occupation numbers as the degrees of freedom in characterizing entanglement is valid even when the particle number is conserved. This physical constraint, as well as the constraints that for fermions n_j is either 0 or 1 and that the number of the relevant modes [14] may be finite are all automatically satisfied by the set of nonzero f. Hence, this approach is a natural one within the standard second-quantization formalism, compatible with the representations of the observables in terms of creation or annihilation operators, which can be viewed as coordinated transformations of occupation numbers of a set of modes. The second-quantized representation of an n-body operator O is $\Sigma a_{i_1'}^\dagger\cdots a_{i_n'}^\dagger\langle i_1'\cdots i_n'|O|i_1\cdots i_n\rangle a_{i_n}\cdots a_{i_1}$. One can observe that, for example, there is no operation which only changes the occupation number of one mode. One may consider "second-quantized computation."

In principle, one can define entanglement with respect to any reference state of the system. In this case, the occupation number of each mode in defining the relative entanglement is the difference with that in the reference state, as conveniently seen by considering the action of creation operators. There are two reference states that are of particular interest. One is the empty state, as we have implicitly considered up to now. Another one is the ground state of the system, which is suitable when all physical processes are in a same bulk of material. In discussing the entanglement in a ground state, it is with respect to the empty state. The considerations can even be extended to relativistic quantum field theory, where the ground state is the vacuum.

An important situation is that the single-particle basis includes both spin and orbit (momentum or position). One can denote the total index as $(\mathbf{o},s)$, where $\mathbf{o}$ substitutes for momentum $\mathbf{k}$ or position $\mathbf{r}$. A special case is half filling, i.e., each orbit is constrained to be occupied by only one particle, i.e., $\Sigma_s n_{\mathbf{o},s}=1$ for each relevant value of $\mathbf{o}$. Then with the orbit modes as the labels with which the particles are effectively distinguished, the entanglement can be viewed as the spin entanglement among the particles in different orbit modes. Under the constraint of half filling, the many-particle state must be a sum of products of $\Pi_s|n_{\mathbf{o},s}\rangle$, under the constraint $\Sigma_s n_{\mathbf{o},s}=1$, for relevant orbits. In the many-particle state, one simply rewrites $\Pi_s|n_{\mathbf{o},s}\rangle$ as $|S_{\mathbf{o}}\rangle$, where $S\mathbf{o}$ is unambiguously the s corresponding to $n_{\mathbf{o},s}=1$. This rigorously justifies the common wisdom that although it is meaningless to identify which particle is in which orbit, it is meaningful to say that the particle in a certain orbit is spin entangled with the particle in another orbit. Hence, the entanglement between Heisenberg spins, which appears as entanglement between distinguishable objects, is in fact a special case of occupation-number entanglement.

Entanglement between Heisenberg spins is the basis of the quantum computing scheme based on electrons in double quantum dots [3]. When the electrons are separated in the two dots, because there are only one-dot potentials, while the Coulomb interaction is negligible, the condition of remoteness [12] is satisfied. One can verify that an antisymmetrization between electrons in different dots has no physical effects. On the other hand, when they are close, and the interaction is appreciable, the antisymmetrization has physical effects, and the entanglement can be characterized by using the full formalism of occupation-number entanglement. During the interaction period, they access the full Hilbert space, which includes the state in which the two electrons, with opposite spins, locate in a same dot, i.e., $|1\rangle_{i,\uparrow}\rangle|1_{i,\downarrow}\rangle$, where $i=1,2$ represents the dots. There are $4!/2!2!=6$ two-particle antisymmetrized basis states, or occupation-number basis states. Nevertheless, as far as the initial and final states are in single occupancy, and the Heisenberg model is a valid description, the interaction period can be viewed as an intermediate process determining the effective spin coupling, while the leakage into the full Hilbert space of two identical particles during a two-particle gate operation does not cause any problem. In terms of the occupation-number states, the spin state of each electron in each dot is $|\uparrow\rangle_i=|1\rangle_{i,\uparrow}|0\rangle_{i,\downarrow}$, $|\downarrow\rangle_i=|0\rangle_{i,\uparrow}|1\rangle_{i,\downarrow}$. Because a spin qubit is in fact an occupation-number state, the loss of identification after separating from the double occupation, as concerned in Ref. [15], does not matter. Note that the intermediate state with double occupancy is *necessary* for the electrons to interact in order to undergo a two-qubit operation.

Finally, we come to the question that what is special about the Yang basis. For two distinguishable particles, the Schmidt basis is clearly the one in which the reduced density matrix of each particle is diagonal: For $\Sigma_i c_i|i\rangle_a|i\rangle_b$ of distinguishable particles a and b, the elements of the reduced density matrix of either a or b are given by $\langle i|\rho_{a(b)}|j\rangle = |c_i|^2\delta_{ij}$. In the following, we show that the Yang basis is the basis in which the one-particle reduced density matrix is diagonal.

In their Yang basis, a two-fermion state is like $|\psi_f\rangle = c_1(|1\rangle|2\rangle-|2\rangle|1\rangle)+c_2(|3\rangle|4\rangle-|3\rangle|4\rangle)+\cdots$ where we use $|i\rangle$ to denote different single-particle basis states. If $k_2' = k_2$, then $k_1'=k_1$ is necessary for any of $\langle k_1'k_2'|\rho|k_1k_2\rangle$, $\langle k_1'k_2'|\rho|k_2k_1\rangle$, $\langle k_2'k_1|\rho|k_1k_2\rangle$ and $\langle k_2'k_1|\rho|k_2k_1\rangle$ to be nonvanishing. Therefore using Eq. (4), one finds $\langle k_1'|\rho^{(1)}|k_1\rangle = \delta_{k_1'k_1}\Sigma_{k_2}{}^{(-)}\langle k_1k_2|\rho|k_1k_2\rangle^{(-)}$. Hence, $\rho^{(1)}$ is diagonal.

In their Yang basis, a two-boson state is like $|\psi_b\rangle = d_1|1\rangle|1\rangle + d_2|2\rangle|2\rangle + \cdots$. Then one finds

$$\langle k_1'k_2'|\rho|k_1k_2\rangle = \langle k_1'k_2'|\rho|k_2'k_1\rangle = \langle k_2'k_1'|\rho|k_1k_2\rangle$$
$$= \langle k_2'k_1'|\rho|k_2k_1\rangle = \delta_{k_1'k_2'}\delta_{k_1k_2}\langle k_1k_1|\rho|k_2k_2\rangle.$$

Consequently, using Eq. (4), one finds $\langle k_1'|\rho^{(1)}|k_1\rangle = \delta_{k_1'k_1}{}^{(+)}\langle k_1k_1|\rho|k_1k_1\rangle^{(+)}$. Hence, $\rho^{(1)}$ is diagonal.

Let us summarize. If one uses the product basis, the coefficients mix the information on (anti)symmetrization and that on entanglement. If, instead, the (anti)symmetrization is made on the basis, then the coefficients unambiguously give the information on entanglement, with respect to the given single-particle basis. (Anti)symmetrized basis is equivalent to particle number representation, and the occupation numbers of different modes are distinguishable degrees of freedom which can be used in quantifying the entanglement even when particle number is conserved. Entanglement of identical particles is a property dependent on which single-particle basis is chosen, as any operation should act on each identical particle in the same way. Indeed, individual particles are excitations of a quantum field, and the single-particle basis defines which set of particles are used in representing the many-particle state. The many-particle state is entangled in the corresponding single-particle basis when it is not a single Slater determinant or permanent. The entanglement is between different single-particle basis states in the given basis. We also show that the entanglement between effectively distinguishable spins of identical particles is a special case of the occupation-number entanglement. We have discussed its use in quantum computing. The (necessary) leakage into the larger Hilbert space *during* the intermediate two-particle process is harmless. Finally it is shown that the two-identical-particle counterpart of the Schmidt basis is the basis in which the one-particle reduced density matrix is diagonal. In addition to quantum computing implementations involving identical particles, the result here is also useful for many-body physics [16].

This publication is an output from project activity funded by The Cambridge-MIT Institute Limited.

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