Necessary and sufficient conditions of separability for fermion wave functions: Theoretical basis of a group-density-analysis method

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A theorem is proved which gives the necessary and sufficient conditions on the p-particle reduced-density operator restricted to a functional subspace that ensures the separability of the wave function of a fermion system. This theorem is the theoretical basis of a general method of analyzing atomic and molecular wave functions, a method which is able to reveal the existence of somehow chemically discernible subsystems of electrons.

INTRODUCTION

Quantum-mechanical methods working with group wave functions[1-6] have been efficiently used to account for the ground-state properties of atomic or molecular many-electron systems,[7-10] which can be considered, from both experimental and theoretical viewpoints, as being formed by the union of cores and bonds localized in some disjoint volumes of the physical space. All these calculations show that good agreement with the experiment requires a careful choice of the mutually orthogonal subspaces in which the group functions are defined. In particular, the basis functions of these subspaces must be rather well localized in the volumes of the physical space associated with each bond or core.[11]

On the other hand, the ground-state properties of a vast class of molecular compounds are still correctly reproduced by using a group wave function, although no suitable partition of the physical space into disjoint volumes can be found either by theoretical methods or by invoking chemical intuition. This is the case of the planar conjugated molecules, for which the criterion leading to the choice of the σ and π functional subspaces is not a localization criterion but a space-symmetry one.[12,13]

Thus it appears that an atomic or molecular electronic system, although it is an assembly of identical strongly interacting particles, can be considered in many cases as the union of interacting discernible subsystems. That these subsystems are discernible follows from the localization or space-symmetry features of the whole system: As the theoretical counterpart, an antisymmetrized (because of the identity of the particles) product of proper functions describing each subsystem is a good approximation of the wave function.

On the other hand, from the analytical viewpoint, we may reasonably postulate that a discernible subsystem can be theoretically revealed in a many-electron system by investigating the ability of the wave function to be fairly well approximated by a separable group function, that is, by an antisymmetrized product of functions defined in a partition of the Hilbert space into two mutually orthogonal subspaces, one associated with the subsystem of interest, the other with the rest of the system. We will deduce afterwards that the subsystem is a localized one if it appears that the basis functions of the associated subspace are well localized in a volume of the physical space.

A general method of analysis of the wave functions can be founded along these lines provided that answers to the following questions can be clearly shown theoretically. First, what are the necessary and sufficient conditions of separability available for any kind of many-particle wave function? Second, how does one characterize quantitatively the extent that the wave function to be analyzed differs from a separable approximation?

The aim of this work is to solve the first of these two problems by having recourse to the properties of the reduced-density operators. Indeed, since we know that a system can be described by a wave function (pure state) if and only if its density operator is a projection operator,[14] it is tempting to admit that a subsystem can be described by a proper function if and only if the density operator of the whole system, reduced to the number of particles of the subsystem and restricted to the associated functional subspace, is a projection operator.

The paper is divided into three sections. In Sec. I, some useful concepts are defined and the theorem is precisely stated. In Sec. II, we give the properties of the reduced density operators of a special kind of function, the event-type functions. A proof of the theorem is given in Sec. III.

I. STATEMENT OF THE SEPARABILITY THEOREM

In what follows we shall use the notion of p-particle reduced-density operator restricted to a given subspace $\mathcal{E}$ spanned by a set of orthonormal p functions $\psi_i^{(p)}$. Let $\hat{P}_{\mathcal{E}}^{(p)}$ be the projection operator defined by

$$\hat{P}_{\mathcal{E}}^{(p)} = \sum_{i \geq 1} |\psi_i^{(p)}\rangle\langle\psi_i^{(p)}| \; ; \tag{1}$$

then the density operator we are defining is given by

$$[\hat{\rho}_n^{(p)}]_{\mathcal{E}} = \hat{P}_{\mathcal{E}}^{(p)} \hat{\rho}_n^{(p)} \hat{P}_{\mathcal{E}}^{(p)} , \tag{2}$$

where $\hat{\rho}_n^{(p)}$ is the p-particle reduced-density operator deduced from the total n-particle wave function according to the usual definition and the normalization convention proposed by Löwdin.[15]

Remembering a definition first proposed by Primas,[16] we will call a primitive function of the wave function $\Psi^{(n)}$ any function $\Phi^{(n)}$ that equals $\Psi^{(n)}$ after projection into the subspaces of functions totally antisymmetric or totally symmetric under any permutation of the space-spin coordinates. Thus we may write

$$\Psi^{(n)}(1 \ldots n) = \mathcal{O}^{(n)}[\Phi^{(n)}(1 \ldots n)] , \tag{3}$$

where $\mathcal{O}^{(n)}$ is the antisymmetrization operator

$$\mathcal{A}^{(n)} = (n!)^{-1/2} \sum_{\pi} (-)^{\pi} \pi ,$$

or the symmetrization operator

$$\mathcal{S}^{(n)} = (n!)^{-1/2} \sum_{\pi} \pi ,$$

according to whether the system is formed by fermions or bosons. Obviously the primitive function is not defined uniquely.

We will consider that the one-particle Hilbert space[17] can be considered as a direct sum of two orthogonal subspaces,

$$\mathcal{H}^{(1)} = \mathcal{H}_{\alpha}^{(1)} \oplus \mathcal{H}_{\beta}^{(1)} , \quad \hat{P}_{\alpha}^{(1)} \cdot \hat{P}_{\beta}^{(1)} = 0 . \tag{4}$$

It follows that the p-particle Hilbert space $\mathcal{H}^{(p)}$, defined as a p-fold tensorial product of $\mathcal{H}^{(1)}$,

$$\mathcal{H}^{(p)} = \mathcal{H}^{(1)} \otimes \cdots \otimes \mathcal{H}^{(1)} , \tag{5}$$

can be considered also as a direct sum of $p+1$ subspaces,

$$\mathcal{H}^{(p)} = \bigoplus_{r=0}^{p} [\mathcal{H}_{\alpha}^{(r)} \otimes \mathcal{H}_{\beta}^{(p-r)}] , \tag{6}$$

where

$$\mathcal{H}_{\alpha}^{(r)} = \mathcal{H}_{\alpha}^{(1)} \otimes \cdots \otimes \mathcal{H}_{\alpha}^{(1)} \tag{7}$$

and

$$\mathcal{H}_{\beta}^{(p-r)} = \mathcal{H}_{\beta}^{(1)} \otimes \cdots \otimes \mathcal{H}_{\beta}^{(1)} .$$

When an element of the partition is particularized (let us say α), it is useful to write

$$\mathcal{H}^{(p)} = \mathcal{H}_{\alpha}^{(p)} \oplus \mathcal{H}_{\bar{\alpha}}^{(p)} , \tag{8}$$

where $\mathcal{H}_{\alpha}^{(p)}$ is defined by Eq. (7) and the orthogonal subspace $\mathcal{H}_{\bar{\alpha}}^{(p)}$ can be derived from Eq. (6).

Putting $p = n$ in Eq. (6), we conclude that any wave function $\Psi^{(n)} \in \mathcal{H}^{(n)}$ can be developed exactly in terms of products of functions $\psi_{Ai_r}^{(r)} \in \mathcal{H}_{\alpha}^{(r)}$ and $\psi_{Bj_r}^{(n-r)} \in \mathcal{H}_{\beta}^{(n-r)}$:

$$\Psi^{(n)}(1 \ldots n) = \sum_{r=0}^{n} \mathcal{O}^{(n)} \Big(\sum_{i_r j_r} c_{i_r j_r}^{r} \psi_{Ai_r}^{(r)}(1 \ldots r) \times \psi_{Bj_r}^{(n-r)}(r+1, \ldots n) \Big) \tag{9}$$

$$= \sum_{r=0}^{n} \Psi_r^{(n)}(1 \ldots n) , \tag{10}$$

with

$$\int |\Psi_r^{(n)}(1 \ldots n)|^2 d1 \ldots dn = \alpha_r = \sum_{i_r j_r} |c_{i_r j_r}^{r}|^2 . \tag{11}$$

The function $\Psi_r^{(n)} \in \mathcal{H}_{\alpha}^{(r)} \otimes \mathcal{H}_{\beta}^{(n-r)}$ is an event-type function analogous to that recently introduced in the so-called "loge theory."[18]

We will say that $\Psi^{(n)}$ is p-separable with respect to the partition $\mathcal{H}_{\alpha}^{(p)} \otimes \mathcal{H}_{\beta}^{(n-p)}$ of $\mathcal{H}^{(n)}$ if it reduces to an event-type function (with the well defined p value of r), the primitive of which can be written as a simple product of functions $\psi_A^{(p)} \in \mathcal{H}_{\alpha}^{(p)}$ and $\psi_B^{(n-p)} \in \mathcal{H}_{\beta}^{(n-p)}$.

The aim of this work is to analyze the properties of the p-particle reduced-density operator restricted to a given subspace in connection with the separability of the wave function. The main result can be expressed as follows.

Theorem. For any n-fermion wave function $\Psi^{(n)} \in \mathcal{H}^{(n)}$, having a p-particle density operator $\hat{\rho}_n^{(p)}$, the two relations

$$([\hat{\rho}_n^{(p)}]_{\alpha})^2 = [\hat{\rho}_n^{(p)}]_{\alpha}$$

and

$$\mathrm{Tr}[\hat{\rho}_n^{(p)}]_{\alpha} = 1 ,$$

which means that $[\hat{\rho}_n^{(p)}]_{\alpha}$ is a projector on a function $\psi_A^{(p)} \in \mathcal{H}_{\alpha}^{(p)}$,

$$[\hat{\rho}_n^{(p)}]_{\alpha} = |\psi_A^{(p)}\rangle\langle\psi_A^{(p)}| ,$$

are necessary and sufficient conditions of p-separability with respect to the partition $\mathcal{H}_{\alpha}^{(p)} \otimes \mathcal{H}_{\beta}^{(n-p)}$ of $\mathcal{H}^{(n)}$, a possible form of the primitive function $\Phi^{(n)}$ being the simple product of $\psi_A^{(p)}$ with a function $\psi_B^{(n-p)} \in \mathcal{H}_{\beta}^{(n-p)}$.

II. PROPERTIES OF THE REDUCED-DENSITY OPERATORS DERIVED FROM EVENT-TYPE FUNCTIONS

Before giving a proof of the theorem, we will emphasize some properties characteristic of the operators $[\hat{\rho}_n^{(p)}]_\alpha$ representable by wave functions like those of Eqs. (9) or (10).

The primitive functions used in this work are always some products of antisymmetrized functions; it is useful to derive an expression of the operator $\hat{\mathcal{O}}^{(n)}$ in terms of tensorial products of operators working in the subspace $\mathcal{H}^{(r)} \otimes \mathcal{H}^{(n-r)}$. It can be easily verified that, for this special case, the kernel of $\hat{\mathcal{O}}^{(n)}$ in the coordinate representation can be reduced to

$$\mathcal{O}^{(n)}(1\ldots n) = (C_n^r)^{-1/2} \sum_{(u_1\ldots u_r)} \delta^{(u_1\ldots u_n)} \mathcal{O}^{(r)}(u_1\ldots u_r) \times \mathcal{O}^{(n-r)}(u_{r+1}\ldots u_n) . \quad (12)$$

In this formula, the set $(u_1\ldots u_n)$ is deduced from the set $(1\ldots n)$ by applying the permutation

$$\begin{pmatrix} u_1\ldots u_n \\ 1\ldots n \end{pmatrix}.$$

The subsets $(u_1\ldots u_r)$ and $(u_{r+1}\ldots u_n)$ are submitted to the conditions

$$u_1 < u_2 < \cdots < u_r ,$$

and

$$u_{r+1} < u_{r+2} < \cdots < u_n .$$

The sum is extended to the C_n^r possible ordered subsets $(u_1\ldots u_r)$. Finally, the factor $\delta^{(u_1\cdots u_n)}$ is defined by $\delta^{(u_1\cdots u_n)} = 1$, for any permutation

$$\begin{pmatrix} u_1\ldots u_n \\ 1\ldots n \end{pmatrix},$$

if $\hat{\mathcal{O}}^{(n)}$ is the symmetrizer, or by

$$\delta^{(u_1\cdots u_n)} = \begin{cases} 1, & \text{for an even permutation} \\ -1, & \text{for an odd permutation,} \end{cases}$$

if $\hat{\mathcal{O}}^{(n)}$ is the antisymmetrizer.

In a first step we consider the following simple product form of the primitive function

$$\Phi^{(n)}(1\ldots n) = \psi_A^{(r)}(1\ldots r)\psi_B^{(n-r)}(r+1,\ldots n) . \quad (13)$$

Using Eq. (12), we can write the n-particle wave function

$$\Psi^{(n)}(1\ldots n) = (C_n^r)^{-1/2} \sum_{(u_1\ldots u_r)} \delta^{(u_1\ldots u_n)} \psi_A^{(r)}(u_1\ldots u_r) \times \psi_B^{(n-r)}(u_{r+1}\ldots u_n) . \quad (14)$$

Now we use Löwdin's definition[15] of the kernel of the p-particle reduced-density operator $\hat{\rho}_n^{(p)}$

$$\rho_n^{(p)}(1\ldots p; 1'\ldots p') = C_n^p \int [\Psi^{(n)}(1\ldots n)\Psi^{*(n)}(1'\ldots n')]_{\substack{(p+1)'=p+1 \\ \cdots \\ n'=n}} \times d(p+1)\cdots dn , \quad (15)$$

together with the expression of $\Psi^{(n)}$ considered above [Eq. (13)], and we obtain

$$\rho_n^{(p)}(1\ldots p; 1'\ldots p') = \frac{C_n^p}{C_n^r} \sum_{(u_1\ldots u_r)} \sum_{(v_1\cdots v_r)} \delta^{(u_1\ldots u_n)}\delta^{(v_1\ldots v_n)} \times \int [\psi_A^{(r)}(u_1\ldots u_r)\psi_B^{(n-r)}(u_{r+1}\ldots u_n)\psi_A^{*(r)}(v_1'\ldots v_r')\psi_B^{*(n-r)}(v_{r+1}'\ldots v_n')]_{\substack{(p+1)'=p+1 \\ \cdots \\ n'=n}} d(p+1)\ldots dn . \quad (16)$$

In this double sum, only the terms for which the subset $(1\ldots p)$ is included in the subsets $(u_1\ldots u_r)$ and $(v_1\ldots v_r)$ will give a contribution to the kernel $\rho_{n\alpha}^{(p)}(1\ldots p; 1'\ldots p')$ of the operator $[\hat{\rho}_n^{(p)}]_\alpha$. These particular subsets are necessarily of the form

$$(12\ldots p, u_{p+1}\ldots u_r), \quad r \geq p ,$$

where $(u_{p+1} < \cdots < u_r)$ can be chosen among the $(n-p)$ remaining elements $(p+1,\ldots n)$. There are exactly C_{n-p}^{r-p} such different subsets $(u_1\ldots u_r)$, the same being true for $(v_1\ldots v_r)$. If we remark that for each $(u_1\ldots u_r)$ there is associated one and only one $(u_{r+1}\ldots u_n)$, we can deduce that all the cross terms arising between the particular subsets $(u_1\ldots u_r)$ and $(v_1\ldots v_r)$ just defined will vanish owing to the strong orthogonality properties[12] [Eq. (4)]. There remain the $C_n^r C_{n-p}^{r-p}$ diagonal terms which contribute equally, so that

$$\rho_{n\alpha}^{(p)}(1\ldots p; 1'\ldots p') = \frac{C_n^p}{C_n^r}\frac{C_{n-p}^{r-p}}{C_r^p}\rho_{Ar}^{(p)}(1\ldots p; 1'\ldots p') = \rho_{Ar}^{(p)}(1\ldots p; 1'\ldots p') , \quad (17)$$

where

$$\rho_{Ar}^{(p)}(1\ldots p;1'\ldots p') = C_r^p \int \psi_A^{(r)}(1\ldots p, u_{p+1}\ldots u_r) \times \psi_A^{*(r)}(1'\ldots p', u_{p+1}\ldots u_r)\, du_{p+1}\cdots du_r . \tag{18}$$

Now we examine the general case [see Eqs. (9) and (10)]

$$\Psi^{(n)}(1\ldots n) = \sum_{r=0}^{n} \sum_{i_r j_r} c_{i_r j_r}^r \mathcal{O}^{(n)}[\psi_{Ai_r}^{(r)}(1\ldots r) \times \psi_{Bj_r}^{(n-r)}(r+1\ldots n)] = \sum_{r=0}^{n} \Psi_r^{(n)}(1\ldots n) ,$$

where $\Psi_r^{(n)}$ is not a normalized function.

We have, by definition,

$$\rho_n^{(p)}(1\ldots p;1'\ldots p') = C_n^p \sum_{r,s=0}^{n} \int [\Psi_r^{(n)}(1\ldots n)\Psi_s^{*(n)}(1'\ldots n')]_{\substack{(p+1)'=p+1 \\ \cdots \\ n'=n}} \times d(p+1)\cdots dn . \tag{19}$$

On the other hand, as was shown above, an expression like

$$\mathcal{O}^{(n)}[\psi_{Ai_r}^{(r)}(1\ldots r)\psi_{Bj_r}^{(n-r)}(r+1,\ldots n)] \tag{20}$$

can be replaced by the sum

$$(C_n^r)^{-1/2} \sum_{(u_1\cdots u_r)} \delta^{(u_1\cdots u_n)} \psi_{Ai_r}^{(r)}(u_1\ldots u_r)\psi_{Bj_r}^{(n-r)}(u_{r+1}\ldots u_n) , \tag{21}$$

restricted to the C_{n-p}^{r-p} subsets $(u_1\ldots u_r)$ containing $(1\ldots p)$. The terms of the double sum in Eq. (19) which give a contribution to the expression of the operator $[\hat{\rho}_n^{(p)}]_\alpha$ are those for which the subset $(1\ldots p)$ is included in the subsets $(u_1\ldots u_r)$ and $(u_1\ldots u_s)$. Thus the double sum can be reduced to the terms for which

$$r \geq p, \quad s \geq p .$$

Moreover, the cross terms $(r \neq s)$ vanish identically owing to the strong orthogonality properties [Eq. (4)], because there always exists at least one point the coordinates of which appear at the same time as arguments of functions $\psi_A^{(r)}$ and $\psi_B^{(n-s)}$ or $\psi_A^{(s)}$ and $\psi_B^{(n-r)}$, which are strongly orthogonal.

Thus we may write

$$\rho_{n\alpha}^{(p)}(1\ldots p;1'\ldots p') = \frac{C_n^p}{C_n^r} \sum_{r\geq p} \sum_{i_r j_r} \sum_{i_r' j_r'} c_{i_r j_r}^r c_{i_r' j_r'}^{*r} \times \frac{C_{n-p}^{r-p}}{C_r^p} \delta_{j_r j_r'} \rho_{Ai_r i_r'}^{(p)}(1\ldots p;1'\ldots p') = \sum_{r\geq p} \sum_{i_r i_r'} \Big(\sum_{j_r} c_{i_r j_r}^r c_{i_r' j_r}^{*r} \Big) \rho_{Ai_r i_r'}^{(p)}(1\ldots p;1'\ldots p') , \tag{22}$$

where

$$\rho_{Ai_r i_r'}^{(p)}(1\ldots p;1'\ldots p') = C_r^p \int \psi_{Ai_r}^{(r)}(1\ldots p, u_{p+1}\ldots u_r) \times \psi_{Ai_r'}^{*(r)}(1'\ldots p', u_{p+1}\ldots u_r) du_{p+1}\ldots du_r \tag{23}$$

is the kernel of a transition p-particle reduced-density operator.[19] This formula can be compared to that of Eq. (18).

On the other hand, if we define

$$\rho_{n,r}^{(p)}(1\ldots p;1'\ldots p') = C_n^p \int [\Psi_r^{(n)}(1\ldots n)\Psi_r^{*(n)}(1'\ldots n')]_{\substack{(p+1)'=p+1 \\ \cdots \\ n'=n}} \times d(p+1)\cdots dn , \tag{24}$$

as the kernel of the p-particle reduced density operator derived from the n function $\Psi_r^{(n)}$, we can rewrite Eq. (22) in the form

$$\rho_{n\alpha}^{(p)}(1\ldots p;1'\ldots p') = \sum_{r\geq p} \rho_{n,r\alpha}^{(p)}(1\ldots p;1'\ldots p') , \tag{25}$$

where the kernel $\rho_{n,r\alpha}^{(p)}(1\ldots p;1'\ldots p')$ can be derived from the one just defined in Eq. (24) by restriction to the subspace $\mathcal{H}_\alpha^{(p)}$.

It can easily be verified that the matrix representing the operator $\hat{\rho}_{n,r}^{(p)}$ in the subspace $\mathcal{H}^{(p)}$ is block diagonal with respect to the partition $\mathcal{H}_\alpha^{(p)} \oplus \mathcal{H}_{\bar{\alpha}}^{(p)} = \mathcal{H}^{(p)}$, so that a diagonalization of each block separately yields the eigenvalues. The same is not true, however, for the operator $\hat{\rho}_n^{(p)}$, because the interaction of different events $(r \neq s)$ causes the appearance of nonvanishing cross terms.

We know [Eq. (23)] that, within Löwdin's normalization convention,

$$\mathrm{Tr}\hat{\rho}_{Ai_r i_r'}^{(p)} = C_r^p \delta_{i_r i_r'} ; \tag{26}$$

then we can derive from Eq. (22) an expression of the trace of the operator $\hat{\rho}_{n\alpha}^{(p)}$

$$\mathrm{Tr}[\hat{\rho}_n^{(p)}]_{\mathcal{A}} = \sum_{r\geq p}\Big(\sum_{i_r j_r} |c^r_{i_r j_r}|^2\Big) C_r^p$$

$$= \sum_{r\geq p} \alpha_r C_r^p , \tag{27}$$

where, according to Eq. (11),

$$\alpha_r = \sum_{i_r j_r} |c^r_{i_r j_r}|^2 \geq 0 , \quad \forall r$$

and (28)

$$\sum_{r\geq p} \alpha_r \leq 1 .$$

If we compare Eq. (27) with Eq. (25), we conclude that

$$\mathrm{Tr}[\hat{\rho}^{(p)}_{n,r}]_{\mathcal{A}} = \alpha_r C_r^p . \tag{29}$$

We will conclude this chapter with a few remarks on the bound conditions for the natural occupation numbers of a p-particle reduced-density operator represented by an event-type function.

For fermion systems, we use the approach proposed by Coleman.[20] We start from the inequality

$$(\rho_n^p)_i \leq C_n^p \langle \chi_i^{(p)} \chi_i^{(n-p)} | A^{(n)} | \chi_i^{(p)} \chi_i^{(n-p)} \rangle , \tag{30}$$

where $\chi_i^{(p)}$ is the natural p function associated with the eigenvalue $(\rho_n^p)_i$, $\chi_i^{(n-p)}$ is the conjugated natural $n-p$ function and $A^{(n)}$ is the antisymmetrizing projector $(n!)^{-1/2}\mathcal{A}^{(n)}$; equality is obtained if and only if,

$$\Psi^{(n)}(1\ldots n) = \mathcal{A}^{(n)}[\chi_i^{(p)}(1\ldots p)\chi_i^{(n-p)}(p+1,\ldots n)] . \tag{31}$$

With the aid of Sasaki's formula[21] we obtain

$$(\rho_n^p)_i \leq \sum_{u=0}^{p} (-1)^u C_p^u C_{n-p}^u \langle \chi_i^{(p)} \chi_i^{(n-p)} | \pi_u | \chi_i^{(p)} \chi_i^{(n-p)} \rangle , \tag{32}$$

where π_u is a permutation operator which interchanges u of the p variables in $\chi_i^{(p)}$ with u of the $n-p$ variables in $\chi_i^{(n-p)}$. Dropping the negative terms, one obtains the rough upper bound[22]

$$(\rho_n^p)_i \leq \sum_{u=0}^{p/2} C_p^{2u} C_{n-p}^{2u} \langle \chi_i^{(p)} \chi_i^{(n-p)} | \pi_{2u} | \chi_i^{(p)} \chi_i^{(n-p)} \rangle . \tag{33}$$

Let us now consider the even-type function $\Psi_r^{(n)}$, with $r \geq p$. From Eq. (31) we know that the upper bound can be attained only if $\chi_i^{(p)}\chi_i^{(n-p)} \in \mathcal{H}_{\mathcal{A}}^{(r)} \otimes \mathcal{H}_{\mathcal{B}}^{(n-r)}$. However, in this case, a certain number of terms in Eq. (33) vanish identically because of the strong orthogonality properties. Therefore, in general, the upper bounds will be smaller than usual for event-type functions.

As an example, it is easy to verify that, for $r=3$, $p=2$, and $\chi_i^{(2)} \in \mathcal{H}_{\mathcal{A}}^{(2)}$, all the terms in Eq. (33) vanish, excepting the one corresponding to the identity permutation. We conclude that

$$(\rho^2_{n,3})_i \leq 1 , \tag{34}$$

whereas the upper bound for $(\rho_n^2)_i$ is $\frac{1}{2}n$.[20]

The upper bounds can easily be obtained in any case by considering that they are realized for event-type functions of extreme type, according to the definition given by Coleman.[20] Thus we find that, for $\chi_i^{(2)} \in \mathcal{H}_{\mathcal{A}}^{(2)}$,

$$(\rho^2_{n,r})_i \leq [\tfrac{1}{2}r] , \tag{35}$$

where the symbol $[x]$ represents the greatest integer less than or equal to the real number x, and we deduce immediately the inequality of Eq. (34).

For boson systems, we know that a full condensation of particles is allowed; the upper bounds are also realized for event-type functions of extreme type, and, in the conditions of the preceding example, we obtain

$$(\rho^2_{n,r})_i \leq C_r^2 . \tag{36}$$

III. PROOF OF THE SEPARABILITY THEOREM

We suppose that the n-particle wave function is p-separable with respect to a partition $\mathcal{H}_{\mathcal{A}}^{(p)} \otimes \mathcal{H}_{\mathcal{B}}^{(n-p)}$ of $\mathcal{H}^{(n)}$,

$$\Psi^{(n)}(1\ldots n) = \mathcal{O}^{(n)}[\psi_A^{(p)}(1\ldots p)\psi_B^{(n-p)}(p+1,\ldots n)] ,$$

where

$$\psi_A^{(p)} \in \mathcal{H}_{\mathcal{A}}^{(p)}, \quad \psi_B^{(n-p)} \in \mathcal{H}_{\mathcal{B}}^{(n-p)} ,$$

and

$$\int \psi_A^{(p)}(\ldots i\ldots)\psi_B^{(n-p)}(\ldots i\ldots)\, di = 0 .$$

Putting $r=p$ in Eq. (18), we obtain immediately the expression of the kernel of $[\hat{\rho}_n^{(p)}]_{\mathcal{A}}$:

$$\rho_{n\mathcal{A}}^{(p)}(1\ldots p; 1'\ldots p') = \rho_{A\mathcal{p}}^{(p)}(1\ldots p; 1'\ldots p')$$

$$= \psi_A^{(p)}(1\ldots p)\psi_A^{*(p)}(1'\ldots p') .$$

We deduce that

$$[\hat{\rho}_n^{(p)}]_{\mathcal{A}} = |\psi_A^{(p)}\rangle\langle\psi_A^{(p)}| ,$$

which shows that $[\hat{\rho}_n^{(p)}]_{\mathcal{A}}$ is just the projector on the p function $\psi_A^{(p)} \in \mathcal{H}_{\mathcal{A}}^{(p)}$. This establishes the direct proposition of the theorem.

On the other hand, let us suppose that the following relations

$$\mathrm{Tr}[\hat{\rho}_n^{(p)}]_{\mathcal{A}} = 1 , \tag{37}$$

$$([\hat{\rho}_n^{(p)}]_{\mathcal{A}})^2 = [\hat{\rho}_n^{(p)}]_{\mathcal{A}} , \tag{38}$$

hold for the p-particle reduced-density operator $[\hat{\rho}_n^{(p)}]_\alpha$ restricted to the subspace $\mathcal{H}_\alpha^{(p)}$.

The general expression of $\hat{\rho}_n^{(p)}$ in terms of natural p functions $\chi_i^{(p)}$ is[14]

$$\hat{\rho}_n^{(p)} = \sum_{i \geq 1} (\rho_n^p)_i \, | \chi_i^{(p)} \rangle \langle \chi_i^{(p)} | \; ; \quad (\rho_n^p)_i \geq 0, \quad \forall i \; . \tag{39}$$

Using this and Eq. (2), defining $[\hat{\rho}_n^{(p)}]_\alpha$, we obtain

$$[\hat{\rho}_n^{(p)}]_\alpha = \sum_{i=1}^{N} (\rho_n^p)_i (\hat{P}_\alpha^{(p)} | \chi_i^{(p)} \rangle \langle \chi_i^{(p)} | \hat{P}_\alpha^{(p)}) \; . \tag{40}$$

It is always possible to expand $\hat{P}_\alpha^{(p)}$ in terms of a set of orthonormalized p functions $a_\mu^{(p)}$ forming an N_α-dimensional basis for the subspace $\mathcal{H}_\alpha^{(p)}$,

$$\hat{P}_\alpha^{(p)} = \sum_{\mu=1}^{N_\alpha} | a_\mu^{(p)} \rangle \langle a_\mu^{(p)} | \; , \tag{41}$$

especially chosen in order to diagonalize $[\hat{\rho}_n^{(p)}]_\alpha$, in this basis

$$[\hat{\rho}_n^{(p)}]_\alpha = \sum_{\mu=1}^{N_\alpha} \left(\sum_{i=1}^{N} (\rho_n^p)_i | \, c_{i\mu}^p |^2 \right) | a_\mu^{(p)} \rangle \langle a_\mu^{(p)} | \; , \tag{42}$$

where

$$c_{i\mu}^p = \langle a_\mu^{(p)} | \chi_i^{(p)} \rangle \tag{43}$$

and

$$0 < \sum_{\mu=1}^{N_\alpha} | \, c_{i\mu}^p |^2 \leq 1, \quad \forall i \leq N \; . \tag{44}$$

The normalization condition accounts for the fact that every natural p function $\chi_i^{(p)}$ does not necessarily have a projection into $\mathcal{H}_\alpha^{(p)}$; we suppose there are only N such functions.

Considering Eqs. (37) and (38), we deduce that there exists a given value of μ (let us say $\mu = 1$) for which

$$\sum_{i=1}^{N} (\rho_n^p)_i | \, c_{i1}^p |^2 = 1 \; , \tag{45}$$

whereas for any other values of $\mu \, (\mu \neq 1)$ we have

$$\sum_{i=1}^{N} (\rho_n^p)_i | \, c_{i\mu}^p |^2 = 0 \; . \tag{46}$$

Moreover, if we take into account the bound conditions (39) and (44), we deduce that the more general solution is

$$\begin{vmatrix} (\rho_n^p)_1^{-1} & | \, c_{21} |^2 & \dots & | \, c_{N1} |^2 \\ 0 & | \, c_{22} |^2 & \dots & | \, c_{N2} |^2 \\ \vdots & \vdots & & \\ 0 & | \, c_{2N_\alpha} |^2 & \dots & | \, c_{NN_\alpha} |^2 \end{vmatrix} \begin{vmatrix} (\rho_n^p)_1 \\ 0 \\ \vdots \\ 0 \end{vmatrix} = \begin{vmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{vmatrix} , \tag{47}$$

where $(\rho_n^p)_1 \geq 1$ in order to agree with the normalization condition (44).

Then, the more general orthogonal transformation which connects the basis of natural p functions $\chi_i^{(p)}$ and the basis formed by the union of the functions $a_\mu^{(p)} \in \mathcal{H}_\alpha^{(p)}$ and $\bar{a}_\nu^{(p)} \in \mathcal{H}_{\bar{\alpha}}^{(p)}$, is represented by the square matrix $\underline{T}$,

$$\left| \begin{array}{cccc|c} (\rho_n^p)_1^{-1/2} & 0 \dots & 0 & & c_{1,N_\alpha+1} \; \dots \\ c_{21} & c_{22} \dots & c_{2N_\alpha} & & c_{2,N_\alpha+1} \; \dots \\ \vdots & \vdots & \vdots & & \vdots \\ c_{N1} & c_{N2} \dots & c_{NN_\alpha} & & c_{N,N_\alpha+1} \; \dots \\ \hline 0 & 0 \dots & 0 & & c_{N+1,N_\alpha+1} \; \dots \\ \vdots & \vdots & \vdots & & \vdots \end{array} \right| , \tag{48}$$

where N_α is the dimension of $\mathcal{H}_\alpha^{(p)}$ and N is the number of natural p functions $\chi_i^{(p)}$ which have a nonvanishing projection into $\mathcal{H}_\alpha^{(p)}$.

We deduce immediately that $N \geq N_\alpha$; in the opposite case, the number of $\bar{\chi}_i^{(p)}$ functions having a vanishing projection into $\mathcal{H}_\alpha^{(p)}$ would be greater than the dimension of $\mathcal{H}_{\bar{\alpha}}^{(p)}$ and thus nonlinearly independent. At this stage, the more general relation connecting the matrices $\underline{R}(\chi)$ and $\underline{R}(a)$, which represent $\hat{\rho}_n^{(p)}$ in the two basis sets $\{\chi, \bar{\chi}\}$ and $\{a, \bar{a}\}$, respectively, is represented in Fig. 1.

Let us examine, first, the case $N = N_\alpha$. The components of the vectors $\vec{c}_j$ $(j > N_\alpha)$ are such that

$$c_{j\nu} = 0, \quad \forall \nu \leq N_\alpha \; . \tag{49}$$

Then the vectors $\vec{c}_i$ $(1 \leq i \leq N_\alpha)$, which form with the vectors $\vec{c}_j$ an orthonormal basis set, must have components such that

$$c_{i\mu} = 0, \quad \forall \mu > N_\alpha \; . \tag{50}$$

Thus, in this case, the transformation matrix $\underline{T}$ is block diagonal; as it is a unitary matrix, we deduce that for $i = 1$

$$c_{1\mu} = \delta_{1\mu} \; , \tag{51}$$

and for $\mu = 1$

$$c_{i1} = \delta_{i1} \; . \tag{52}$$

It follows from Eq. (45) that

$$(\rho_n^p)_1 = 1 \; , \tag{53}$$

and from Eq. (43) that

$$a_1^{(p)} = \chi_1^{(p)} \; . \tag{54}$$

This last relation means that, in the case of interest, the natural p functions $\chi_1^{(p)}$, corresponding to the eigenvalue $(\rho_n^p)_1$, belong to $\mathcal{H}_\alpha^{(p)}$. Finally, we remark that the matrix $\underline{R}(a)$ is block diagonal, too.

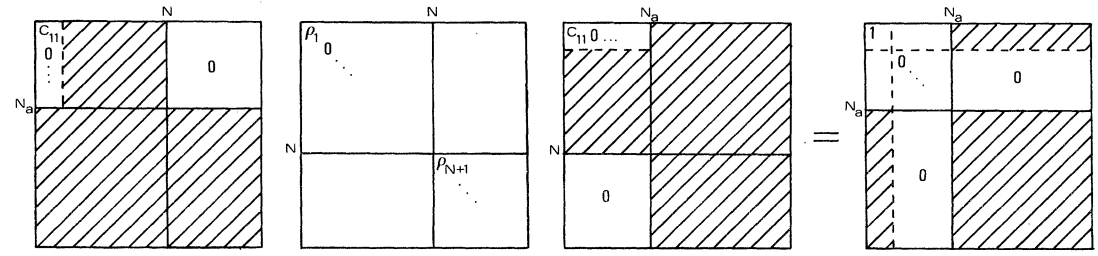

FIG. 1. General relation connecting the matrices $\underline{R}(\chi)$ and $\underline{R}(a)$.

Let us now examine the case $N > N_a$. In order to realize the more general situation symbolized in Fig. 1, we must consider the wave function to be a sum of event-type functions, so that nonvanishing cross terms with respect to the partition $\mathcal{H}_{\alpha}^{(p)} \oplus \mathcal{H}_{\bar{\alpha}}^{(p)} = \mathcal{H}^{(p)}$ can arise in the matrix $\underline{R}(a)$. At the same time, we must impose that [see Eq. (37)]

$$\mathrm{Tr}[\hat{\rho}_n^{(p)}]_{\alpha} = 1 ; \tag{55}$$

then, using Eqs. (27) and (29),

$$\mathrm{Tr}[\hat{\rho}_n^{(p)}]_{\alpha} = \sum_{r \geq p} \mathrm{Tr}[\hat{\rho}_{n,r}^{(p)}]_{\alpha} = \sum_{r \geq p} \alpha_r C_r^p = 1 . \tag{56}$$

Such relations can be satisfied only if

$$\sum_{r \geq p} \alpha_r < 1 , \tag{57}$$

which implies that in the development of the wave function both classes of terms, those having $r > p$ and those having $r < p$, must be introduced simultaneously in addition to the term $r = p$.

Let us work in the basis $\{a\}$ which diagonalizes the operator $[\hat{\rho}_n^{(p)}]_{\alpha}$ [Eq. (42)]. In order to agree with the general situation of Fig. 1 again, the diagonal elements must be given by [see Eq. (38) and Eqs. (45) and (46)]

$$(\rho_n^p)_{\mu} = \delta_{\mu 1} , \quad \forall \mu . \tag{58}$$

In such a basis the matrices representing the operators $[\hat{\rho}_{n,r}^{(p)}]_{\alpha}$ are not diagonal *a priori*. However, from Eqs. (25) and (58), we obtain a relation satisfied by their diagonal elements $(\rho_{n,r}^p)_{\mu}$,

$$\sum_{r \geq p} (\rho_{n,r}^p)_{\mu} = (\rho_n^p)_{\mu} = \delta_{\mu 1} , \quad \forall \mu . \tag{59}$$

Comparing Eq. (59) with (56), we are led to the conclusion that

$$(\rho_{n,r}^p)_1 = \mathrm{Tr}[\hat{\rho}_{n,r}^{(p)}]_{\alpha} , \tag{60}$$

and consequently that

$$(\rho_{n,r}^p)_{\mu} = 0 , \quad \forall \mu \neq 1 . \tag{61}$$

Since we know that the inequality

$$\rho_{\mu\mu} \rho_{\nu\nu} \geq | \rho_{\mu\nu} |^2 \tag{62}$$

holds for the elements of any reduced-density matrix,[23] we conclude that the matrices representing the operators $[\hat{\rho}_n^{(p)}]_{\alpha}$ and $[\hat{\rho}_{n,r}^{(p)}]_{\alpha}$, must be simultaneously diagonalized in order to realize the general situation of Fig. 1. If we remember now that a diagonalization of $[\hat{\rho}_{n,r}^{(p)}]_{\alpha}$ yields the eigenvalues of $\hat{\rho}_{n,r}^{(p)}$ we see, from the Eqs. (53) and (29), that there necessarily exists an eigenvalue

$$(\rho_{n,r}^p)_1 = \alpha_r C_r^p , \quad \forall r \geq p . \tag{63}$$

This condition is compatible with the bound conditions for the eigenvalues of a boson system, but not at all with that of a fermion system, as shown by Eqs. (35) and (36).

Thus, for a fermion system, we have only to consider the case $N = N_a$ studied above. As the value of $(\rho_n^p)_1$ obtained in Eq. (53) is the greatest possible, we conclude, taking account of Eq. (31), that

$$\Phi^{(n)}(1 \ldots n) = \chi_1^{(p)}(1 \ldots p) \chi_1^{(n-p)}(p+1 \ldots n) , \tag{64}$$

where $\chi_1^{(p)} \in \mathcal{H}_{\alpha}^{(p)}$, according to Eq. (54), and $\chi_1^{(n-p)} \in \mathcal{H}_{\bar{\alpha}}^{(n-p)}$, since $\Phi^{(n)} \in \mathcal{H}_{\alpha}^{(p)} \otimes \mathcal{H}_{\bar{\alpha}}^{(n-p)}$. This achieves the proof of the theorem.

For boson systems, however, no conclusion can be given.

DISCUSSION AND CONCLUSION

It seems to us particularly interesting to emphasize the following points.

First, we have shown that the bound conditions on the eigenvalues of a p-particle reduced-density matrix representable by an event-type function alone are more restrictive than the classical bound conditions[20] derived for any sort of totally antisymmetrized wave function. The upper bounds are found to be the same only if we consider the limiting-case event-type functions $\Psi_0^{(n)}$ or $\Psi_n^{(n)}$ defined in the trivial partitions $\mathcal{H}^{(0)} \otimes \mathcal{H}^{(n)}$ or $\mathcal{H}^{(n)} \otimes \mathcal{H}^{(0)}$ of $\mathcal{H}^{(n)}$.

Now, as we have pointed out from the beginning, a great number of calculations on atomic or molecular systems show that their ground-state wave

functions are correctly approximated by a separable function which is a kind of event-type function. This implies necessarily that the occupation numbers of the natural p functions usually encountered in the study of this class of systems never reach the classical upper bounds foreseen by the theory. Indeed, the study of the two-particle reduced-density matrices representable by an atomic or molecular wave function reveals that the order of magnitude of the greatest eigenvalues is about unity.[24]

On the other hand, some considerations of these bound conditions can lead, in some special cases, to the selection of the only convenient event-type function. For instance, in the theory of superconductivity some wave functions of extreme type are used so that the classical upper bounds for the two-particle density matrix are reached[25]; clearly, only a limiting-case event-type function defined in the trivial partition of the Hilbert space is suitable for such a wave function. The impossibility of finding any proper partitions of the number of particles and of the Hilbert space other than the trivial ones can be considered as further evidence of the well-known collective and delocalization features of the superconductivity phenomenon.

When the wave function $\Psi^{(n)}$ is p-separable with respect to the partition $\mathcal{K}_\alpha^{(p)} \otimes \mathcal{K}_\beta^{(n-p)}$ of $\mathcal{K}^{(n)}$, we have shown that the p-particle function $\psi_A^{(p)}$, which enters in the expression of the primitive function $\Phi^{(n)}$, is also a natural p function. This suggests that, when there is no degeneracy of the occupation numbers, the p-natural analysis will yield the best group of p functions, $\psi^{(p)}$, for the system of interest.

The main point is, however, the validity of the theorem for any fermion system regardless of the kind of wave function used. Henceforth we are able to decide if the system can be represented by a separable function and consequently to bring to light the existence of a subsystem.

Naturally, a fermion wave function is in general a linear combination of event-type functions. As we have pointed out in the Introduction, the problem is now to define a procedure which allows us to determine quantitatively to what extent a separable function alone can give a good approximation of the wave function; this will be investigated in a later paper. Nevertheless, the method of analysis founded on the above theorem is simple to handle[26]; the idempotency is immediately revealed after diagonalizing the matrix representing the p-particle reduced-density operator restricted to a given subspace. Moreover, the dimension of this matrix, characteristic of the subspace, does not depend on the size of the whole system.

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