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N Completeness, *N* Representability, and Geminal Expansions

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The complete solution is presented for the N-completeness problem, i.e., the problem of determining when a set of p-particle functions generates symmetric or antisymmetric functions without applying a symmetrizing or antisymmetrizing operator. Then it is shown that a symmetric or antisymmetric function has finite 2 rank if, and only if, it has finite 1 rank. Finally, the relation between N representability of N completeness is discussed.

I. INTRODUCTION

This paper is concerned with several problems which arise when one tries to expand a symmetric or antisymmetric N-particle function in terms of p-particle functions. Such expansions are of greatest interest when $p=2$, and are then called geminal (i.e., 2-particle) expansions. For example, if $N=4$, $p=2$, a geminal expansion has the form

$$\Psi(1,2,3,4)=\sum_{kl} c_k \phi_k(12)\phi_l(34).$$

Given a symmetric or antisymmetric N-particle function, one can always find a geminal basis in which the N-particle function can be written as a geminal expansion.[1] Furthermore, the geminal expansion will have the proper permutational symmetry to begin with and no symmetrizing or antisymmetrizing operators need be applied. As geminals are being increasingly used to study physical problems, e.g., correlation, the properties of such expansions and their associated basis sets have become increasingly important. Indeed, one might consider the geminal expansion as the 2-particle generalization of the Slater-determinant expansions.

Unfortunately, it is easy to see that not all sets of geminals will give rise to such symmetric or antisymmetric expansions. Thus one is naturally led to consider the so-called N-completeness problem which was originally introduced in connection with the so-called N-representability problem.[2–14] A set of orthonormal p-particle functions is said to be N complete if there exists at least one symmetric or antisymmetric N-particle function which can be written as a p-particle (e.g., geminal if $p=2$) expansion using only the given p-particle functions. In this paper we present a complete solution to the N-completeness problem.

In a previous paper,[1] a partial solution to the N-completeness problem was presented. It expressed the final result in terms of a set of transposition matrices (to be defined) and a very awkward condition[15] of the form $\mathcal{O}_\epsilon\Psi=\Psi$. We now show that this latter condition is completely unnecessary. Both necessary and sufficient conditions can be expressed in terms of the transposition matrices alone. Furthermore, we can now state the solution as one simple condition on the final transposition matrix, rather than as a long series of conditions. We also drop the restriction to finite rank. A detailed exposition of these results forms the content of Sec. III.

In Ref. 1, we raised the following question[16]: Can a symmetric or antisymmetric function have finite 2 rank and infinite 1 rank? We now show that, except in the trivial case $N=2$, the answer is no. This and other results concerning rank are discussed in Sec. IV.

In a previous paper,[1] we showed that one could make considerable progress in the difficult problem of N representability [2–14] by studying the N completeness of the natural p states. (Natural spin geminals when $p=2$.) In Sec. V, we use our improved results on N completeness to state some improved N-representability theorems. Furthermore, we show that failure to consider N completeness has led to some erroneous results.[9]

II. REVIEW

An N-particle *pure state* is described by a normalized square-integrable function

$$\Psi(1\cdots N).$$

An N-particle statistical mixture is described by the *ensemble density matrix*

$$\rho^N=\sum_j \alpha_j \Psi_j(1\cdots N)\Psi_j^*(1'\cdots N'), \qquad (1)$$

where

$$0\leqslant\alpha_j\leqslant 1$$

and

$$\sum_j \alpha_j=1.$$

The pth-*order reduced-density matrix*[17] of a pure state or statistical mixture is

$$D^p(x;x')=\int \Psi(x,y)\Psi^*(x,y)\,dy \qquad (2)$$

or

$$D^p(x;x')=\int \rho^N(x,y;x'y)\,dy\ , \qquad (3)$$

where x and y represent, respectively, the coordinates of the first p and last $(N-p)$ particles. A p *matrix*,[17] also denoted D^p, is any p-particle operator which is Hermitian, is non-negative, has trace 1, and has the appropriate permutational symmetry. The *rank* R_p of a p matrix is the number of nonzero eigenvalues it has. The p *rank* of an N-particle function is the rank R_p of its pth-order reduced-density matrix.

A p matrix is pure or ensemble N *representable* if it can be derived according to (2) or (3) from an N-particle pure state or ensemble density matrix of a certain permutational symmetry. The (not necessarily unique) N-particle function or ensemble from which a p matrix can be derived is called its *preimage*. In particular, one speaks of boson N representability if the preimage is symmetric, and fermion N representability if the preimage is antisymmetric.

The *natural* p *states* of any N-particle (pure or ensemble) state are the eigenfunctions belonging to nonzero eigenvalues of its pth-order reduced-density matrix. It will be useful to extend this concept to any set of functions.

Definition. Let $\{\Phi_k\}$ be an orthonormal set of s-particle states. The *natural* q *states* of the set $\{\Phi_k\}$ are the q-particle functions obtained by orthoganalizing

$$\bigcup_k \text{(natural } q \text{ states of } \Phi_k). \qquad (4)$$

They are defined only up to unitary equivalence, and it is easy to show that the natural q states are unitarily equivalent to the eigenfunctions of any s matrix whose range is identical to the space spanned by $\{\Phi_k\}$

The following well-known results will be extremely useful.

Theorem 2.1. Any p matrix can be written in the form

$$D^p(x;x')=\sum_k \lambda_k^p\,\phi_k^p(x)\,\phi_k^p(x')\ , \qquad (5)$$

where λ_k^p and ϕ_k^p are the eigenvalues and eigenfunctions of D^p.

Theorem 2.2. If[2,18] D^p and D^{N-p} are the reduced-density matrices of an N-particle pure state Ψ, then they have the same nonzero eigenvalues. Thus $R_p=R_{N-p}$. Further, Ψ can be expanded in its natural p and $(N-p)$ states as

$$\Psi=\sum_k (\lambda_k^p)^{1/2}\,\phi_k^p(1\cdots p)\phi_k^{N-p}(p+1\cdots N). \qquad (6)$$

Theorem 2.3. Any[1,19] symmetric or antisymmetric N-particle function can be expanded in its natural p and q states as

$$\Psi=\sum_{ik_1\cdots k_\nu} c_{ik_1\cdots k_\nu}\,\phi_i^q(w)\,\phi_{k_1}^p(x_1)\cdots\phi_{k_1}^p(x_\nu)\ , \qquad (7)$$

where $N=q+\nu p$, and w and x_i represent the coordinates of disjoint sets of q and p particles, respectively. Further[20] the eigenfunctions of any ensemble density matrix (i.e., N matrix) can also be expanded in this way.

The above expansions of Ψ suggest another problem, called N completeness, which is closely related to N representability and interesting in itself.

Definition. A set $\{\psi_k\}$ $(k=1\cdots M_0)$ of orthonormal symmetric (antisymmetric) p-particle states is said to be boson (fermion) N complete if there exists an N-particle function which can be expanded in terms of $\{\psi_k\}$ and its natural q states in the form (7) (with $N=\nu p+q$ and $\phi_k^p\rightarrow\psi_k$).

We now state without proof some trivial results on N completeness.

Theorem 2.4. A set of p-particle states is N complete if and only if there exists a set of (not necessarily orthonormal) $(N-p)$-particle states $\{\chi_k\}$ and an N-particle function of the appropriate symmetry which can be expanded in the form

$$\Psi=\sum_k \psi_k(1\cdots p)\,\chi_k(p+1\cdots N). \qquad (8)$$

Theorem 2.5. Any set of orthonormal 1-particle states is boson N complete. A set of 1-particle states is fermion N complete if and only if it spans a space of dimension $\geq N$.

III. N COMPLETENESS

In Ref. 1, the N-completeness conditions were expressed in terms of several so-called transposition matrices. The definition below is a slight generalization of the matrices considered previously.[1,21–23]

Definition. Let $\{\psi_k\}$ be an orthonormal set of p-particle states. The associated *transposition matrix* $\underline{T}(p, q, r)$ is defined as the (double-index) matrix whose elements are given by

$$\tau_{ki,lj} = \int \psi_k^*(w, x)\, \theta_i^*(y, z)\, \psi_l(y, x)\, \theta_j(w, z)\,, \tag{9}$$

where

$$p \geq q \geq r, \quad p \neq r$$

$w, x, y,$ and z represent disjoint sets of coordinates of, respectively, r, $(p-r)$, r, and $(q-r)$ particles, and $\{\theta_i\}$ are the natural q states of $\{\psi_k\}$. $\underline{T}(p, q, r)$ is defined up to a restricted class[24] of unitary transformations.

Associated with any transposition matrix $\underline{T}(p, q, r)$ is a series of matrices,[25] $\underline{\Omega}^\alpha$, which are defined below. The full motivation for constructing these matrices is given in Ref. 1, but two points are worth noting here. First, if $\underline{T}$ satisfies the $(\nu p + q)$-completeness conditions, then $\underline{\Omega}^\alpha$ will satisfy the $[(\nu - \alpha + 1)p + q]$- completeness conditions. Further, if $p > q = r$, then one can write $\underline{T}$ in the form (10) given below for $\underline{\Omega}^\alpha$ by expanding the $\{\psi_k\}$ in its natural q and $(p-q)$ states. In order to treat bosons and fermions simultaneously we let, $\epsilon = +1$ for bosons, $\epsilon = -1$ for fermions, and use appropriate powers, e.g., ϵ^p.

Definition. Let the orthonormal ϵ^r *eigenvectors* (eigenvectors belonging to eigenvalue ϵ^r) of $\underline{T}(p, q, r)$ by denoted[26] by

$$\underline{A}^m = (a_{ki}^m)$$

and the ϵ^r rank (i.e., degeneracy of ϵ^r) of $\underline{T}$ by M_1. Note that the $\underline{A}^m$ are defined only up to a unitary transformation among themselves, and that we have written them as (single-index) matrices rather than as column vectors. Then $\underline{\Omega}^2$ is defined by

$$\omega_{km,ln} = \textstyle\sum_i a_{ki}^n a_{li}^{m*} = (\underline{A}^n \underline{A}^{m\dagger})_{kl}\,. \tag{10}$$

One then defines a sequence of such matrices, using the ϵ^p eigenvectors of each $\underline{\Omega}^\alpha$ to define $\underline{\Omega}^{\alpha+1}$. Let the ϵ^p rank and ϵ^p eigenvectors of $\underline{\Omega}^\alpha$ be M_α and

$${}^\alpha\underline{U}^{m_\alpha} = (u_{km_{\alpha-1}}^{m_\alpha})\,,$$

respectively.[25–27] $\underline{\Omega}^{\alpha+1}$ is defined as

$$\omega_{km_\alpha, ln_\alpha}^{\alpha+1} = \sum_{m_{\alpha-1}} u_{km_{\alpha-1}}^{n_\alpha} u_{lm_{\alpha-1}}^{m_\alpha *}\,. \tag{11}$$

If $M_\alpha = 0$, define $\underline{\Omega}^{\alpha+1} = 0$. Occasionally it will be convenient to consider $\underline{T}$ itself as an $\underline{\Omega}^\alpha$ matrix. For this purpose, one defines $\underline{\Omega}^1 = \underline{T}$ and $M_0 =$ the number of ψ_k.

Theorem 3.1. The matrices $\underline{T}\,(=\underline{\Omega}^1)$ and $\underline{\Omega}^\alpha$ defined above have the following properties:

(a) $\underline{\Omega}^\alpha = (\underline{\Omega}^\alpha)^\dagger$ $\quad(\alpha = 1, 2, \ldots)$;

(b) $0 \leq \omega_{km,km}^\alpha \leq 1$ $\quad(\alpha = 1, 2, \ldots)$;

(c) $|\omega_{km,ln}^\alpha|^2 \leq \omega_{kn,kn}^\alpha\, \omega_{lm,lm}^\alpha \leq 1$ $\quad(\alpha = 1, 2, \ldots)$;

(d) spectral radius of $\underline{\Omega}^\alpha \leq 1$ $\quad(\alpha = 1, 2, \ldots)$;

(e) $\sum_{ln} |\omega_{km,ln}^\alpha|^2 \leq 1$ $\quad(\alpha = 1, 2, \ldots)$;

(f) $\mathrm{Tr}\underline{\Omega}^\alpha = M_{\alpha-1} = \epsilon^p$ rank of $\underline{\Omega}^{\alpha-1}$ $\quad(\alpha = 3 \ldots)$;
$\mathrm{Tr}\underline{\Omega}^2 = M_1 = \epsilon^r$ rank of $\underline{T}$,
$\mathrm{Tr}\,\underline{T}\,(p, q, q) = M_0 =$ number of ψ_k;

(g) $\mathrm{Tr}(\underline{\Omega}^\alpha)^\dagger \underline{\Omega}^\alpha \leq [\mathrm{Tr}\underline{\Omega}^\alpha]^2$ $\quad(\alpha = 1, 2, \ldots)$;

(h) $\underline{\Omega}^\alpha$ defines a bounded self-adjoint operator on a (possibly infinite-dimensional) Hilbert space.

Proof.

(a) Trival.

(b) The only nontrivial part is

$$\tau_{ki,ki} = \int D_\psi^r(y, w)\, D_\theta^r(y, w) \leq [\mathrm{Tr}(D_\psi^r)^2\, \mathrm{Tr}(D_\theta^r)^2]^{1/2} \leq 1\,,$$

where D_ψ^r and D_θ^r are the rth-order reduced-density matrices of ψ_k and θ_i, respectively. The first step is just the Schwarz inequality for the trace norm.

(c) This follows from (b) and various applications of the Schwarz inequality:

$$|\tau_{ki,lj}|^2 = \left|\int F_{kj}(x, z) F_{li}^*(x, z)\right|^2 \leq \int |F_{kj}(x, z)|^2 \int |F_{li}^*(x, z)|^2 = \tau_{kj,kj}\tau_{li,li}\,,$$

where $F_{kj}(x, z) = \int dw\, \psi_k^*(w, x)\, \theta_j(w, z)$;

$$|\omega_{km,ln}|^2 = \left|\textstyle\sum_i a_{ki}^n a_{li}^{m*}\right|^2 \leq \textstyle\sum_i |a_{ki}^n|^2 \sum_i |a_{li}^m|^2 = \omega_{kn,kn}\,\omega_{lm,lm}\,.$$

(d) Let λ be any eigenvalue of $\underline{\Omega}^\alpha$ and $\underline{V} = \{v_{km_{\alpha-1}}\}$ be the corresponding eigenfunction. Consider the $(\alpha p + q)$-particle function:

$$\Psi_\lambda = \sum_{ik_1\cdots k_\alpha} b_{ik_1\cdots k_\alpha}\, \theta_i(w)\, \psi_{k_1}(x_1) \cdots \psi_{k_\alpha}(x_\alpha)\,, \tag{12}$$

where

$$b_{ik_1\cdots k_\alpha} = \sum_{m_1\cdots m_{\alpha-1}} a_{k_1 i}^{m_1} u_{k_2 m_1}^{m_2} \cdots u_{k_{\alpha-1} m_{\alpha-2}}^{m_{\alpha-1}} v_{k_\alpha m_{\alpha-1}}, \tag{13}$$

w, $x_1 \cdots x_\alpha$ represent disjoint sets of q- and p-particle coordinates, and $a_{k_1 i}^{m_1}$, $u_{k m_{B-1}}^{m_B}$ are the ϵ^r and ϵ^p eigenvectors of $\underline{T}$ and $\underline{\Omega}^\beta$ defined previously.

Let P_α be the operator which permutes $x_{\alpha-1}$ and x_α or, equivalently, interchanges $k_{\alpha-1}$ and k_α in $b_{ik_1\cdots k_\alpha}$. Then a simple calculation shows that

$$\langle \Psi_\lambda, P_\alpha \Psi_\lambda \rangle = \lambda . \tag{14}$$

Since $(P_\alpha)^2 = 1$,

$$\begin{aligned} |\lambda|^2 &= |\langle \Psi_\lambda, P_\alpha \Psi_\lambda \rangle|^2 \\ &\leq \|\Psi_\lambda\| \cdot \|P_\alpha \Psi_\lambda\| \\ &= \|\Psi_\lambda\|^2 = 1 . \end{aligned} \tag{15}$$

(e) $$\begin{aligned} \sum_{ln} |\omega_{km,ln}^\alpha|^2 &= [\underline{\Omega}^\alpha (\underline{\Omega}^\alpha)^\dagger]_{km,km} \\ &\leq \text{spectral radius of } \underline{\Omega}^\alpha (\underline{\Omega}^\alpha)^\dagger \\ &= [\text{spectral radius of } \underline{\Omega}^\alpha]^2 \\ &\leq 1 . \end{aligned} \tag{16}$$

(f) $$\sum_{km_{\alpha-1}} \omega_{km_{\alpha-1},km_{\alpha-1}}^\alpha = \sum_{i,k,m_{\alpha-1}} |u_{ki}^{m_{\alpha-1}}|^2 = \sum_{m_{\alpha-1}} 1 = M_{\alpha-1} .$$

(g) This follows from (c).

(h) Since this is trivial in finite demensions, we consider only the infinite-demensional case, i.e., $M_0 = \infty$. The argument given when proving (d) is equally valid for any truncation of $\underline{\Omega}^\alpha$, so that all truncations also have spectral radius ≤ 1. This is a sufficient condition[28] for $\underline{\Omega}^\alpha$ to define a bounded operator on some Hilbert space. Furthermore, it implies that all later theorems are valid for both finite and infinite sets of $\{\psi_k\}$.

The complete solution to the N-completeness problem can now be stated in a simple way.

Theorem 3.2. Let $N = \nu p + q$. Then a set of (symmetric or antisymmetric) p-particle states is (boson or fermion) N complete if and only if the associated $\underline{\Omega}^\nu$ matrix has ϵ^p (ϵ^r if $\nu = 1$) as an eigenvalue.

Remark. By the definition of $\underline{\Omega}^\alpha$, whenever the above condition is satisfied one also has (i) ϵ^r is an eigenvalue of $\underline{T}(p,q,r)$; (ii) ϵ^p is an eigenvalue of $\underline{\Omega}^\alpha$ for $2 \leq \alpha \leq \nu$.

Proof. Necessity was shown previously,[1] therefore, we consider only sufficiency here. Let Ψ be an N-particle function of the sort considered in the proof of part (d) of the previous theorem with $\lambda = \epsilon^p$, i.e.,

$$\Psi = \sum_{ik_1\cdots k_\nu} b_{ik_1\ldots k_\nu} \theta_i(w) \psi_{k_1}(x_1) \cdots \psi_{k_\nu}(x_\nu), \tag{17}$$

where

$$b_{ik_1\ldots k_\nu} = \sum_{m_1\cdots m_{\nu 1}} a_{k_1 i}^{m_1} u_{k_2 m_1}^{m_2} \circ \cdots u_{k_\nu m_{\nu-1}}^{m_\nu}, \tag{18}$$

$w, x_1 \cdots x_\nu$ are disjoint sets of q- and p-particle coordinates, and we have omitted the superscript m_ν on Ψ and b. Now, let P be one of the following kinds of permutations: Class A—P interchanges particles completely within any w or x_α; class B—P interchanges r particles in w with r particles in x_α; class C—P interchanges x_α and x_β, or, equivalently, interchanges k_α and k_β in $b_{ik_1\cdots k_\nu}$. Let σ be either the sign of P or $+1$ depending on whether fermions or bosons are under consideration. Clearly, $P\Psi = \sigma\Psi$ for permutations of class A. For classes B and C, a slight extension of the argument given in the proof of part (d) of the previous theorem shows that

$$\langle \Psi, P\Psi \rangle = \sigma . \tag{19}$$

Since the projector onto the subspace generated by eigenfunctions to eigenvalue σ of P is $\mathcal{O}_\sigma = \frac{1}{2}(1 + \sigma P)$, (19) implies that $\|\mathcal{O}_\sigma \Psi\| = 1$. Therefore,

$$\mathcal{O}_\sigma \Psi = \Psi , \quad P\Psi = \sigma\Psi . \tag{20}$$

Since any permutation can be decomposed into a product of permutations of the above classes, Ψ is actually symmetric or antisymmetric as desired.

IV. RANK

In Ref. 1 the following question was raised. Can a symmetric or antisymmetric function have finite 2 rank and infinite 1 rank? The next theorem shows that this can only happen in the trivial case $N = 2$.

Theorem 4.1. Let $1 \leq p$, $q < N$. Then the p rank of any symmetric or antisymmetric N-particle function is finite (infinite) if and only if the q rank is finite (infinite).

Proof. By theorem 2.2 we can assume without loss of generality that $p < q \leq \frac{1}{2}N$. Let w, x, y, z, respectively, represent disjoint sets of p-, $(q-p)$-, $(q-p)$-, and $(N+p-2q)$-particle coordinates, and expand Ψ in its natural p, $(q-p)$, and $(N-q)$ states as

$$\Psi = \sum_{mik} b_{mik} \phi_m^p(w) \phi_i^{q-p}(x) \phi_k^{N-q}(y,z) . \tag{21}$$

Consider the transposition matrix $\underline{T}(N-q, q-p, q-p)$ formed from $\{\phi_k^{N-q}\}$ and $\{\phi_i^{q-p}\}$. For each m, b_{mik} defines an ϵ^{q-p} eigenvector, $\underline{A}^m = (a_{ki}^m = b_{mik})$ of $\underline{T}$. Since the ϕ_m^p are eigenfunctions of D^p,

$$\mathrm{Tr}(\underline{A}^m \underline{A}^{n\dagger}) = \sum_{ik} b_{mik} b_{nik}^* = \lambda_m^p \delta_{mn} . \tag{22}$$

Thus, the $\underline{A}^m$ define R_p orthogonal ϵ^{q-p} eigenvectors of $\underline{T}$. Since $\epsilon^2 = 1$ and $(\underline{T}\,\underline{T}^\dagger)\,\underline{A}^m = (\epsilon^2)\,\underline{A}^m$, $\mathrm{Tr}(\underline{TT}^\dagger) \geq R_p$. But theorem 2.2 and parts (f) and (g) of theorem 3.1 imply that

$$\mathrm{Tr}(\underline{\mathrm{T}}\underline{\mathrm{T}}^\dagger) \leq (\mathrm{Tr}\,\underline{\mathrm{T}})^2 = R_{N-q}^2 = R_q^2 .$$

Thus

$$R_p \leq \mathrm{Tr}(\underline{\mathrm{T}}\underline{\mathrm{T}}^\dagger) \leq R_q^2 \quad (p < q), \tag{23}$$

and R_p is finite whenever R_q is finite.

Conversely, suppose R_p is finite and let $q = \mu p + s$ $(1 \leq s < p)$. By theorem 2.3, all ϕ_i^q lie in the space spanned by

$$\{\phi_i^s(w)\, \phi_{k_1}^p(x_1) \cdots \phi_{k_\mu}^p(x_\mu)\}.$$

By the first part of the theorem, R_s = the number of ϕ_i^s is finite. Therefore, we have $R\,q \leq R_s R_p^\mu < \infty$.

Coleman[5,29] has shown that the p rank of an antisymmetric N-particle function is $\geq \binom{N}{p}$. One can easily translate this into an N-completeness condition.

Theorem 4.2. If $\{\psi_k\}$ is fermion N complete, then

(a) the number of $\psi_k = M_0 \geq \binom{N}{p}$;

(b) the ϵ^r rank of $\underline{\mathrm{T}} = M_1 \geq \binom{N}{p+q}$;

(c) the ϵ^prank of $\underline{\Omega}^\alpha = M_\alpha \geq \binom{N}{p\alpha + q}$ $(\alpha = 2 \ldots)$.

V. N REPRESENTABILITY

As mentioned earlier, there is a close connection between N completeness and N representability. In particular, it follows from theorem 2.3 that a necessary condition for N representability of a p matrix is that its eigenfunctions to nonzero eigenvalues form an N-complete set. In fact, one can say more. For this, let $\{\psi_k\}$ be a basis in which D^p can be expanded in the form

$$D^p = \textstyle\sum_k d_{kl}\psi_k(x)\, \psi_l^*(x') . \tag{24}$$

Such bases always exist. In particular, one can choose $\{\psi_k\}$ to be the eigenfunctions of D^p; then $\psi_k = \phi_k^p$ and $d_{kl} = \lambda_k^p \delta_{kl}$.

Theorem 5.1. Let $N = \nu p + q$. A p matrix D^p is (boson or fermion) pure N representable if and only if $\{\psi_k\}$ is (boson or fermion) N complete and one of the ϵ^p eigenvectors (ϵ^r if $\nu = 1$) $\underline{\mathrm{W}}$ of $\underline{\Omega}^\nu$ satisfies

$$\underline{\mathrm{W}}\,\underline{\mathrm{W}}^\dagger = D, \tag{25}$$

where $\{\psi_k\}$ and $\underline{\mathrm{D}} = (d_{kl})$ are as in (24).

Theorem 5.2. Let $N = \nu p + q$. A p matrix D^p is (boson or fermion) ensemble N representable if and only if $\{\psi_k\}$ is N complete and there exist positive numbers α_n and normalized ϵ^p (ϵ^r if $\nu = 1$) eigenvectors $\underline{W}^n$ of $\underline{\Omega}^\nu$ such that

$$\underline{\mathrm{D}} = \textstyle\sum_n \alpha_n \underline{\mathrm{W}}^n \underline{\mathrm{W}}^{n\dagger}, \tag{26}$$

where $\{\psi_k\}$ and $\underline{\mathrm{D}} = (d_{kl})$ are as in (24).

These theorems represent a considerable improvement over the results of Ref. 1, where it was actually necessary to generate the preimage in order to check for N representability. However, Eq. (17) still gives a means of generating the preimage, so that testing for N representability is still implicitly equivalent to generating the preimage.

It is not clear whether theorems 5.1 and 5.2 actually represent a solution or merely a restatement of the N-representability problem. In fact, both extremes can occur. The extent to which these results actually simplify the N-representability problem depends on M_ν, the ϵ^p degeneracy of $\underline{\Omega}^\nu$. The smaller M_ν, the greater the simplification. This aspect of the problem, together with some examples, is discussed in more detail in Ref. 1.

Recently, Kiang[9] has suggested that the N-representability problem is contentless, i.e., every p matrix is N representable. This is clearly false as examples[30–33] of p matrices which are not N representable exist in the literature. The errors in Kiang's paper arise, in part, from a failure to consider the N-completeness aspect of the N-representability problem.

Before discussing Kiang's work, we point out that the N-completeness problem itself is not contentless. The results of Sec. IV provide an easy method of generating sets of functions which are not N complete. However, large rank is not sufficient in itself. One can construct examples of non-N-complete sets of functions of arbitrarily large or small rank.

Kiang's theorem[9] is stated in somewhat nonstandard terminology. It can be restated as follows: (i) Every p matrix has a preimage, which does not necessarily correspond to any special permutational symmetry. (ii) Every p matrix has a preimage of prescribed permutational symmetry.

Part (i) is a well-known result of Von Neumann[34] and will not be considered further here. To prove (ii), Kiang expands D^p in the form (24) and then assumes that symmetric N-particle functions of the form (8) always exist, i.e., that $\{\psi_k\}$ is N complete. Since we have already shown that this assumption is false, this explains the contradiction between Kiang's theorem and the known fact that p matrices do exist which are not N representable.

Even in an N-complete basis set, however, Kiang's argument still fails. First, N-completeness conditions may reduce the number of independent parameters; this corresponds to small ϵ^p degeneracy of $\underline{\Omega}^\nu$. Second, the existence of solutions of nonlinear equations does not simply depend on the number of parameters alone; indeed, his argument gives erroneous results even when $p = 1$ and N completeness is trivial.

VI. CONCLUSION

We have presented a number of important new results. In particular, theorem 3.2 contains the complete solution to the N-completeness problem.

Theorem 5.2 will greatly add to our understanding of the complicated N-representability problem. In view of Eqs. (17) and (18) we have an algorithm for constructing all possible preimages of any p matrix. This will discourage those who hoped that they could greatly simplify N-particle calculations by using 2 matrices. But the results will be very useful for further study of N-representability and related problems, e.g., when does a p matrix have a unique preimage.

Theorem 4.1 has a number of interesting consequences. It has long been assumed (but never proved!) that the eigenfunctions of Hamiltonians containing $1/r_{12}$ interactions will have infinite 1 rank. We now know that, if this is true and $N \neq 2$, these eigenfunctions will also have infinite 2 rank. Many people have tried to approximate N-particle eigenfunctions by antisymmetrizing a simple (i.e., one term with no permutational symmetry) product of geminals. We now know that the resultant antisymmetric function will have infinite 2 rank if any of the geminals have infinite 1 rank.

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[15]See Ref. 1, theorems 3–6.

[16]See Ref. 1, theorem 1 and discussion.

[17]The terms "pth-order reduced-density matrix" and "p matrix" have been used interchangeably in the literature. We feel that the distinction adopted here should help to avoid confusion.

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[24]See Ref. 1, Eqs. (20)–(23). In this case $\sigma_{ki,ij} = \delta_{ki} u_{ij}$.

[25]The system of numbering $\underline{\Omega}^{\alpha}$ is exactly the reverse of that used in Ref. 1.

[26]Since $\underline{T}$ is a double-index matrix, the eigenvectors can be written as single-index matrices.

[27]When no confusion can result, we drop α for simplicity.

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