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# The *p*-body rank of an *n*-electron state

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Received 3 November 1988

Abstract. Extreme subsets of the set  $\mathscr{P}_n^p$  of all *p*-body matrices are discussed. The concept of *p*-body rank of an *n*-electron wavefunction is defined and its physical meaning is investigated.

### 1. Introduction

The purpose of this paper is to investigate the intrinsic correlation structure of antisymmetric wavefunctions. The correlation implied by a wavefunction is revealed by the suitability of that wavefunction as a ground state of certain kinds of operators. The ground state of a non-interacting *n*-electron system can simply be determined by the fermion statistics, and it is found that these ground states can be described by determinantal wavefunctions which are regarded as having no dynamical correlation. When interaction is introduced into the *n*-electron system the motion of the electrons becomes very complicated. Even when the interaction changes smoothly, the ground state of the system may change abruptly, as occurs in the cases treated by the method of quasi-averages [1]. The solutions of some model Hamiltonians can be helpful for understanding the correlation of electrons. The recently constructed *n*-electron states with symplectic symmetry [2], which are antisymmetrised products of a geminal power with some mutually orthogonal geminals besides some spin orbitals and which can serve as the ground states of some model Hamiltonians with symplectic or quasispin symmetry, can be regarded as describing the correlation associated with such a special kind of interactions.

In density functional theory the ground state is uniquely related to the ground-state density [3]. But this theory requires a *local* 1-body potential. If the potential is non-local, the one-to-one relation between ground-state wavefunctions and densities breaks down. Instead of density, the 1-matrix (the first-order reduced density matrix) must be used [4]. Furthermore, if one relaxes the restriction to a 2-body Coulomb interaction and uses a non-local 2-body potential, then it is obvious that the one-to-one relation will be between the ground-state wavefunctions and 2-matrices (the secondorder reduced density matrices). A non-local 1- or 2-body interaction occurs more often than one might think. It makes its appearance in two cases at least: when the interaction is mediated by other kinds of particles or when it is approximated in a finite-dimensional Hilbert space. The latter includes almost every numerical calculation. An operator A, approximated by a finite-dimensional matrix  $(a_{ij})$ , can also be represented by an integral operator with kernel  $A(x, x') = \sum a_{ij}\varphi_i(x)\varphi_j^*(x')$ , while the *i*th vector is represented by the function  $\varphi_i(x)$  in the position representation of that finite-dimensional Hilbert space. So A(x, x') can never have, as a factor, the  $\delta$  function  $\delta(x-x')$  to make the integration a multiplication<sup>†</sup>. The non-degenerate ground state is uniquely related to either the density, the 1-matrix or the 2-matrix, depending on the nature of the potential and the interaction between the electrons. If we include density into the hierarchy of reduced density matrices, we can still say roughly that if the electrons interact with each other through a *p*-body potential, then the *p*-matrix (the *p*th-order reduced density matrix) contains all the information needed to describe the correlation of the electrons.

The purpose of this paper is to deduce a physical concept from the general theory of reduced density matrices [5-7], i.e. the *p*-body rank of an *n*-electron state. The significance of this new term is that if a particular *n*-electron wavefunction becomes the ground state of a *p*-body operator, then the ground state must possess degenerancy not less than the *p*-body rank of that wavefunction.

In §§ 2 and 3 we shall introduce the structure of the extreme subsets of  $\mathcal{P}^n$  and  $\mathcal{P}^p_n$ , respectively, generalising some results of [6, 7], then we shall give the definition of the *p*-body rank of an *n*-electron state in § 4. By the term '*p*-body' we always mean something associated with every set of *p* electrons contained in an *n*-electron system, and the word 'body' may be omitted as in the example '*p*-matrix'.

# 2. The geometrical structure of $\mathcal{P}^n$

The geometrical structure of the set  $\mathcal{P}^n$  consisting of all the *n*-electron density matrices is obvious and was discussed in [8]. In this section we shall give a detailed description of its extreme subsets.

To avoid most mathematical troubles, we suppose the dimension r of the oneparticle state space  $\mathcal{V}$  to be finite. The *n*-electron state space will be denoted by  $\mathscr{V}^{n\Lambda}$ . It is the *n*-fold antisymmetrised product space of  $\mathcal{V}$  with dimension  $M = \binom{r}{n}$ .

All the Hermitian operators defined on  $\mathcal{V}^{n\Lambda}$  consitute a real Euclidean space  $\mathcal{H}^n$  with dimension  $M^2$ , in which all the operators with trace equal to 1 constitute a hyperplane. Denoting the identity operator on  $\mathcal{H}^n$  as  $I^n$ , and taking  $X = (1/M)I^n$  as origin, we then get a real Euclidean space  $\overline{\mathcal{H}}^n$  with dimension  $M^2 - 1$  from that hyperplane [8].  $\mathcal{P}^n$  is a convex set in  $\overline{\mathcal{H}}^n$  with interior points which are the density matrices without zero eigenvalues. The boundary of  $\mathcal{P}^n$  consists of the density matrices which do possess some zero eigenvalues.

Now, let V be a non-empty subspace of  $\mathcal{V}^{n\Lambda}$ , and denote all the desnity matrices with range in V by  $\mathcal{P}^{n}(V)$ , which has the following properties.

(i)  $\mathcal{P}^n(V)$  is a convex subset in  $\mathcal{P}^n$ . A density matrix  $D \in \mathcal{P}^n(V)$  without zero eigenvalue on V is a relative interior point of  $\mathcal{P}^n(V)$ ; otherwise it is a relative boundary point.

(ii) If a mixture  $D = \lambda D_1 + (1 - \lambda) D_2$ ,  $(0 < \lambda < 1, D_1, D_2 \in \mathcal{P}^n)$ , belongs to  $\mathcal{P}^n(V)$ , then  $D_1$  and  $D_2$  also belong to  $\mathcal{P}^n(V)$ .

(iii) If D is a relative interior point of  $\mathcal{P}^n(V)$  then, for every point  $D_1$  in  $\mathcal{P}^n(V)$ , except D itself, there is a line segment in  $\mathcal{P}^n(V)$  with D as an interior point and  $D_1$  an end point.

<sup>&</sup>lt;sup>†</sup> It is wrong to call such a finite-dimensional matrix a local operator and it is doubtful that it is worthwhile discussing the problem of whether a matrix is deduced from a local or non-local operator, since in this case the density is not enough to determine the ground state.

(i) This statement is obvious.

(ii) Let  $V_1$ ,  $V_2$  and V be the ranges of  $D_1$ ,  $D_2$  and D, respectively. Since  $\lambda$  is a positive number and  $D_1$  and  $D_2$  are both positive operators, it is obvious that both  $V_1$  and  $V_2$  are contained in V, so property (ii) results.

(iii) Since D is a relative interior point of  $\mathcal{P}^n(V)$ , a positive number  $\varepsilon$  can always be found such that  $\varepsilon$  is less than the minimal eigenvalue of D. Let x be the maximal eigenvalue of  $D_1$ , of course we can choose  $\varepsilon < x$ . Then  $D_2 = aD_1 + (1-a)D$ , with  $a = -[\varepsilon/(x-\varepsilon)] < 0$ , belongs to  $\mathcal{P}^n(V)$ , and the line segment  $D(\lambda) = \lambda D_1 + (1-\lambda)D_2$ ,  $0 < \lambda < 1$ , also belongs to  $\mathcal{P}^n(V)$ . D is an interior point of this line segment with  $\lambda = -[a/(1-a)] = \varepsilon/x$ , i.e.  $D = D(\varepsilon/x)$ , which implies property (iii).

An extreme subset E of a set K is defined [9] as a subset of K, such that if x and y are two points of K and the interior of the line segment xy has a common point with E, then both x and y belong to E. An extreme subset of a convex set is also convex, and if it contains an inner point of a line segment in that convex set, it will contain the whole line segment.

The subset  $\mathcal{P}^n(V)$  and the extrme subsets of  $\mathcal{P}^n$  are connected through the following theorem.

Theorem 1. E is an extreme subset of  $\mathcal{P}^n$  if and only if there is a subspace  $V \subset \mathcal{V}^{n\Lambda}$  such that  $E = \mathcal{P}^n(V)$ .

**Proof.** From the definition of extreme subset and the property (ii) of the subset  $\mathcal{P}^n(V)$ , it is obvious that  $\mathcal{P}^n(V)$  is an extreme subset of  $\mathcal{P}^n$ . To prove that if E is an extreme subset of  $\mathcal{P}^n$ , then there is a subspace  $V \subset \mathcal{V}^{n\Lambda}$  such that  $E = \mathcal{P}^n(V)$ , we need the following lemma.

Lemma 1. If E is a convex subset in  $\mathcal{P}^n$ , then there is a subspace  $V \subset \mathcal{V}^{n\Lambda}$  such that  $E \subset \mathcal{P}^n(V)$  and E has at least one common point with the relative interior of  $\mathcal{P}^n(V)$ .

Proof. The proof of this lemma is simple and can be stated as follows.

The range of a mixture must be the union of the ranges of each density matrix taking part in the convex combination to form the mixture. So by considering convex combinations of the elements of E, we can find at least one element with the largest range V, i.e. the ranges of all other elements of E are contained in V. Thus,  $E \subset \mathcal{P}^n(V)$  and the elements with the largest range V are the points common to E and the relative interior of  $\mathcal{P}^n(V)$ .

From lemma 1, we know that if E is an extreme subset of  $\mathcal{P}^n$ , then there is a subspace  $V \subset \mathcal{V}^{n\Lambda}$  such that  $E \subset \mathcal{P}^n(V)$  and E and  $\mathcal{P}^n(V)$  have at least one point in common. According to the property (iii) of  $\mathcal{P}^n(V)$  and the fact that E is an extreme subset of  $\mathcal{P}^n$ , we know that any point in  $\mathcal{P}^n(V)$  is contained in E, therefore  $E = \mathcal{P}^n(V)$ . Thus the theorem 1 is established.

Now we give the extreme subsets, and the boundary of  $\mathscr{P}^n$ , a matrix representation. Let  $\lambda_i$ , i = 1, 2, ..., m, be *m* positive numbers, with  $\sum_{i=1}^m \lambda_i = 1$ . Then  $UAU^{-1}$  is an element of  $\mathscr{P}^n(V)$ , where *A* is a density matrix with range in *V* and *U* is a unitary matrix on *V*. When *U* is a unitary matrix on  $\mathscr{V}^{n\Lambda}$ , then  $UAU^{-1}$  may be an element of another extreme subset. The form  $UAU^{-1}$  with m = 1, 2, ..., M - 1, can represent all the boundary elements of  $\mathscr{P}^n$ . Let  $\mathscr{H}^n(V)$  denote the set of all the Hermitian operators with range in  $V \subset \mathscr{V}^{n\Lambda}$ ;  $\mathscr{H}^n(V)$  is a hyperplane and  $\mathscr{P}^n(V)$  is the intersection of  $\mathscr{P}^n$  with  $\mathscr{H}^n(V)$ .

## 3. The extreme subsets of $\mathcal{P}_n^p$

The set  $\mathscr{P}_n^p$ , consisting of all the *n*-representable *p*-matrices, is the image of the set  $\mathscr{P}^n$ under the mapping of the (n, p) contraction operator  $L_n^p$ , i.e.  $\mathscr{P}_n^p = L_n^p(\mathscr{P}^n)$  [6].  $L_n^p$  is a linear operator; it maps a convex set into a convex set, and the full pre-image of a convex set is also convex. The image of an extreme subset is not necessarily an extreme subset, but the full pre-image of an extreme subset will be extreme. As to this point, let us prove a second theorem.

Theorem 2. S is an extreme subset of  $\mathcal{P}_n^p$  if and only if the full pre-image of S in  $\mathcal{P}^n$  under the mapping of  $L_n^p$  is an extreme subset of  $\mathcal{P}^n$ .

*Proof.* Let E be the full pre-image in  $\mathcal{P}^n$  of an extreme subset S of  $\mathcal{P}^p_n$ ; then  $S = L^p_n(E)$ . According to theorem 1, we need to prove that there is a subspace  $V \subset \mathcal{V}^{n\Lambda}$  such that  $E = \mathcal{P}^n(V)$ .

Since S is convex, E is also convex. According to lemma 1, there is a subspace  $V \subset \mathcal{V}^{n\Lambda}$  such that  $E \subset \mathcal{P}^n(V)$  and E contains at least one relative interior point of  $\mathcal{P}^n(V)$ . From the property (iii) and the definition of extreme subset, E should contain all the elements of  $\mathcal{P}^n(V)$  if it contains one relative interior point of  $\mathcal{P}^n(V)$ . So  $E \supset \mathcal{P}^n(V)$  and furthermore  $E = \mathcal{P}^n(V)$ . That is, if S is extreme in  $\mathcal{P}^p_n$ , then its full pre-image E in  $\mathcal{P}^n$  is also extreme.

Now, suppose the full pre-image of S in  $\mathcal{P}^n$  is an extreme subset  $\mathcal{P}^n(V)$ ; we need to prove that S is an extreme subset of  $\mathcal{P}_n^p$ . To this end, let  $D_1^p$ ,  $D_2^p \in \mathcal{P}_n^p$ ,  $D^p = \lambda D_1^p + (1-\lambda)D_2^p$ ,  $0 < \lambda < 1$ , and  $D^p \in S$ . We need to prove  $D_1^p \in S$  and  $D_2^p \in S$ . Since  $L_n^p$  is linear, there must be pre-images  $D_1$ ,  $D_2$ , and D of  $D_1^p$ ,  $D_2^p$ , and  $D^p$ , respectively, such that  $D = \lambda D_1 + (1-\lambda)D_2$  and  $D \in \mathcal{P}^n(V)$ . Let the range of D be  $V' \subset V$  and the ranges of  $D_1$  and  $D_2$  be  $V_1$  and  $V_2$ , respectively; then the convex combination relation immediately leads to  $V \supset V' \supset V_1$  and  $V_2$ . Therefore  $D_1 \in \mathcal{P}^n(V)$  and  $D_2 \in \mathcal{P}^n(V)$ . The proof is finished.

An extreme subset containing only one point is an extreme point. As a corollary one immediately gets the theorem in [6, 7], which is as follows.

 $D^p$  is an extreme point of  $\mathscr{P}_n^p$  if and only if there is a subspace  $V \subset \mathscr{V}^{n\Lambda}$  such that the full pre-image of  $D^p$  in  $\mathscr{P}^n$  is just  $\mathscr{P}^n(V)$ .

As an example we discuss the extreme subsets of  $\mathcal{P}_n^1$ .

 $\mathscr{P}_n^1$  is the set of all 1-matrices. It is known [5] that the set of all the extreme points of  $\mathscr{P}_n^1$  consists of all the 1-matrices of determinantal wavefunctions. For any subspace  $\mathscr{V}_0 \subset \mathscr{V}$  with dimension *n*, there is only one determinantal wavefunction in  $\mathscr{V}_0^{n\Lambda}$  and there is only one 1-matrix with range in  $\mathscr{V}_0$ .

For any subspace  $\mathcal{V}_1$  with dimension more than n in  $\mathcal{V}$ , denote the set of all the 1-matrices with range in  $\mathcal{V}_1$  by  $\mathcal{P}_n^1(\mathcal{V}_1)$  and denote the set of all the density matrices with range in  $\mathcal{V}_1^{n\Lambda}$  by  $\mathcal{P}^n(\mathcal{V}_1^{n\Lambda})$ ; then it is obvious that the full pre-image of  $\mathcal{P}_n^1(\mathcal{V}_1)$  in  $\mathcal{P}^n$  is  $\mathcal{P}^n(\mathcal{V}_1^{n\Lambda})$ . Therefore,  $\mathcal{P}_n^1(\mathcal{V}_1)$  is an extreme subset of  $\mathcal{P}_n^1$ .

Suppose  $\mathcal{V}_0$  is a subspace of  $\mathcal{V}$  with dimension  $m \leq n$ , while  $\mathcal{V}_1$  is another subspace of  $\mathcal{V}$  with dimension greater than n - m, and there is no intersection between  $\mathcal{V}_0$  and  $\mathcal{V}_1$ . Denote by  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  the set of all the 1-matrices with range  $\mathcal{V}_0 \cup \mathcal{V}_1$  and such that  $\mathcal{V}_0$  is a subspace of the eigenspace belonging to the eigenvalue 1/n of each 1-matrix. Then one can easily know that the full pre-image of  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  in  $\mathcal{P}^n$  is  $\mathcal{P}^n(\mathcal{V}_0^{n\Lambda} \wedge \mathcal{V}_1^{(n-m)\Lambda})$ , i.e. the set of all the density matrices with range in the antisymmetric product space  $\mathcal{V}_0^{m\Lambda} \wedge \mathcal{V}_1^{(n-m)\Lambda}$  of  $\mathcal{V}_0^{m\Lambda}$  and  $\mathcal{V}_1^{(n-m)\Lambda}$ . So  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  is also an extreme subset of  $\mathcal{P}_n^1$ , and it is the general form of an extreme subset of  $\mathcal{P}_n^1$ . When m = n, all the 1-matrices in  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  should have their range in  $\mathcal{V}_0$ , since the trace of a 1-matrix must be equal to 1, so  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  reduces to  $\mathcal{P}_n^1(\mathcal{V}_0)$ , which contains only one element—the 1-matrix of the determinantal wavefunction in  $\mathcal{V}_0^{n\Lambda}$ . When m = 0,  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  reduces to  $\mathcal{P}_n^1(\mathcal{V}_1)$ , which has been discussed above.

It can be proved that any other convex subset S which cannot be expressed in the form  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  is not an extreme subset of  $\mathcal{P}_n^1$ . The proof is simple. Again using the fact that the range of the convex combination of several positive operators is just the union of the ranges of each individual operator taking part in that combination, we can find all the elements in S having the largest range. They must have a common range with the ranges of all other elements contained in it. Furthermore, since 1/n is the largest possible eigenvalue of any 1-matrix, the degenerancy of the eigenvalue 1/nfor a convex combination of several 1-matrices will be less than the degeneracies of the same eigenvalue for the 1-matrices taking part in that combination. Then we can find the elements with the lowest degeneracy of the eigenvalue 1/n among the elements with the largest range, again by making convex combinations. Suppose  $D_0^1$  is such an element, and  $\mathcal{V}_0 \cup \mathcal{V}_1$  is its range, where  $\mathcal{V}_0$  is its eigenspace belonging to the eigenvalue 1/n. S must be contained in  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$  and has a common point  $D_0^1$  with the interior of  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$ . On the other hand, S cannot contain all the elements of  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$ , otherwise S would be equal to  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$ . Since  $D_0^1$  is in the interior of  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$ , for any point  $D_1^1$  in  $\mathscr{P}_n^1(\mathscr{V}_0, \mathscr{V}_1)$  there must be a line segment completely contained in  $\mathcal{P}_{\mathbf{r}}^{1}(\mathcal{V}_{0},\mathcal{V}_{1})$  and with  $D_{\mathbf{i}}^{1}$  is an end point while  $D_{\mathbf{i}}^{0}$  is an interior point, according to lemma 1. If we choose such a  $D_1^1$  which is not in S, then we have found a line segment in  $\mathcal{P}_n^1$  such that S contains one of its inner points, but does not contain the whole line segment. So S cannot be an extreme subset of  $\mathcal{P}_n^1$ .

To conclude, the extreme subsets of  $\mathcal{P}_n^1$  are all of the form  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$ , which consists of the 1-matrices whose eigenspaces, corresponding to eigenvalue 1/n, contain  $\mathcal{V}_0$  and whose range is in  $\mathcal{V}_0 \cup \mathcal{V}_1$ .

#### 4. The *p*-body rank of an *n*-electron state

The extreme subsets of  $\mathcal{P}_n^p$  are connected with the extreme subsets of  $\mathcal{P}^n$  through theorem 2, and provide a tool for analysing the intrinsic correlation structure of the *n*-electron wavefunction and density matrix. This is what we shall do in this section. To begin with, we make two definitions.

**Definition 1.** If the full pre-image of an extreme subset E of  $\mathcal{P}_n^p$  in  $\mathcal{P}^n$  is  $\mathcal{P}^n(V)$ , then call  $\mathcal{P}^n(V)$  a *p*-extreme subset of  $\mathcal{P}^n$ , and V a *p*-subspace of  $\mathcal{V}^{n\Lambda}$ .

Theorem 2 gives a one-to-one relation between the extreme subsets of  $\mathcal{P}_n^p$  and the *p*-extreme subsets of  $\mathcal{P}^n$  or the *p*-subspaces of  $\mathcal{V}^{n\Lambda}$ . Of course, not all of the extreme subsets of  $\mathcal{P}^n$  are *p*-extreme subsets and not all of the subspaces of  $\mathcal{V}^{n\Lambda}$  are *p*-subspaces.

It is known that all extreme points are exposed [7]. This result can be simply generalised to give that all the extreme subsets of  $\mathcal{P}_n^p$  are exposed subsets in our finite-dimensional case. Therefore the *p*-subspaces here are the same as those in [6].

 $\mathcal{P}_n^p$  is an extreme subset of itself, therefore  $\mathcal{V}^{n\Lambda}$  and  $\mathcal{P}^n$  are a *p*-space and a *p*-extreme subset, respectively. From this view point, any wavefunction belongs to some *p*-subspace and any density matrix belongs to some *p*-extreme subset. We make the following further definition.

**Definition 2.** If a *p*-extreme subset  $\mathcal{P}^n(V)$  contains *D*, and there is no other *p*-extreme subset containing *D* contained in  $\mathcal{P}^n(V)$ , then  $\mathcal{P}^n(V)$  will be called the minimal *p*-extreme subset containing *D*, while the dimension of *V* will be called the *p*-body rank of *D*.

If the minimal *p*-extreme subset containing  $D(\psi)$  is  $\mathcal{P}^n(V)$ , then call V the minimal *p*-subspace containing  $\psi$  and the dimension of V the *p*-body rank of  $\psi$ .

The concept of the minimal *p*-extreme subset containing a density matrix and the minimal *p*-subspace containing a wavefunction connects the geometrical structure of  $\mathcal{P}_n^p$  with the intrinsic correlation structure of the wavefunction. The physical meaning of these new terms is given by the following theorem.

Theorem 3. If  $\psi$  is a ground state of a *p*-body operator *H*, and the *p*-body rank of  $\psi$  is *S*, then if the minimal *p*-subspace containing  $\psi$  is *V*, the degeneracy of the ground state of *H* is at least *S*, and the ground-state eigenspace contains *V*.

**Proof.** Suppose E is the minimal extreme subset containing  $D^p(\psi)$ . E is a convex set whose boundary consists of its extreme subsets, which are also extreme subsets of  $\mathscr{P}_n^p$ . So  $D^p(\psi)$  must be in the relative interior of E, otherwise it would be contained in another extreme subset of E, contrary to the minimal condition. For each point  $D_1^p$  in E, except  $D^p(\psi)$ , there must be a line segment with  $D_1^p$  as an end point and  $D^p(\psi)$  as an interior point, i.e.  $D^p(\psi) = \lambda D_1^p + (1-\lambda)D_2^p$  ( $0 < \lambda < 1$ ), where  $D_2^p$  is another point contained in E.

Now, since  $\psi$  is a ground state,  $\langle H \rangle_{(\psi)} = \text{Tr}(HD(\psi)) = \binom{n}{p}\text{Tr}(H^pD^p(\psi))$  is the minimum of the average values of H. Where  $\Gamma_p^n(H^p) = H$  and  $\Gamma_p^n$  is the expansion operator [6]. The fact that

$$\langle H \rangle_{(\psi)} = \binom{n}{p} \left[ \lambda \operatorname{Tr}(H^p D_1^p) + (1 - \lambda) \operatorname{Tr}(H^p D_2^p) \right]$$

tells us that

$$\langle H \rangle_{(\psi)} = {n \choose p} \operatorname{Tr}(H^p D_1^p) = {n \choose p} \operatorname{Tr}(H^p D_2^p)$$

otherwise  $\binom{n}{p}$  Tr $(H^p D_1^p)$  or  $\binom{n}{p}$  Tr $(H^p D_2^p)$  will be less than  $\langle H \rangle_{(\psi)}$ . When  $D_1^p$  runs over all the elements in E, except  $D^p(\psi)$ , its pre-images in  $\mathcal{P}^n(V)$  run over all the elements in  $\mathcal{P}^n(V)$ , except that of  $D^p(\psi)$ . So we conclude that, for any element D in  $\mathcal{P}^n(V)$ ,  $\langle H \rangle_{(\psi)} = \text{Tr}(HD)$ . The theorem follows.

*Example.* The 1-body rank of  $\psi = c_1 |123\rangle + c_2 |456\rangle$ , where  $|c_1|^2 + |c_2|^2 = 1$ . Here we have denoted the normalised determinantal wavefunction with one electron in each of the spin orbitals  $|i\rangle$ ,  $|j\rangle$  and  $|k\rangle$  by  $|ijk\rangle$ .

The 1-matrix of  $\psi$  is given by

$$D'(\psi) = |c_1|^2 D^1(123) + |c_2|^2 D^1(456)$$

with

$$D^{1}(123) = \frac{1}{3}(|1\rangle\langle 1| + |2\rangle\langle 2| + |3\rangle\langle 3|)$$
$$D^{1}(456) = \frac{1}{3}(|4\rangle\langle 4| + |5\rangle\langle 5| + |6\rangle\langle 6|).$$

Denote the one-particle space spanned by  $|1\rangle$ ,  $|2\rangle$ , ...,  $|6\rangle$  by  $\mathcal{V}_1$ , and let  $V = \mathcal{V}_1^{3\Lambda}$ ; the dimension of V is  $20 = \binom{6}{3}$ . The image of  $\mathcal{P}^3(V)$  is  $\mathcal{P}_3^1(\mathcal{V}_1)$  which consists of the 1-matrices with ranges in  $\mathcal{V}_1$ . The full pre-image of  $\mathcal{P}_3^1(\mathcal{V}_1)$  in  $\mathcal{P}^3$  is  $\mathcal{P}^3(V)$ , so  $\mathcal{P}_3^1(\mathcal{V}_1)$  is an extreme subset of  $\mathcal{P}_3^1$ .  $D^1(\psi)$  is a relative interior point of  $\mathcal{P}_3^1(\mathcal{V}_1)$ .  $\mathcal{P}_3^1(\mathcal{V}_1)$  is the minimal extreme subset containing  $D^1(\psi)$ . Therefore,  $\mathcal{P}^3(V)$  is the minimal 1-body extreme subset containing  $D^1(\psi)$ , and V is the minimal 1-subspace containing  $\psi$ . The one-body rank of  $\psi$  is 20. If a 1-body operator has  $\psi$  as its ground state, then the degeneracy of its ground state is at least 20. The simplest 1-body operator with  $\psi$  as its ground state may be

$$H=\sum_{i=7}^r a_i^+a_i.$$

It is obvious that the ground-state eigenvalue of H is zero, its ground-state eigenspace is V with degeneracy 20.

In general, if the eigenspace of  $D^1(\psi)$  belonging to eigenvalue 1/n is  $\mathcal{V}_0$ , while the range of  $D^1(\psi)$  is  $\mathcal{V}_0^{m_\Lambda} \cup \mathcal{V}_1^{(n-m)\Lambda}$ , then the minimal extreme subset containing  $D^1(\psi)$  is  $\mathcal{P}_n^1(\mathcal{V}_0, \mathcal{V}_1)$ . The 1-subspace containing  $\psi$  is  $\mathcal{V}_0^{m_\Lambda} \cup \mathcal{V}_1^{(n-m)\Lambda}$ , where *m* is the dimension of  $\mathcal{V}_0$ . Suppose the dimension of  $\mathcal{V}_1$  is *s*; the 1-body rank of  $\psi$  is  $\binom{s}{n-m}$ .

#### Acknowledgment

This work is supported by the National Natural Science Foundation of China.

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