

## Eigenvalues of Fermion Density Matrices\*

FUKASHI SASAKI†

Quantum Chemistry Group, Uppsala University, Uppsala, Sweden

(Received 30 December 1964)

The least upper bound of the eigenvalues of second-order reduced density matrices for a system of fermions is proved to be  $n$  for a system of  $2n$  or  $2n+1$  identical fermions. It is also shown that this limiting state may be interpreted as a system of identical pairs behaving as quasibosons.

### 1. INTRODUCTION

IT is known that certain features of a system are illuminated by the spectrum of its first-order density matrix. For example, an eigenvalue of this matrix may be interpreted as the occupation number of the corresponding spin orbital, and if all the eigenvalues are equal to 1, the state can be described by a single Slater determinant.<sup>1</sup> We might expect that the spectrum of a higher order reduced density matrix would also characterize the structure of the system. However, it seems that little has been done along this line.<sup>2</sup> In this paper, we discuss the range of the eigenvalues of a many-particle density matrix in order to approach this problem.

For this purpose, it is convenient to use a wave function expanded in terms of the eigenfunctions of density matrices.<sup>3</sup> The expansion is obtained by the use of the following theorems.<sup>3-5</sup>

*Theorem 1.* If  $A$  is a linear and completely continuous transformation<sup>4</sup> of one Hilbert space into another, and  $f$  is an element of the first Hilbert space,  $Af$  can be written in the form

$$Af = \sum_i \mu_i g_i (f_i, f).$$

Here  $\{f_i\}$  and  $\{g_i\}$  are orthonormal sets in the two Hilbert spaces involved, and  $\{\mu_i\}$  is a nonincreasing

\*The results of this paper were originally presented at the Hylleraas Symposium on Atomic and Molecular Quantum Mechanics at Sanibel Island, 1962, and were preliminarily reported in Technical Note No. 77 from the Uppsala Quantum Chemistry Group, 1962 (unpublished). The work has been sponsored in part by the King Gustaf VI Adolf's 70-Years Fund for Swedish Culture, Knut and Alice Wallenberg's Foundation, The Swedish Natural Science Research Council, and in part by the Aeronautical Research Laboratory, OAR, through the European Office, Aerospace Research, U. S. Air Force.

†This work was performed while the author was on leave from the Department of Physics, University of Tokyo, Tokyo, Japan.

<sup>1</sup> Per-Olov Löwdin, Phys. Rev. **97**, 1474 (1955).

<sup>2</sup> See, however, the preliminary report of A. J. Coleman, Can. Math. Bull. **4**, No. 2 (1961). Further progress has been reported by him at Sanibel Island, Winter Institute in Quantum Chemistry and Solid State Physics, January 1962 (unpublished).

<sup>3</sup> J. von Neumann, *Mathematische Grundlagen der Quantenmechanik* (Julius Springer, Verlag, Berlin, 1932) (English transl.: Princeton University Press, Princeton, New Jersey, 1955, Chap. VI); B. C. Carlson, and J. M. Keller, Phys. Rev. **121**, 659 (1961).

<sup>4</sup> See, e.g., F. Riesz and B. Sz-Nagy, *Functional Analysis* (Frederick Ungar Publishing Company, New York, 1955), p. 206.

<sup>5</sup> A. T. Amos and G. G. Hall, Proc. Roy. Soc. (London) **A263**, 483 (1961). Detailed proofs of these theorems have been given in F. Sasaki, Technical Report 77, Uppsala Quantum Chemistry Group, 1962 (unpublished).

sequence of positive numbers. The sequence can be finite or infinite, and in the latter case it tends to zero.

Corollary 1:

$$\sup | (Af, g) | / [ (f, f) (g, g) ]^{1/2} = \mu_1.$$

*Theorem 2.* If there exists a normal operator  $S$  such that  $AS = A$ , every  $f_i$  is an eigen-element of  $S$ , i.e.,  $Sf_i = f_i$ .

A normalized wave function  $\Psi(x_1, x_2, \dots, x_N)$  of  $N$  fermions may be regarded as a kernel of the operator  $A$ , which transforms absolute-square-integrable functions of  $M$  fermions into functions of  $N-M$  fermions:

$$\begin{aligned} g(x_1, \dots, x_{N-M}) \\ = \int \dots \int dx'_1 \dots dx'_M \\ \times \Psi(x_1, \dots, x_{N-M}, x'_1, \dots, x'_M) f(x'_1, \dots, x'_M), \end{aligned}$$

or, in a brief form

$$g(x) = \int \Psi(x, y) f(y) dy,$$

where  $x$  and  $y$  denote  $(x_1 \dots x_{N-M})$  and  $(x'_1 \dots x'_M)$ , respectively. Since the wave function  $\Psi(x, y)$  is normalized:

$$\iint |\Psi(x, y)|^2 dx dy = 1,$$

it corresponds necessarily to a completely continuous transformation. By the use of theorem 1, we obtain the following expansion of the wave function  $\Psi$ :

$$\Psi(x, y) = \sum_i \mu_i g_i(x) f_i(y), \quad (1.1)$$

where

$$\int g_i^*(x) g_j(x) dx = \delta_{ij},$$

$$\int f_i^*(y) f_j(y) dy = \delta_{ij},$$

and

$$\mu_i \geq \mu_j > 0 \quad \text{for } i < j.$$

Since the density matrix of order  $M$  of this pure state is defined by

$$\Gamma_M(y, y') = \binom{N}{M} \int \Psi(x, y) \Psi^*(x, y') dx,$$

we obtain immediately the diagonal expansion of the density matrix from (1.1) in the form

$$\Gamma_M(y, y') = \binom{N}{M} \sum_i \mu_i^2 f_i(y) f_i^*(y').$$

Similarly, the density matrix of order  $N - M$  is found to be

$$\Gamma_{N-M}(x, x') = \binom{N}{M} \sum_i \mu_i^2 g_i(x) g_i^*(x').$$

In order to evaluate the symmetry property of  $f_i$ , it is convenient to introduce the antisymmetry projection operator defined with respect to the coordinates  $y = (x_1' \cdots x_M')$ :

$$O_{AS, y} = \frac{1}{M!} \sum_P \epsilon_P P.$$

Here  $P$  is a permutation operator which permutes only the coordinates  $y$  and  $\epsilon_P$  is its parity. It is easy to see that  $O_{AS, y}$  is self-adjoint and that

$$\begin{aligned} & \int \Psi(x, y) O_{AS, y} f(y) dy \\ &= \int O_{AS, y} \Psi(x, y) f(y) dy = \int \Psi(x, y) f(y) dy. \end{aligned}$$

Thus by using theorem 2, it follows that  $O_{AS, y} f = f$ , i.e., that if the function  $\Psi$  is antisymmetric,  $f_i$  and  $g_i$  in the expansion (1.1) should also be antisymmetric.

2. THE LEAST UPPER BOUND

The largest eigenvalue of a density matrix of order  $M$  may be regarded as a functional of  $\Psi$ :

$$\lambda_{M, N}(\Psi) = \binom{N}{M} \mu_1^2.$$

Introducing a projection operator  $O_\Psi$  which projects out the state  $\Psi$ :

$$O_\Psi = \Psi(\Psi),$$

we obtain the following equality from (1.1);

$$\lambda_{M, N}(\Psi) = \binom{N}{M} (g_1 f_1 O_\Psi g_1 f_1).$$

Introducing the total antisymmetry projection operator

$$O_{AS} = \frac{1}{N!} \sum_P \epsilon_P P,$$

it is found for any function  $\omega = \omega(x, y)$  that

$$\begin{aligned} (\omega(O_{AS} - O_\Psi)\omega) &= (\omega(1 - O_\Psi)O_{AS}(1 - O_\Psi)\omega) \\ &= ((1 - O_\Psi)\omega O_{AS}(1 - O_\Psi)\omega) \geq 0. \end{aligned}$$

Thus we obtain the following inequality

$$\begin{aligned} \lambda_{M, N}(\Psi) &\leq \binom{N}{M} (g_1 f_1 O_{AS} g_1 f_1) \\ &\leq \binom{N}{M} \sup_{f, g} (g f O_{AS} g f), \end{aligned} \tag{2.1}$$

where  $f$  and  $g$  are normalized functions of  $M$  and  $N - M$  particles, respectively. Since the last term of (2.1) does not depend on  $\Psi$ , it follows that

$$\lambda_{M, N} \equiv \sup_\Psi \lambda_{M, N}(\Psi) \leq \binom{N}{M} \sup_{f, g} (g f O_{AS} g f). \tag{2.2}$$

We shall now prove that the last term of (2.2) is equal to  $\lambda_{M, N}$ . Let  $\{f^{(k)}\}$  and  $\{g^{(k)}\}$  be the sets of normalized functions which give a solution of the above extremum problem:

$$0 < \lambda^{(k)} = \binom{N}{M} (g^{(k)} f^{(k)} O_{AS} g^{(k)} f^{(k)}) \rightarrow \binom{N}{M} \sup (g f O_{AS} g f)$$

as  $k \rightarrow \infty$ .

Since a set of functions  $\{\Psi^{(k)}\}$  defined by the equation

$$\Psi^{(k)} = \left( \binom{N}{M} / \lambda^{(k)} \right)^{1/2} O_{AS} g^{(k)} f^{(k)}$$

consists of normalized antisymmetric functions, it follows from corollary 1 that

$$\lambda_{M, N}(\Psi^{(k)}) \geq \binom{N}{M} |(g^{(k)} f^{(k)}, \Psi^{(k)})|^2 = \lambda^{(k)},$$

i.e., that

$$\lim_{k \rightarrow \infty} \lambda_{M, N}(\Psi^{(k)}) \geq \lim_{k \rightarrow \infty} \lambda^{(k)}. \tag{2.3}$$

By comparing (2.3) with (2.2), it is found that

$$\lambda_{M, N} = \binom{N}{M} \sup_{f, g} (g f O_{AS} g f). \tag{2.4}$$

<sup>6</sup> We note that for a system of identical bosons, the whole argument is valid after replacing the antisymmetry projection operators by the symmetry projection operators. Thus the least upper bound of the eigenvalues for bosons is given by the equation

$$\lambda_{M, N} = \binom{N}{M} \sup_{f, g} (g f O_S g f) \tag{2.5}$$

under the condition  $(f, f) = (g, g) = 1$ . Here the total symmetry projection operator  $O_S$  is given by the equation

$$O_S = (1/N!) \sum_P P.$$

It is readily seen from (2.5) that

$$\lambda_{M, N} = \binom{N}{M} \text{ (for a system of bosons).}$$

3. UPPER BOUNDS

It is convenient to write the antisymmetry projection operator in the form

$$\begin{aligned} & \binom{N}{M} O_{AS}(1, \dots, N) \\ &= O_{AS}(1, \dots, M) O_{AS}(M+1, \dots, N) \\ & \times \sum_{i=0}^{\min\{N-M, M\}} (-)^i \binom{N-M}{i} \binom{M}{i} \\ & \times P\{(1, M+1)(2, M+2) \dots (i, M+i)\} \\ & \times O_{AS}(1, \dots, M) O_{AS}(M+1, \dots, N), \end{aligned} \quad (3.1)$$

where  $O_{AS}(\dots)$  denotes the antisymmetry projection operator defined with respect to the coordinates in the parenthesis, and  $P\{(1, M+1)(2, M+2) \dots (i, M+i)\}$  denotes the operation of replacing the coordinate 1 by  $M+1$ ,  $M+1$  by 1,  $\dots$ ,  $i$  by  $M+i$  and  $M+i$  by  $i$ . This shows that the  $f$  and  $g$  that give the extremum in Eq. (2.4) should be antisymmetric. Therefore we may introduce the density matrices of the  $i$ th order  $\Gamma_{i,f}$  and  $\Gamma_{i,g}$  reduced from  $f$  and  $g$ . By the use of these density matrices, we obtain

$$\lambda_{M,N} = 1 + \sup \sum_{i=1}^{\min\{M, N-M\}} (-)^i \text{tr} \Gamma_{i,f} \Gamma_{i,g}. \quad (3.2)$$

Since density matrices are positive definite, it is easy to see that

$$\begin{aligned} 0 &\leq \text{tr} \Gamma_{i,f} \Gamma_{i,g} \leq \min(\text{tr} \Gamma_{i,f} \lambda_{i, N-M}; \text{tr} \Gamma_{i,g} \lambda_{i, M}) \\ &= \min \left[ \binom{M}{i} \lambda_{i, N-M}; \binom{N-M}{i} \lambda_{i, M} \right]. \end{aligned} \quad (3.3)$$

From (3.2) and (3.3) we obtain an upper bound of the eigenvalues by the recurrence equation<sup>7</sup>

$$\begin{aligned} \lambda_{M,N} \leq \Lambda_{M,N} = 1 + \sum_{i=1}^{\min\{\lfloor \frac{1}{2}M \rfloor, \lfloor \frac{1}{2}(N-M) \rfloor\}} \min \left[ \binom{M}{2i} \Lambda_{2i, N-M}; \right. \\ \left. \binom{N-M}{2i} \Lambda_{2i, M} \right]. \end{aligned} \quad (3.4)$$

The solutions of (3.4) are

$$\begin{aligned} \Lambda_{0,N} &= 1, \\ \Lambda_{1,N} &= 1, \\ \Lambda_{2,N} &= \lceil \frac{1}{2}N \rceil, \quad N \geq 4 \\ \Lambda_{3,N} &= 1 + 3 \lceil \frac{1}{2}(N-3) \rceil, \quad N \geq 6 \\ \Lambda_{4,N} &= 1 + (\lceil \frac{1}{4}N \rceil - 1)(1 + 6 \lceil \frac{1}{2}N \rceil - 6 \lceil \frac{1}{4}N \rceil) \\ & \quad + (N - 4 \lceil \frac{1}{4}N \rceil)(N - 4 \lceil \frac{1}{4}N \rceil - 1), \quad N \geq 8 \\ \Lambda_{5,N} &= 1 + 10 \lceil \frac{1}{2}(N-5) \rceil + 5 \Lambda_{4, N-5}, \quad N \geq 10 \\ & \vdots \end{aligned}$$

<sup>7</sup>  $\lceil x \rceil$  stands for the integral part of  $x$ .

It should be noticed that

$$\Lambda_{M,N} = O(N^{\lfloor M/2 \rfloor}).$$

This is the same order of magnitude as the largest eigenvalue of  $\Gamma_{\lfloor M/2 \rfloor}$  for a system of  $\lfloor N/2 \rfloor$  bosons.<sup>8</sup>

Since the eigenvalues of the first-order density matrix of a single-determinant wave function are 1, it follows that  $\Lambda_{1,N}$  is equal to  $\lambda_{1,N}$ . It is shown in Sec. 5 that  $\Lambda_{2,N}$  is also equal to  $\lambda_{2,N}$ .

4. EXTREME PROPERTIES OF WAVE FUNCTIONS

In this section we study the case where the largest eigenvalue of the  $M$ th-order density matrix is almost equal to the least upper bound  $\lambda_{M,N}$ . Suppose we have a wave function  $\Psi$  such that

$$(f \Gamma_{M, \Psi} f) = \lambda_{M,N} - \epsilon,$$

where  $\epsilon$  is a small non-negative number and  $f$  is a normalized function of  $M$  particles. It should be noted that  $f$  may or may not be an eigenfunction of  $\Gamma_{M, \Psi}$ . Define a function  $\Phi$  by the equation

$$\Phi(1, \dots, N) = \left[ \binom{N}{M} / \lambda_{M,N} \right]^{1/2}$$

$$\times O_{AS} f(1, \dots, M) g(M+1, \dots, N),$$

where

$$g(M+1, \dots, N)$$

$$= \left[ \binom{N}{M} / (\lambda_{M,N} - \epsilon) \right]^{1/2}$$

$$\times \int \dots \int \Psi(1, \dots, N) f^*(1, \dots, M) dx_1 \dots dx_M.$$

It is easy to see that

$$(g, g) = (\lambda_{M,N} - \epsilon)^{-1} (f \Gamma_{M, \Psi} f) = 1,$$

$$(\Psi, \Phi) = \left[ \binom{N}{M} / \lambda_{M,N} \right]^{1/2} (\Psi O_{AS} f g)$$

$$= \left[ \binom{N}{M} / \lambda_{M,N} \right]^{1/2} (\Psi, f g)$$

$$= (1 - \epsilon / \lambda_{M,N})^{1/2},$$

<sup>8</sup> This was conjectured by C. N. Yang, Rev. Mod. Phys. 34, 694 (1962). (See also footnote 9.)

and

$$(\Phi, \Phi) = \binom{N}{M} (fg O_{AS} fg) / \lambda_{M,N} \leq 1.$$

Then it follows that

$$\begin{aligned} 0 \leq (\Psi - \Phi, \Psi - \Phi) &= (\Psi, \Psi) + (\Phi, \Phi) - (\Psi, \Phi) - (\Phi, \Psi) \\ &\leq 2 - 2(1 - \epsilon / \lambda_{M,N})^{1/2} \leq 2\epsilon / \lambda_{M,N}. \end{aligned} \quad (4.1)$$

From the first three terms of (4.1), we obtain

$$(\Phi, \Phi) \geq 2(1 - \epsilon / \lambda_{M,N})^{1/2} - 1 \geq 1 - 2\epsilon / \lambda_{M,N}.$$

Summarizing the results obtained above, we have a theorem.

*Theorem 3.* If a normalized  $M$ -particle function  $f$  satisfies the following equation

$$(f \Gamma_{M, \Psi} f) = \lambda_{M,N} - \epsilon,$$

the wave function  $\Psi$  can be expressed as

$$\begin{aligned} \Psi = & \left[ \binom{N}{M} / \lambda_{M,N} \right]^{1/2} \\ & \times O_{AS} f(1, \dots, M) g(M+1, \dots, N) + h(1, \dots, N), \end{aligned}$$

where  $(g, g) = 1$ ,  $(h, h) \leq 2\epsilon / \lambda_{M,N}$ , and  $1 \geq (\Psi - h, \Psi - h) \geq 1 - 2\epsilon / \lambda_{M,N}$ .

We apply the above theorem to the first-order density matrix. We know that some of the eigenvalues of the first-order density matrix can be  $\lambda_{1,N} (= 1)$ ,

$$\Gamma_{1, \Psi}(1, 1') = \sum_{i=1}^p f_i(1) f_i^*(1') + \sum_{i=p+1}^N \lambda_i f_i(1) f_i^*(1'). \quad (4.2)$$

In such a case, it follows from theorem 3 that the wave function  $\Psi$  can be expressed as

$$\Psi = N^{1/2} O_{AS} f_1(1) g_1(2, \dots, N). \quad (4.3)$$

Using (3.1), we obtain

$$\begin{aligned} 1 = (\Psi, \Psi) &= N (f_1 g_1 O_{AS} f_1 g_1) = 1 - \int \dots \int dx_2 \dots dx_{N-1} \\ & \times \left| \int f_1^*(1) g_1(1, 2, \dots, N-1) dx_1 \right|^2, \end{aligned}$$

i.e.,

$$\int dx_1 f_1^*(1) g_1(1, 2, \dots, N-1) \equiv 0. \quad (4.4)$$

The first-order density matrix of  $g$  is found from (4.3) and (4.4) to be

$$\Gamma_{1, \theta_1} = \Gamma_{1, \Psi} - \Gamma_{1, f_1}. \quad (4.5)$$

Comparing (4.2) with (4.5), we see that the largest eigenvalue of  $\Gamma_{1, \theta_1}$  is also 1 if  $p > 1$ . Thus, by repeated

application of the previous discussion, it is found that

$$\begin{aligned} \Psi = & \left[ \frac{N!}{(N-p)!} \right]^{1/2} \\ & \times O_{AS} f_1(1) \dots f_p(p) g(p+1, \dots, N), \end{aligned} \quad (4.6)$$

$$\Gamma_{1, \Psi} = \sum_{i=1}^p f_i (f_i + \Gamma_{1, \theta_i}) \quad (4.7)$$

and

$$\int dx_1 f_i^*(1) g(1, 2, \dots, N-p) \equiv 0 \quad (i=1, \dots, p). \quad (4.8)$$

### 5. THE LEAST UPPER BOUND OF THE EIGENVALUES OF THE SECOND-ORDER DENSITY MATRICES

In this section, we prove that the upper bound  $\Lambda_{2,N}$  derived in Sec. 3 is actually the smallest.

Define functions  $F_{2n}(1 \dots 2n)$  and  $F_{2n+1}(1 \dots 2n+1)$  by the equations

$$\begin{aligned} F_{2n}(1, \dots, 2n) &= O_{AS} f(1, 2) f(3, 4) \dots f(2n-1, 2n), \\ F_{2n+1}(1, \dots, 2n+1) &= O_{AS} f(1, 2) f(3, 4) \dots \\ & \times f(2n-1, 2n) g(2n+1), \end{aligned} \quad (5.1)$$

where  $f(1, 2)$  is a normalized antisymmetric function of two particles and  $g(1)$  is an arbitrary normalized function of a particle.

Then it is found that

$$(F_{2n}, F_{2n}) = 2^n n! / (2n)! + O(\epsilon^2), \quad (5.2)$$

$$(F_{2n+1}, F_{2n+1}) = 2^n n! / (2n+1)! + O(\epsilon), \quad (5.2')$$

where

$$\begin{aligned} \epsilon^2 = \text{tr}(\Gamma_{1, f})^2 &= \int \int \int \int f(1, 2) f(3, 4) f^*(1, 3) \\ & \times f^*(2, 4) dx_1 dx_2 dx_3 dx_4. \end{aligned} \quad (5.3)$$

Proof:

$$\begin{aligned} (F_{2n}, F_{2n}) &= (O_{AS} f \dots f, O_{AS} f \dots f) \\ &= (f \dots f, O_{AS} f \dots f) \\ &= (1 / (2n)!) \sum_P \epsilon_P (f \dots f, P f \dots f) \\ &= (1 / (2n)!) \sum_P a_P, \end{aligned}$$

where  $a_P = \epsilon_P (f \dots f, P f \dots f)$ . In order to evaluate the above sum, we consider a subgroup  $H$  of the symmetric group  $S_{2n}$ . The subgroup  $H$  is generated from  $n$  transpositions,  $(12), (34), \dots, (2n-1, 2n)$ , and two other permutations,  $(13)(24)$  and  $(135 \dots 2n-1)(246 \dots 2n)$ . There are  $2^n n!$  permutations in  $H$ . It is easy to see that  $a_P = 1$  for such a permutation since  $\epsilon_P P f \dots f = f \dots f$ , but otherwise  $a_P$  is of the order of  $\text{tr}[(\Gamma_{1, f})^2]$ .

For odd  $N$ , (5.2') can be similarly proven. In this case some of the permutations will give integrals of the order  $\text{tr}(\Gamma_{1, f} \Gamma_{1, \theta})$ , but

$$\begin{aligned} 0 \leq \text{tr} \Gamma_{1, f} \Gamma_{1, \theta} &\leq [\text{tr}(\Gamma_{1, f})^2 \text{tr}(\Gamma_{1, \theta})^2]^{1/2} \\ &= [\text{tr}(\Gamma_{1, f})^2]^{1/2} = \epsilon. \quad \text{Q.E.D.} \end{aligned}$$

Let

$$\Psi^N(1, \dots, N) = F_N(1, \dots, N) / [F_N, F_N]^{1/2}. \quad (5.4)$$

Using (3.1), (5.2), and (5.2') we obtain

$$\begin{aligned} (\Psi^N, \Psi^N) &= 1 \\ &= \frac{(F_{N-2}, F_{N-2})}{(F_N, F_N)} (f\Psi^{N-2}, O_{AS}f\Psi^{N-2}) \\ &= \frac{1 - \text{tr}\Gamma_{1,r}\Gamma_{1,\Psi^{N-2}} + (f\Gamma_{2,\Psi^{N-2}}f)}{[N/2] + O(\epsilon)}. \end{aligned}$$

Here we have used a trivial equality

$$\begin{aligned} O_{AS}(1, \dots, N) &= O_{AS}(3, \dots, N)O_{AS}(1, \dots, N)O_{AS}(3, \dots, N). \end{aligned}$$

Since  $\text{tr}\Gamma_{1,r}\Gamma_{1,\Psi^{N-2}} = O(\epsilon)$ , we finally obtain

$$(f\Gamma_{2,\Psi^N}f) = [\frac{1}{2}N] + O(\epsilon). \quad (5.5)$$

It is possible to make  $\text{tr}(\Gamma_{1,r})^2$  as small as we wish, and therefore the largest eigenvalue of  $\Gamma_{2,\Psi^N}$  can be arbitrarily close to  $\Lambda_{2,N}$ .

It is found further that a wave function  $\Psi$  can be approximated by the form (5.4), if the largest eigenvalue is close to  $\Lambda_{2,N}$ . To prove this, suppose we have an  $N$ -particle wave function  $\Psi$  and a 2-particle function  $f$  such that

$$(f\Gamma_{2,\Psi}f) = [N/2] - \epsilon. \quad (5.6)$$

Then using theorem 3 and (3.1), we obtain

$$\Psi = \left[ \binom{N}{2} / \Lambda_{2,N} \right]^{1/2} O_{AS}fg_1 + h_1,$$

where  $(h_1|h_1) < 2\epsilon/\Lambda_{2,N}$ , and

$$\begin{aligned} 1 - \frac{2\epsilon}{\Lambda_{2,N}} &\leq \binom{N}{2} (fg_1 O_{AS}fg_1) / \Lambda_{2,N} \\ &= \{1 - \text{tr}\Gamma_{1,r}\Gamma_{1,g_1} + (f\Gamma_{2,g_1}f)\} / \Lambda_{2,N}. \end{aligned}$$

Since  $\text{tr}\Gamma_{1,r}\Gamma_{1,g} > 0$ , we see that

$$(f\Gamma_{2,g_1}f) \geq \Lambda_{2,N-2} - 2\epsilon, \quad (5.7)$$

showing that the function  $g_1$  can be again expressed as

$$g_1 = \left[ \binom{N-2}{2} / \Lambda_{2,N-2} \right]^{1/2} O_{AS}fg_2 + h_2,$$

where  $(h_2|h_2) < 4\epsilon/\Lambda_{2,N-2}$ . Repeating the procedure, we obtain a decomposition of the total wave function  $\Psi$ :

$$\begin{aligned} \Psi &= \left[ \binom{N}{2} / \Lambda_{2,N} \right]^{1/2} O_{AS}f \left[ \left( \binom{N-2}{2} / \Lambda_{2,N-2} \right)^{1/2} \right. \\ &\quad \left. \times O_{AS}f[\cdot[\dots]\cdot] + h_2 \right] + h_1 \\ &= \frac{N!}{2^{N/2}(N/2)!} O_{AS}f(1,2)f(3,4)\dots \\ &\quad \times f(N-1,N) + h(1, \dots, N), \quad (N \text{ even}) \\ &= \frac{N!}{2^{(N-1)/2}[(N-1)/2]!} O_{AS}f(1,2)f(3,4)\dots \\ &\quad \times f(N-2,N-1)g(N) + h(1, \dots, N), \quad (N \text{ odd}), \quad (5.8) \end{aligned}$$

where

$$(h|h) = O(\epsilon). \quad \text{Q.E.D.}$$

By using (5.3), the first-order density matrix can be written in the form

$$\begin{aligned} \Gamma_{1,\Psi} &\simeq \frac{1}{2}N\Gamma_{1,f}, \quad (N \text{ even}) \\ \Gamma_{1,\Psi} &\simeq \frac{1}{2}(N-1)\Gamma_{1,r+g}(g). \quad (N \text{ odd}) \end{aligned} \quad (5.9)$$

The expressions (5.8) and (5.9) suggest that such a state may be interpreted as a system of fermion pairs which occupy the same state. These electron pairs behave like quasibosons and, since they are all in the same state, the limiting wave function corresponds to a situation with complete Bose-Einstein condensation.<sup>9</sup>

#### ACKNOWLEDGMENTS

The author is indebted to Professor P. O. Löwdin, Professor A. J. Coleman, and Dr. L. B. Redei for helpful discussions and criticism. To Professor Löwdin, the author would like to express his gratitude for giving him the opportunity of being in the stimulating atmosphere of the Quantum Chemistry Group.

<sup>9</sup> This paper was originally submitted for publication in the proceedings of the Hylleraas symposium together with the papers by A. J. Coleman, *Rev. Mod. Phys.* **35**, 668 (1963), and by T. Ando, *ibid.* **35**, 690 (1963), containing similar results. However, since the paper was accidentally omitted in the printed volume, it was later resubmitted to the Physical Review. During the interim, there has been an intense discussion of the interpretation of the results as to Bose-Einstein condensation; see particularly M. Girardeau, *J. Math. Phys.* **4**, 1096 (1963); J. M. Blatt, *Math. Rev.* **28**, 173 (1964); A. J. Coleman, *Phys. Rev. Letters* **13**, 406 (1964); F. Bloch, *Phys. Rev.* **137**, A787 (1965); A. J. Coleman, *J. Math. Phys.* (to be published).