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TECHNICAL NOTE

EIGENVALUES OF FERMION DENSITY MATRICES

by

Fukashi Sasaki

Quantum Chemistry Group
For Research in Atomic, Molecular and Solid-State Theory
Uppsala University, Uppsala, Sweden

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[*]   This work was performed while the author
         was on leave from the Department of
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ABSTRACT

The least upper bound of the eigenvalues of second order 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 n identical pairs behaving as quasi-bosons.

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1. INTRODUCTION

It is known that some features of a system are illustrated 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 [1]. We might expect that the spectrum of a higher-order density matrix would also characterize the structure of the system. However, it seems that little has been done along this line [2]. In this paper, we discuss the range of the eigenvalues of a many-particle density matrix in order to approach this problem.

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[1] Per-Olov Löwdin, Phys. Rev. **97**, 1474 (1955)

[2] See, however, the preliminary report of A. J. Coleman, Canad. Math. Bull. **4**, No. 2, May (1961). Further progress has been reported by him at Sanibel Island, Winter Institute in Quantum Chemistry and Solid State Physics, January 2-13, 1961.

For this purpose, it is convenient to use a wave function expanded in terms of the eigenfunctions of density matrices [3]. The expansion is obtained

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[3] B. C. Carlson and J. M. Keller, Phys. Rev. **121**, 659 (1961)

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by the use of the following theorems.

Theorem 1. If A is a linear operator which renders a completely continuous transformation [4] of one Hilbert space into another, and f is an element of the first Hilbert space, Af can be written in the form

$$A f = \sum_{i} \mu_i \, g_i \, (f_i \, f).$$

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[4] See e.g. F. Riesz and B. Sz.-Nagy, Functional Analysis, (Frederick Ungar Publishing Company, New York 1955) pp 206

Here $\{f_i\}$ and $\{g_i\}$ are orthonormal sets in the two Hilbert spaces involved, and $\{\mu_i\}$ is a non-increasing sequence of positive numbers. The sequence can be finite or infinite, and in the latter case it tends to zero.

Corollary 1:

$$\sup \; |(Af, g)| \; / \; \sqrt{(f,f)(g,g)} \; = \; \mu_1 .$$

$\underline{\text{Theorem 2}}$. If there exists a normal operator S such that $AS = A$, every f_i is an eigenelement of S, i.e. $Sf_i = f_i$.

Although special cases of Theorem 1 have been proven by others [3,5], it would be useful to present it in a more general form. The proof of the above theorems is given in the Appendix A.

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[5] A.T. Amos and G.G. Hall, Proc. Roy. Soc. A$\underline{263}$, 483 (1961).

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

$$g(x_1, \ldots, x_{N-M}) = \int \cdots \int dx_1' \cdots dx_M' \; \Psi(x_1, \ldots, x_{N-M}, x_1', \ldots, x_M') f(x_1'; \ldots; x_M'),$$

or, in a brief form

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

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

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

it renders necessarily a completely continuous transformation (for a proof, see the Appendix B). By the use of Theorem 1, we obtain the following expansion of the wave function Ψ :

$$\Psi(x, y) = \sum_i \mu_i \, g_i(x) \, f_i(y) , \qquad (1\text{-}1)$$

where

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

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

and

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

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 $y = (x_1' \cdots x_M')$:

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

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

$$\int \Psi(x, y) \; O_{AS, y} \, f(y) \, dy \; = \; \int O_{AS, y} \; \Psi(x, y) \, f(y) \, dy \; = \; \int \Psi(x, y) \, f(y) \, dy.$$

Thus by using Theorem 2, it follows that $O_{AS, y} f = f$, i.e. that if the function Ψ 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 Ψ :

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

Introducing a projection operator O_Ψ which projects out the state Ψ :

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

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

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

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

$$(\omega (O_{AS} - O_\Psi) \omega) = (\omega (1 - O_\Psi) O_{AS} (1 - O_\Psi) \omega) =$$

$$= ((1 - O_\Psi) \omega \; O_{AS} (1 - O_\Psi) \omega) \geq 0 .$$

Thus we obtain the following inequality

$$\lambda_{M,N}(\Psi) \leq \binom{N}{M} (g_1 f_1 O_{AS} g_1 f_1) \leq$$

$$\leq \binom{N}{M} \sup_{f,g} (g f O_{AS} g f), \qquad (2\text{-}1)$$

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 Ψ , it follows that

$$\lambda_{M,N} \equiv \sup_\Psi \lambda_{M,N}(\Psi) \leq \binom{N}{M} \sup_{f,g} (g f O_{AS} g f). \quad (2\text{-}2)$$

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:

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

as $k \rightarrow \infty$.

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

$$\Psi^{(k)} = \sqrt{\binom{N}{M}/\lambda^{(k)}} \ O_{AS} \ g^{(k)} f^{(k)}$$

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

$$\lim_{k \rightarrow \infty} \lambda_{M,N} (\Psi^{(k)}) \geq \lim_{k \rightarrow \infty} \lambda^{(k)}. \qquad (2-3)$$

By comparing (2-3) with (2-2), it is found that

$$\lambda_{M,N} = \binom{N}{M} \sup_{f,g} (g f O_{AS} g f)^{6)}. \qquad (2-4)$$

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6)   We note that for a system of identical bosons, the whole argument
     is valid by 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

$$\lambda_{M,N} = \binom{N}{M} \sup_{f,g} (g f O_S g f) \qquad (2-5)$$

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

$$O_S = \frac{1}{N!} \sum_P P$$

It is readily seen from (2-5) that

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

3. UPPER BOUNDS

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

$$\binom{N}{M} O_{AS}(1,\cdots,N) = O_{AS}(1,\cdots,M) O_{AS}(M+1,\cdots,N) \times$$

$$\times \sum_{i=0}^{\min\{N-M,\,M\}} (-)^i \binom{N-M}{i}\binom{M}{i} P\{(1,M+1)(2,M+2)\cdots(i,M+i)\} O_{AS}(1,\cdots,M) O_{AS}(M+1,\cdots;N) \qquad (3-1)$$

where $O_{AS}(p\cdots g)$ denotes the antisymmetry projection operator defined with respect to the coordinates in the parenthesis, and

$P\{(1,M+1)(2,M+2)\cdots(i,M+i)\}$ denotes the operation of replacing the coordinate 1 by $M+1$, $M+1$ by 1, ..., i by $M+i$ and $M+i$ by i. This shows that f and g which give the extremum in the equation (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

$$\lambda_{M,N} = 1 + \sup \sum_{i=1}^{\min(M,\,N-M)} (-)^i \, tr \, \Gamma_{i,f} \Gamma_{i,g}. \qquad (3-2)$$

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

$$0 \le tr \, \Gamma_{i,f} \Gamma_{i,g} \le \min(tr\,\Gamma_{i,f}\,\lambda_{i,N-M}\,;\,tr\,\Gamma_{i,g}\,\lambda_{i,M}) =$$

$$= \min\left[\binom{M}{i}\lambda_{i,N-M}\,;\,\binom{N-M}{i}\lambda_{i,M}\right]. \qquad (3-3)$$

From (3-2) and (3-3) we obtain an upper bound of the eigenvalues by the recurrence equation

$$\lambda_{M,N} \le \Lambda_{M,N} = 1 + \sum_{i=1}^{\min\{[\frac{M}{2}],\,[\frac{N-M}{2}]\}^{7)}} \min\left[\binom{M}{2i}\Lambda_{2i,N-M}\,;\binom{N-M}{2i}\Lambda_{2i,M}\right]. \qquad (3-4)$$

The solutions of (3-4) are

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7)   [x] stands for the integral part of x.

$$\Lambda_{0,N} = 1$$

$$\Lambda_{1,N} = 1$$

$$\Lambda_{2,N} = \left[\frac{N}{2}\right] \qquad\qquad N \geq 6$$

$$\Lambda_{3,N} = 1 + 3\left[\frac{N-3}{2}\right] \qquad\qquad N \geq 6$$

$$\Lambda_{4,N} = 1 + \left(\left[\frac{N}{4}\right]-1\right)\left(1 + 6\left[\frac{N}{2}\right] - 6\left[\frac{N}{4}\right]\right) + \left(N - 4\left[\frac{N}{4}\right]\right)\left(N - 4\left[\frac{N}{4}\right] - 1\right)$$
$$N \geq 8$$

$$\Lambda_{5,N} = 1 + 10\left[\frac{N-5}{2}\right] + 5\Lambda_{4,N-5} \qquad\qquad N \geq 10$$

$$\vdots$$

It should be noticed that

$$\Lambda_{M,N} = O\left(N^{\left[\frac{M}{2}\right]}\right).$$

This is the same order of magnitude as the largest eigenvalue of $\Gamma_{\left[\frac{M}{2}\right]}$ for a system of $\left[\frac{N}{2}\right]$ bosons.

Since the eigenvalues of the first order density matrix of a single determinant wave function are 1, $\Lambda_{1,N}$ is equal to $\lambda_{1,N}$. It is shown in Section 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 Ψ such that

$$\left(f\,\Gamma_{M,\Psi}\,f\right) = \lambda_{M,N} - \varepsilon$$

where ε 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 Φ by the equation

$$\Phi(1,\cdots,N) = \sqrt{\binom{N}{M}/\lambda_{M,N}}\ \mathcal{O}_{AS}\ f(1,\cdots,M)\,g(M+1,\cdots,N)$$

where

$$g(M+1,\cdots,N) = \sqrt{\binom{N}{M}/(\lambda_{M,N} - \varepsilon)} \int\cdots\int \Psi(1,\cdots,N)\, f^*(1,\cdots,M)\, dx_1\cdots dx_M.$$

It is easy to see that

$$(g,g) = \frac{1}{\lambda_{M,N} - \varepsilon}\, (f\, \Gamma_{M,\Psi}\, f) - 1 \quad,$$

$$(\Psi,\Phi) = \sqrt{\binom{N}{M}/\lambda_{M,N}}\, (\Psi\, O_{AS}\, fg) =$$

$$= \sqrt{\binom{N}{M}/\lambda_{M,N}}\, (\Psi,\, fg) =$$

$$= \sqrt{1 - \frac{\varepsilon}{\lambda_{M,N}}}$$

and

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

Then it follows that

$$0 \leq (\Psi-\Phi,\Psi-\Phi) = (\Psi,\Psi) + (\Phi,\Phi) - (\Psi,\Phi) - (\Phi,\Psi) \leq$$

$$\leq 2 - 2\sqrt{1 - \frac{\varepsilon}{\lambda_{M,N}}} \leq \frac{2\varepsilon}{\lambda_{M,N}} \tag{4-1}$$

From the first three terms of (4-1), we obtain

$$(\Phi,\Phi) \geq 2\sqrt{1 - \frac{\varepsilon}{\lambda_{M,N}}} - 1 \geq 1 - \frac{2\varepsilon}{\lambda_{M,N}}$$

Summarizing the results obtained above, we have a theorem.

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

$$(f \ T_{M,\Psi} \ f) = \lambda_{M,N} - \varepsilon,$$

the wave function Ψ can be expressed as

$$\Psi = \sqrt{\binom{N}{M}/\lambda_{M,N}} \ O_{AS} \ f(1,\cdots,M) g(M+1,\cdots N) + h(1,\cdots,N),$$

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

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 $\lambda_{1,N}(=1)$,

$$T_{1,\Psi} (1, 1') = \sum_{i=1}^{p} f_i(1) f_i^*(1') + \sum_{i=m+1} \lambda_i f_i(1) f_i^*(1').$$

In such a case, it follows from Theorem 3 that the wave function Ψ can be expressed as

$$\Psi = \sqrt{N} \ O_{AS} \ f_1(1) g_1(2,\cdots,N) \tag{4-3}$$

Using (3-1), we obtain

$$1 = (\Psi,\Psi) = N (f_1 g_1, O_{AS} f_1 g_1) = 1 - \int\cdots\int dx_2\cdots dx_{N-1} |\int f_1^*(1) g_1(1,2,\cdots,N-1) dx_1|^2$$

i.e.

$$\int dx_1 \ f_1^*(1) g_1(1,2,\cdots,N-1) = 0. \tag{4-4}$$

The first order density matrix of g is found from (4-3) and (4-4) to be

$$T_{1, g_1} = T_{1,\Psi} - T_{1, f_1}. \tag{4-5}$$

Comparing (4-2) with (4-5), we see that the largest eigenvalue of T_{1,g_1} is also 1 if $p > 1$. Thus by repeated application of the previous discussion, it

is found that

$$\Psi = \sqrt{\frac{N!}{(N-p)!}} \; O_{AS} \; f_1(1) \cdots f_p(p) \; g(p+1, \cdots, N), \qquad (4\text{-}6)$$

$$\Gamma_1 \Psi = \sum_{i=1}^{p} f_i X f_i + \Gamma_{1,g} \qquad (4\text{-}7)$$

and

$$\int dx_1 \; f_i^*(1) \; g(1, 2, \cdots, N-p) = 0 \; . \qquad (4\text{-}8)$$

$$(i = 1, \cdots, p)$$

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 Section 3 is actually the smallest.

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

$$F_{2n}(1, \cdots, 2n) = O_{AS} \; f(1,2) \; f(3,4) \cdots f(2n-1, 2n)$$

$$(5\text{-}1)$$

$$F_{2n+1}(1, \cdots, 2n+1) = O_{AS} \; f(1,2) \; f(3,4) \cdots f(2n-1, 2n) \; g(2n+1)$$

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

$$(F_{2n}, F_{2n}) = \frac{2^n n!}{(2n)!} + O(\epsilon^2) \qquad (5\text{-}2)$$

$$(F_{2n+1}, F_{2n+1}) = \frac{2^n n!}{(2n+1)!} + O(\epsilon) \; , \qquad (5\text{-}2')$$

where

$$\varepsilon^2 = tr\, (\Gamma_{1,f})^2 = \iiiint f(1,2) f(3,4) f^*(1,3) f^*(2,4)\ dx_1 dx_2 dx_3 dx_4. \quad (5\text{-}3)$$

Proof

$$(F_{2n}, F_{2n}) = (O_{AS}\, f \cdots f\, ,\ O_{AS}\, f \cdots f) =$$

$$= (f \cdots f\ O_{AS}\, f \cdots f) =$$

$$= \frac{1}{(2n)!} \sum_{P} \varepsilon_P\, (f \cdots f\ P\, f \cdots f)$$

$$= \frac{1}{(2n)!} \sum_{P} a_P ,$$

where $a_P = \varepsilon_P (f \ldots f\, p\, f \ldots f)$. There exist $2^n n!$ permutations which interchange the particles keeping every pair. It is easy to see that $a_P = 1$ for such a permutation since $\varepsilon_P P f \ldots f = f \ldots f$, but otherwise a_P is the order of $tr (\Gamma_{1,f})^2$.

For odd N, (5-2') can be similarly proven. In this case some of the permutations will give integrals of the order $tr(\Gamma_{1,f} \Gamma_{1,g})$, but

$$0 \le tr\, \Gamma_{1,f}\, \Gamma_{1,g} \le \sqrt{tr\, (\Gamma_{1,f})^2\, tr\, (\Gamma_{1,g})^2} = \sqrt{tr\, (\Gamma_{1,f})^2} = \varepsilon .$$

$$\text{Q.E.D.}$$

Let $\quad \Psi^N (1, \cdots, N) = F_N (1, \cdots, N) / \sqrt{(F_N, F_N)} . \qquad (5\text{-}4)$

Using (3-1), (5-2) and (5-2') we obtain

$$(\Psi^N, \Psi^N) = 1 =$$

$$= \frac{(F_{N-2}, F_{N-2})}{(F_N, F_N)} (f\, \Psi^{N-2}\ O_{AS}\, f\, \Psi^{N-2}) =$$

$$= \frac{1 - tr\, \Gamma_{1,f}\, \Gamma_{1,\Psi^{N-2}} + (f\, \Gamma_{2,\Psi^{N-2}}\, f)}{\left[\frac{N}{2} \right] + O(\varepsilon)}$$

Here we have used a trivial equality

$$O_{AS}(1,\cdots,N) = O_{AS}(3,\cdots;N)\,O_{AS}(1,\cdots;N)\,O_{AS}(3,\cdots;N).$$

Since $\operatorname{tr}\Gamma_{1,f}\,\Gamma_{1,\psi^{N-2}} = O(\varepsilon)$, we finally obtain

$$(f\,\Gamma_{2,\psi^N}\,f) = \left[\frac{N}{2}\right] + O(\varepsilon). \tag{5-5}$$

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

It is found further that a wave function Ψ 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 Ψ and a 2-particle function f such that

$$(f\,\Gamma_{2,\Psi}\,f) = \left[\frac{N}{2}\right] - \varepsilon \tag{5-6}$$

Then using Theorem 3 and (3-1), we obtain

$$\Psi = \sqrt{\left(\tbinom{N}{2}\right)/\Lambda_{2,N}}\;O_{AS}\,f g_1 + h_1$$

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

and

$$1 - \frac{2\varepsilon}{\Lambda_{2,N}} \leq \left(\tbinom{N}{2}\right)(f g_1\,O_{AS}\,f g_1)/\Lambda_{2,N} =$$

$$= \left\{1 - \operatorname{tr}\Gamma_{1,f}\Gamma_{1,g_1} + (f\,\Gamma_{2,g_1}\,f)\right\}/\Lambda_{2,N}.$$

Since $\operatorname{tr}\Gamma_{1,f}\Gamma_{1,g} > 0$, we see that

$$(f\,\Gamma_{2,g_1}\,f) \geq \Lambda_{2,N-2} - 2\varepsilon \tag{5-7}$$

showing that the function g_1 can be again expressed as

$$g_1 = \sqrt{\left(\tbinom{N-2}{2}\right)/\Lambda_{2,N-2}}\;O_{AS}\,f g_2 + h_2$$

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

$$\Psi = \sqrt{\binom{N}{2}}/\Lambda_{2,N} \; O_{AS} \; f\left[\sqrt{\binom{N-2}{2}}/\Lambda_{2,N-2} \; O_{AS} \; f\left[[\cdots]\cdots\right] + h_2\right] + h_1$$

$$= \frac{N!}{2^{\frac{N}{2}} (N/2)!} \; O_{AS} \; f(1,2) f(3,4) \cdots f(N-1,N) + h(1,\cdots,N) \quad \text{(N: even)}$$

$$= \frac{N!}{2^{\frac{N-1}{2}} (\frac{N-1}{2})!} \; O_{AS} \; f(1,2) f(3,4) \cdots f(N-2,N-1) g(N) + h(1,\cdots; N) \quad \text{(N: odd)}$$

where $(h|h) = O(\mathcal{E})$.   Q.E.D.

By using (5-3), the first order density matrix can be written in the form

$$\Gamma_{1,\Psi} \simeq \frac{N}{2} \; \Gamma_{1,f} \qquad \text{(N: even)}$$

$$\text{(5-9)}$$

$$\Gamma_{1,\Psi} \simeq \frac{N-1}{2} \; \Gamma_{1,f} + g)(g . \qquad \text{(N: odd)}$$

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 quasi-bosons and, since they are all in the same state, the limiting wave function corresponds to a situation with complete Bose-Einstein condensation.

ACKNOWLEDGEMENT

APPENDIX A

Let f and g be elements of two Hilbert spaces E and E' respectively, and A be a linear operator which is completely continuous and hence transforms every infinite and bounded set in E into a compact set in E'. If A is not a zero operator, there exists a sequence $\{f^{(n)}\}$ such that

$$\| f^{(n)} \| = 1 \quad \text{and} \quad \| A f^{(n)} \| \rightarrow \sup_{f \in E} \| A f \| / \| f \| = \mu_1$$

where $\mu_1 > 0$. From the compactness of $\{A f^{(n)}\}$, it follows that the sequence $\{A f^{(n)} / \mu_1\} \equiv \{g^{(n)}\}$ contains a subsequence $\{g^{(n_k)}\}$ which converges to an element g_1 of E'. The norm of g_1 is 1, since

$$\| g^{(n_k)} \| = \frac{1}{\mu_1} \| A f^{(n_k)} \| \rightarrow 1 .$$

In addition, the sequence $\{f^{(n_k)}\}$ itself converges to an element f_1 of E. Consider a linear functional $K(f) = (Af, g_1)$. The least upper bound of $|K(f)| \equiv \nu$ on the sphere $\| f \| = 1$ is equal to μ_1. To prove $\nu \geq \mu_1$, consider the sequence $\{f^{(n_k)}\}$. Then

$$\nu \geq | K(f^{(n_k)}) | = | (A f^{(n_k)}, g_1) | \rightarrow \mu_1 \qquad (k \rightarrow \infty).$$

On the other hand

$$\nu = \lim_{m \to \infty} | (A f'^{(m)}, g_1) | = \frac{1}{\mu_1} \lim_{m \to \infty} \lim_{k \to \infty} | (A f'^{(m)}, A f^{(n_k)}) | \leq$$

$$\leq \frac{1}{\mu_1} \overline{\lim_{m \to \infty}} \| A f'^{(m)} \| \lim_{k \to \infty} \| A f^{(n_k)} \| \leq \mu_1$$

where $\{f'^{(m)}\}$ is a sequence which gives

$$| K(f'^{(m)}) | \rightarrow \nu \qquad \text{as} \qquad m \rightarrow \infty .$$

Thus we obtain

$$\| f^{(n_k)} - f^{(n_l)} \|^2 = 4 - \| f^{(n_k)} + f^{(n_l)} \|^2 \leq$$

$$\leq 4 - \frac{| K(f^{(n_k)} + f^{(n_l)}) |^2}{\mu_1^2} = 4 - \frac{| K(f^{(n_k)}) + K(f^{(n_l)}) |^2}{\mu_1^2}$$

$$\rightarrow 4 - \frac{| \mu_1 + \mu_1 |^2}{\mu_1^2} = 0 ,$$

since $|K(f)| < \mu_1 \parallel f \parallel$ for any $f \in E$. Thus we can conclude that $f^{(n_k)}$ converges to an element f_1 of E as a result of the completeness of E.

It is easy to see that the elements f_1 and g_1 satisfy the equation

$$A f_1 = g_1 \mu_1$$

since $A f^{(n_k)} = \mu_1 g^{(n_k)}$ for any n_k.

We note that

$$\sup_{\substack{f \in E \\ g \in E'}} |(A f, g)| = \mu_1$$

under the condition $\parallel f \parallel = \parallel g \parallel = 1$, since

$$\mu_1 = (A f_1, g_1) \leq \sup |(A f, g)| \leq \sup |A f| \cdot |g| = \mu_1.$$

Repeating the above procedure in the subspace of E which consists of all the elements orthogonal to f_1, we obtain a pair of elements (f_2 and g_2) and μ_2, if A is not a zero operator in the subspace. In general, f_k and g_k are obtained as a solution of the following extremum problem;

$$(A f_k, g_k) = \sup_f |A f| / |f| = \mu_k > 0 \qquad \text{(A-1)}$$

under the conditions $\parallel f_k \parallel = \parallel g_k \parallel = 1$ and $(f_i, f) = 0$ ($i = 1, 2, \ldots, k-1$). This procedure terminates when μ_k vanishes. It follows that

$$A f_k = \mu_k g_k$$

and moreover that the set $\{g_k\}$ is an orthonormal set. This follows from the evaluation

$$|\alpha g_k + \beta g_\ell|^2 = |\alpha|^2 + |\beta|^2 + 2 \mathcal{R} (\bar{\alpha} \beta (g_k, g_\ell)) =$$

$$= \parallel A (\frac{\alpha}{\mu_k} f_k + \frac{\beta}{\mu_\ell} f_\ell) \parallel^2 \leq$$

$$\leq \mu_k^2 | \frac{\alpha}{\mu_k} f_k + \frac{\beta}{\mu_\ell} f_\ell |^2 = |\alpha|^2 + \frac{\mu_k^2}{\mu_\ell^2} |\beta|^2$$

$$(k < \ell).$$

Setting $\beta = \alpha (g_\ell, g_k) \dfrac{\mu_\ell^2}{\mu_k^2}$ we obtain

$$| (g_k, g_\ell)|^2 \left(1 + \frac{\mu_\ell^2}{\mu_k^2}\right) \leq 0.$$

Hence $(g_k, g_\ell) = 0.$

The sequence $\{\mu_n\}$ is evidently composed of monotonically decreasing and positive terms

$$\mu_1 \geq \mu_2 \geq \cdots \quad > 0.$$

We can prove that $\mu_k \to 0$ as $k \to \infty$ if the sequence is infinite. If $\mu_k \to \mu > 0$, the sequence $\{\mu_k g_k\} = A\{f_k\}$, which is a bounded sequence $\{f_k\}$ transformed by A, would not contain a convergent subsequence, since

$$\| \mu_k g_k - \mu_\ell g_\ell \|^2 = \mu_k^2 + \mu_\ell^2 \geq 2\mu^2 > 0 \quad \text{for } k \neq \ell.$$

An arbitrary element of E may be expressed as

$$f = \sum_{i=1}^{n} (f_i, f) f_i + f^{(n)},\tag{A2}$$

where $f^{(n)}$ is orthogonal to f_i $(i = 1, 2, \ldots n)$ and

$$\| f^{(n)} \|^2 = \| f - \sum_{i=1}^{n} (f_i, f) f_i \|^2 = \| f \|^2 - \sum_{i=1}^{n} |(f_i, f)|^2 \leq \| f \|^2.$$

Therefore if the sequence $\{\mu_i\}$ is infinite,

$$\| A f^{(n)} \| \leq \mu_{n+1} \| f^{(n)} \| \leq \mu_{n+1} \| f \| \to 0$$

as $n \to \infty$. Operating by A on both sides of (A-2) and taking the limit, we obtain

$$A f = \sum_{i=1}^{\infty} (f_i, f) A f_i = \sum_{i=1}^{\infty} \mu_i (f_i, f) g_i$$

In the case where the sequence $\{\mu_i\}$ terminates at μ_k, it follows from (A-1) that

$$\| A f^{(k)} \| = 0.$$

Thus we obtain

$$A f = \sum_{i=1}^{k} \mu_i (f_i, f) g_i$$

This proves Theorem 1.

It follows from Theorem 1 that

$$(A f, g) - \sum_i \mu_i (f, f_i)(g_i, g) \leq \sqrt{\sum_i \mu_i^2 |(f, f_i)|^2 \sum_j |(g_j, g)|^2} \leq$$

$$\leq \mu_1 \| f \| \| g \|$$

Setting $f = f_1$ and $g = g_1$, we obtain

$$(A f_1, g_1) - \mu_1$$

Thus, we have proven Corollary 1.

To prove Theorem 2, let S be a normal operator such that

$$AS = A .$$

Then

$$\| (1-S) f_i \|^2 - ((1-S^\dagger)(1-S) f_i, f_i) - ((1-S)(1-S^\dagger) f_i, f_i) -$$

$$- \frac{1}{\mu_i} (A (1-S)(1-S^\dagger) f_i, g_i) - \frac{1}{\mu_i} (0, g_i) - 0.$$

This proves Theorem 2.

APPENDIX B

In order to prove that the transformation under consideration is completely continuous, we shall show that any weakly convergent sequence $\{f_n(y)\}$ is transformed by $\Psi(x,y)$ into a strongly convergent sequence $\{g_n(x)\}$.

From (1-1) it follows that the function

$$k(x) = \int |\Psi(x,y)|^2 \, dy$$

has a definite and finite value for almost all x. Therefore, since $\{f_n(y)\}$ is weakly convergent,

$$g_n(x) - g_m(x) = \int \Psi(x,y) f_n(y) \, dy - \int \Psi(x,y) f_m(y) \, dy$$

tends to 0 almost everywhere when $m, n \to \infty$.

Using Schwarz's inequality, we have

$$|g_n(x)|^2 = \iint \Psi(x,y) f_n(y) \Psi(x,y') f_n(y') \, dy \, dy' \le$$

$$\le \int |\Psi(x,y)|^2 dy \int |f_n(y)|^2 dy \le M \, k(x)$$

Here a finite number M is an upper bound of a sequence $\{\int |f_n(y)|^2 dy\}$. Then

$$|g_n(x) - g_m(x)|^2 \le |g_n(x)|^2 + |g_m(x)|^2 + 2|g_n(x) g_m(x)| \le 4M \, k(x)$$

Since $4Mk(x)$ is a Lebesgue-integrable function and we have shown that $|g_n(x) - g_m(x)|^2$ tends to 0 almost everywhere, it follows from Lebesgue's theorem that

$$\int |g_n(x) - g_m(x)|^2 \, dx \longrightarrow 0$$

when $n, m \to \infty$.

$$\text{Q.E.D.}$$

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