PRELIMINARY REPORT

DENSITY MATRICES OF n-FERMION SYSTEMS

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The energy of a system of indistinguishable particles in two-body interaction may be expressed in terms of the one and two-particle density matrices. In order to work directly with the density matrices we must know what restrictions are imposed on them by the statistics of the system. This report summarizes some results giving a partial answer to the question "What functions can arise as density matrices of a system of n fermions?".

NOTATION. The system is characterized by the normalized antisymmetric function $\psi = \psi(1, 2, 3, \ldots, n)$. The p-th order density matrix

$$D^p(x; x') = \int_{p+1, \ldots, n} \psi(1, 2, \ldots, n)\, \overline{\psi}(1', \ldots, p', p+1, \ldots, n) \tag{1}$$

may be regarded as the kernel of the hermitian integral equation of trace 1:

$$\int_y D^p(x; y)\, \psi_i^p(y) = \lambda_i^p \psi_i^p(x).$$

Here, ψ_i^p is a function of p particles which, in analogy with Löwdin, we call a <u>natural p-state of ψ</u> corresponding to the <u>p-th order eigenvalue of ψ</u>, λ_i^p. These eigenvalues are positive and $\Sigma_i \lambda_i^p = 1$. We assume they are ordered monotonically, $\lambda_i^p \geq \lambda_{i+1}^p$. Superscripts are integers between 1 and n indicating the number of particles involved in the corresponding function; throughout

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this report, $p + q = n$; the product $f^p f^q$ stands for $f^p(1, 2, \ldots, p) f^q(p+1, \ldots, n)$. The <u>p-rank of ψ</u> is the number of non-zero λ_i^p, though, for convenience, we shall refer to the 1-rank simply as the <u>rank of ψ</u> and denote it by r.

A function $D^p(x;y)$ will be called <u>n-representable</u> if there exists an antisymmetric function ψ of n particles satisfying equation (1). In this language, a basic problem of many particle physics is to obtain intrinsic criteria for recognizing when a given function is n-representable. A similar problem may be formulated for bosons, or more generally for functions of arbitrary symmetry type. We denote by A the idempotent operator which antisymmetrizes a function of n particles.

THEOREM 1. For m a finite natural number, $1 \leq i \leq m$, c^i complex numbers, and f_i^p, f_i^q functions of p and q particles respectively, the difference

$$d^2 = \|\psi - \Sigma c^i f_i^p f_i^q\|^2$$

attains its minimum, $1 - \Sigma_{i=1}^{i=m} \lambda_i^p$, if and only if the f's are proportional to the corresponding natural states of ψ, and $|c^i|^2 = \lambda_i^p = \lambda_i^q$.

THEOREM 2. ψ and the ψ_i^p may be expanded in terms of the r ψ_i^1 for which $\lambda_i^1 \neq 0$.

If a little more care is taken in defining the p and q natural states, theorem 1 is independent of the symmetry type of ψ; theorem 2 is valid for fermions and bosons.

THEOREM 3. For fermions, $n\lambda_i^1 \leq 1$; $(n - p + 1)\lambda_i^p < 1$ for $p > 1$.

Thus the 2-rank of ψ is at least n.

THEOREM 4. The condition that D^1 be n-representable can be expressed in terms of the first order eigenvalues alone.

THEOREM 5. A sufficient condition that D^1 be n-representable is that each of the first order eigenvalues of ψ be degenerate with multiplicity divisible by n.

THEOREM 6. D^1 is 2-representable if and only if the first order eigenvalues are evenly degenerate.

THEOREM 7. If D^1 is n-representable, $r \neq n + 1$.

THEOREM 8. If $r = n + 2$, a n.a.s.c. that D^1 be n-representable is as follows:

(i) if n is odd, $\lambda_1^1 = n^{-1}$ and the remaining first order eigenvalues are evenly degenerate and less than n^{-1};

(ii) if n is even, the first order eigenvalues are evenly degenerate and all less than n^{-1}.

THEOREM 9. If $D^1(x;y)$ is n-representable and $\lambda_1^1 = \lambda_2^1 = \ldots = \lambda_k^1 = n^{-1}$, then

$$D^1 = n^{-1}[\psi_1^1(x)\overline{\psi}_1^1(y) + \ldots + \psi_k^1(x)\overline{\psi}_k^1(y)] + D_2^1$$

where $D_2^1(x;y)$ is $(n-k)$-representable.

THEOREM 10. $D^1(x;y)$, of rank r, is n-representable by ψ, if and only if it may be put into the form

$$D^1 = \lambda_1^1 \psi_1^1(x)\overline{\psi}_1^1(y) + (n-1)\lambda_1^1 D_1^1 + (1 - n\lambda_1^1) D_2^1,$$

where D_1^1 is $(n-1)$-representable and orthogonal to ψ_1^1, and D_2^1 has rank at most $r - 1$ and is n-representable by $\psi - cA(\psi_1^1 \psi_1^{n-1})$ where c is an appropriately chosen constant.

The first part of theorem 1 was suggested by and generalizes a result of Löwdin [1] for $n = 2$; the last equality was recently noticed by Carlson and Keller [2]. The first part of theorem 3 was known to Löwdin [3] and has as a consequence that if $r = n$, D^1 is the Dirac density matrix corresponding to the Hartree-Fock approximation. Theorem 10 provides a double induction algorithm by which, in principle, the n-representability of any alleged one particle density matrix of finite rank could be decided. For two particle matrices the result analogous to theorem 5 is considerable more complicated since λ_i^2 do not provide a complete set of unitary invariants; my results in this connection so far are partial and scattered.

Numerical calculations have been initiated to test the practical usefulness of theorem 10. Preliminary results of these calculations together with proofs of the above will be given in a paper now being prepared for publication.

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REFERENCES

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2. ...., 121 (1961), 659-661.

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