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CROCKER NUCLEAR LABORATORY

University of California, Davis

MASTER

PROPERTIES OF THE 2-MATRIX DUE TO THE INTEGER CHARACTER
OF OCCUPATION NUMBERS

Claude Garrod

August, 1967

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standpoint to the publication or
dissemination of this document:

California Patent Group, USAEC

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The simple fact that the number of particles in any quantum state can only be an integer has nontrivial consequences for the properties of reduced density matrices. In this paper we shall investigate some of the simpler inequalities involving density matrix elements which can be traced to the discreteness of the particles.

We consider only the diagonal elements of the 1-matrix and 2-matrix. These elements can be written as expectation values of number operators in the following way:

$$D_1(n|n) = \langle N_n \rangle \equiv \rho(n) \quad (1)$$

$$D_2(n,m|n,m) = \langle N_n N_m \rangle - \delta_{nm} \langle N_n \rangle \quad (2)$$

In terms of these elements we define a "fluctuation matrix" $K(n,m)$ as follows:

$$K(n,m) = \langle (N_n - \rho(n))(N_m - \rho(m)) \rangle = D_2(n,m|n,m) + \delta_{nm} \rho(n) \rho(m). \quad (3)$$

The diagonal element $K(n,n)$ is just the mean square fluctuation in the value of the occupation number of the n th quantum state. It is obvious from its definition that $K(n,m)$ is a non-negative matrix; that is, it has no negative eigenvalues. In reference 1 this fact was noted and some use was made of inequalities derived therefrom. We shall now see that some of the inequalities may be strengthened.

Let us consider the diagonal elements of K . Obviously they must be greater than or equal to zero. Since N_n has only integer eigenvalues

$K(n,n)$ can be zero only if $\rho(n)$ is an integer. If $\rho(n)$ is not an integer then we may get a non-zero lower bound on $K(n,n)$ as follows. We first express $\rho(n)$ as the sum of the nearest smaller integer plus a number smaller than one.

$$\rho(n) = I + E \quad (4)$$

We shall then show that:

$$K(n,n) \geq E(1 - E). \quad (5)$$

Proof: Let $P_n(N)$ be the probability that the n th state contain exactly N particles. We must show that

$$\text{Min} \sum_n N^2 P_n(n) = (\rho(n))^2 + E(1 - E) \quad (6)$$

where the minimization is done with the constraints that:

$$P_n(N) \geq 0, \quad (7)$$

$$\sum_n P_n(N) = \rho(n), \quad (8)$$

$$\text{and } \sum_n P_n(N) = 1. \quad (9)$$

We are thus looking for the minimum of a linear function of the parameters $P_n(N)$ with linear constraints. This is a classical minimum problem. (See, for instance, reference 2.) The minimum is found by changing as many as possible of the inequality constraints without the violating two equality

constraints. The maximum number of the $P_n(N)$ which we can set equal to zero is all but two. The minimum occurs for some combination of only two non-zero $P_n(N)$. It is now a trivial matter to show that the two $P_n(N)$'s which we want to be non-zero are those which bracket $\rho(n)$. Thus

$$P_n(I) = \alpha \quad \text{and} \quad P_n(I+1) = 1 - \alpha \quad (10)$$

Equation 8 demands that:

$$I\alpha + (I+1)(1-\alpha) = I + E \quad (11)$$

or:

$$\alpha = 1 - E. \quad (12)$$

Thus:

$$\sum N^2 P_n(N) = I^2(1-E) + (I+1)^2 E = (I+E)^2 - E(1-E) \quad (13)$$

which proves the theorem.

For fermion systems $0 \leq \rho(n) \leq 1$ and $D_2(n,n|n,n) = 0$. This makes the inequality 5 and identity. However, for boson systems it is a non-trivial constraint on the elements of D_2 .

The fact that K is a non-negative matrix implies also that the principle 2×2 determinants are non-zero.

$$K(n,n) K(m,m) - (K(n,m))^2 \geq 0 \quad (14)$$

or:

$$|K(n,m)| \leq \sqrt{K(n,n) K(m,m)}. \quad (15)$$

This inequality may also be strengthened by making use of the fact that N_n and N_m must be integers. In order to develop a stronger bound on $K(n,m)$ we must determine the largest value of $|K(n,m)|$ consistent with given values of $\rho(n)$, $\rho(m)$, $K(n,n)$, and $K(m,m)$. Without any loss in generality we may assume that $n = 1$ and $m = 2$. Let $P(N_1, N_2)$ be the probability that exactly N_1 particles are in state 1 while N_2 particles are in state 2. We thus want to find the maximum and minimum values of the function:

$$F = \sum_{N_1, N_2} (N_1 - \rho(1))(N_2 - \rho(2)) P(N_1, N_2) \quad (16)$$

with the constraints:

$$P(N_1, N_2) \geq 0 \quad (17)$$

$$\sum (N_1 - \rho(1)) P(N_1, N_2) = 0, \quad (18)$$

$$\sum (N_2 - \rho(2)) P(N_1, N_2) = 0, \quad (19)$$

$$\sum (N_1 - \rho(1))^2 P(N_1, N_2) = K(1,1) \quad (20)$$

$$\text{and:} \quad \sum (N_2 - \rho(2))^2 P(N_1, N_2) = K(2,2) \quad (21)$$

The problem is the same type as that considered before. This time, since we have four equality constraints we can expect to have four non-zero P 's. For given $\rho(1)$, $\rho(2)$, $K(1,1)$ and $K(2,2)$ the numerical problem of testing all reasonable combinations of four non-zero P 's to see which

yields a minimum or maximum for F is a fairly simple one. The result of the calculation yields upper and lower bounds for $K(1,2)$.

REFERENCES

1. C. Garrod and J. K. Percus, J. Math. Phys., 5, 1756, (1964).
2. Charnes, Cooper, and Henderson, An Introduction to Linear Programming, John Wiley & Sons, New York, (1953).

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