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The conditions on the one-matrix for three-body fermion wavefunctions with one-rank equal to six

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Abstract. The necessary and sufficient conditions for a one-body reduced density matrix of rank 6 to be derivable from a three-body fermion wavefunction are presented. For this case it can be shown explicitly that the information content of the one-matrix is less than that of the wavefunction. The extension of these conditions to the cases of a three-body function of one-rank 7 and a four-body function of one-rank 8 are also discussed. We have obtained sufficient conditions for these two cases. Numerical studies reported in this paper lead us to believe that these conditions are the necessary and sufficient conditions.

1. Introduction

In a previous paper (Borland and Dennis 1970) a numerical investigation of the properties of some real N-body antisymmetric wavefunctions was presented. It was found that when the wavefunctions were constructed from a finite number, M, of natural spin orbitals, they had a simplified form in the general case $M = N+2$, and the special case $N = 3$, $M = 6$.

The general three-body wavefunction expressed in terms of 6 orbitals would have 20 configurations. However, it was found that in the natural spin orbital representation the only non-zero configuration coefficients were A_{123}, A_{145}, A_{246}, A_{356}, A_{124}, A_{135}, A_{236} and A_{456}. Here A_{ijk} is the coefficient of the Slater determinant formed from orbitals ϕ_i, ϕ_j and ϕ_k. This reduction in the number of determinants has since been confirmed analytically by M B Ruskai and R L Kingsley (private communications). The numerical results were for real wavefunctions, but the analytical proofs show that the reduction also holds for the more general complex case. This reduced form simplifies the derivation of the necessary and sufficient conditions for three-representability of the one-matrix in this case.

We make no apology for the consideration of such a special case. The general N-representability problem for one and two body reduced density matrices is so difficult and yet so fundamental to many branches of science that each concrete result is useful in shedding light on the nature of the solution of the more general problem.

We follow the notation used by Borland and Dennis (1970). All references in the present paper to density matrices mean one-body reduced density matrices, and all wavefunctions are fermion wavefunctions.

2. Sufficient conditions for the case $N = 3$, $M = 6$

Consider a wavefunction consisting of just the four normalized Slater determinants whose coefficients are A_{123}, A_{145}, A_{246} and A_{356}. For convenience, we label these coefficients α_1, α_2, α_3 and α_4 respectively. Normalization of the wavefunction demands that

$$\sum_{i=1}^{4} |\alpha_i|^2 = 1. \tag{1}$$

It is clear that the density matrix formed from such a wavefunction is diagonal, as no two orbitals occur together in more than one determinant. The eigenvalues are given by

$$\lambda_1 = |\alpha_1|^2+|\alpha_2|^2 \tag{2a}$$

$$\lambda_2 = |\alpha_1|^2+|\alpha_3|^2 \tag{2b}$$

$$\lambda_3 = |\alpha_1|^2+|\alpha_4|^2 \tag{2c}$$

$$\lambda_4 = |\alpha_2|^2+|\alpha_3|^2 \tag{2d}$$

$$\lambda_5 = |\alpha_2|^2+|\alpha_4|^2 \tag{2e}$$

$$\lambda_6 = |\alpha_3|^2+|\alpha_4|^2. \tag{2f}$$

It can be seen from (1) and (2) that

$$\lambda_1+\lambda_6 = 1 \tag{3a}$$

$$\lambda_2+\lambda_5 = 1 \tag{3b}$$

$$\lambda_3+\lambda_4 = 1. \tag{3c}$$

We can now insist without loss of generality that the eigenvalues are ordered $\lambda_i \geqslant \lambda_{i+1}$.

Solving equations (2) for the $|\alpha_i|^2$ and using equations (3) we obtain

$$2|\alpha_1|^2 = \lambda_1+\lambda_2+\lambda_3-1 = \lambda_1+\lambda_2-\lambda_4 \tag{4a}$$

$$2|\alpha_2|^2 = \lambda_1+\lambda_4+\lambda_5-1 = \lambda_1+\lambda_5-\lambda_3 \tag{4b}$$

$$2|\alpha_3|^2 = \lambda_2+\lambda_4+\lambda_6-1 = \lambda_4+\lambda_6-\lambda_5 \tag{4c}$$

$$2|\alpha_4|^2 = \lambda_3+\lambda_5+\lambda_6-1 = \lambda_5+\lambda_6-\lambda_4. \tag{4d}$$

Since $|\alpha_i|^2$ is non-negative the right hand sides of equation (4) must be greater than or equal to zero. The ordering of the eigenvalues ensures this for equations (4*a*), (4*b*) and (4*c*) but equation (4*d*) gives the non-trivial condition $\lambda_5+\lambda_6 \geqslant \lambda_4$. The eigenvalues therefore satisfy the conditions

$$\lambda_1+\lambda_6 = 1 \tag{5a}$$

$$\lambda_2+\lambda_5 = 1 \tag{5b}$$

$$\lambda_3+\lambda_4 = 1 \tag{5c}$$

$$\lambda_5+\lambda_6 \geqslant \lambda_4 \tag{5d}$$

$$\lambda_i \geqslant 0 \tag{5e}$$

with the eigenvalues enumerated so that $\lambda_i \geqslant \lambda_{i+1}$.

These conditions are sufficient conditions for three-representability of the one-matrix because if they are satisfied we can, from equations (4), determine a set of four coefficients α_1, α_2, α_3 and α_4 defining a wavefunction from which the one-matrix can be derived. That these sufficient conditions (5) are also necessary will be shown in § 3.

3. Necessary conditions for the case $N = 3$, $M = 6$

In the natural orbital representation any three-body wavefunction approximated using six basis orbitals consists of only the eight determinants whose coefficients are A_{123}, A_{124}, A_{135}, A_{145}, A_{236}, A_{246}, A_{356} and A_{456}. We label these coefficients $\beta_1 \ldots \beta_8$ respectively, and as usual normalization requires

$$\sum_{i=1}^{8} |\beta_i|^2 = 1. \tag{6}$$

The eigenvalues of the density matrix formed from this wavefunction are given by

$$\lambda_1 = |\beta_1|^2 + |\beta_2|^2 + |\beta_3|^2 + |\beta_4|^2 \tag{7a}$$

$$\lambda_2 = |\beta_1|^2 + |\beta_2|^2 + |\beta_5|^2 + |\beta_6|^2 \tag{7b}$$

$$\lambda_3 = |\beta_1|^2 + |\beta_3|^2 + |\beta_5|^2 + |\beta_7|^2 \tag{7c}$$

$$\lambda_4 = |\beta_2|^2 + |\beta_4|^2 + |\beta_6|^2 + |\beta_8|^2 \tag{7d}$$

$$\lambda_5 = |\beta_3|^2 + |\beta_4|^2 + |\beta_7|^2 + |\beta_8|^2 \tag{7e}$$

$$\lambda_6 = |\beta_5|^2 + |\beta_6|^2 + |\beta_7|^2 + |\beta_8|^2. \tag{7f}$$

It is immediately obvious from (6) and (7) that

$$\lambda_1 + \lambda_6 = 1$$

$$\lambda_2 + \lambda_5 = 1$$

$$\lambda_3 + \lambda_4 = 1$$

which shows the necessity of equations (5*a*), (5*b*) and (5*c*).

We can as usual insist that the eigenvalues are completely ordered so that $\lambda_i \geqslant \lambda_{i+1}$. Subtraction of (7*f*) from (7*c*) and of (7*f*) from (7*d*) gives, respectively

$$|\beta_1|^2 + |\beta_3|^2 = |\beta_6|^2 + |\beta_8|^2 + \lambda_3 - \lambda_6 \tag{8}$$

and

$$|\beta_2|^2 + |\beta_4|^2 = |\beta_5|^2 + |\beta_7|^2 + \lambda_4 - \lambda_6. \tag{9}$$

Because the density matrix is diagonal, the off-diagonal elements are zero. This means that

$$\beta_1^*\beta_5 + \beta_2^*\beta_6 + \beta_3^*\beta_7 + \beta_4^*\beta_8 = 0 \tag{10a}$$

$$\beta_1^*\beta_3 + \beta_2^*\beta_4 + \beta_5^*\beta_7 + \beta_6^*\beta_8 = 0 \tag{10b}$$

and

$$\beta_1^*\beta_2 + \beta_3^*\beta_4 + \beta_5^*\beta_6 + \beta_7^*\beta_8 = 0 \tag{10c}$$

where β_i^* is the complex conjugate of β_i. We wish to show that $\lambda_5+\lambda_6 \geqslant \lambda_4$, that is

$$|\beta_3|^2+|\beta_5|^2+2|\beta_7|^2+|\beta_8|^2-|\beta_2|^2 \geqslant 0. \tag{11}$$

Addition of (10*a*) and (10*c*) gives

$$\beta_1^*(\beta_2+\beta_5)+\beta_6(\beta_2^*+\beta_5^*) = -\beta_3^*(\beta_4+\beta_7)-\beta_8(\beta_4^*+\beta_7^*). \tag{12}$$

Subtraction of (10*c*) from (10*a*) and complex conjugation gives

$$\beta_1(\beta_5^*-\beta_2^*)+\beta_6^*(\beta_2-\beta_5) = \beta_3(\beta_4^*-\beta_7^*)+\beta_8^*(\beta_7-\beta_4). \tag{13}$$

Multiplying (12) by (13), rearranging and collecting up the real parts of the resultant equation, we obtain

$$(|\beta_2|^2-|\beta_5|^2)(|\beta_1|^2-|\beta_6|^2) = (|\beta_3|^2-|\beta_8|^2)(|\beta_4|^2-|\beta_7|^2). \tag{14}$$

Inserting (8) and (9) in (14) leads to

$$\frac{\lambda_3-\lambda_6}{\lambda_4-\lambda_6} = \frac{|\beta_3|^2-|\beta_8|^2}{|\beta_2|^2-|\beta_5|^2} \geqslant 1. \tag{15}$$

To prove the inequality (11) we consider the two possibilities:

(i) $|\beta_2|^2-|\beta_5|^2 \leqslant 0.$

In this case, it is clear immediately that (11) is satisfied.

(ii) $|\beta_2|^2-|\beta_5|^2 > 0.$

Then we have from (15) that

$$|\beta_3|^2-|\beta_8|^2 \geqslant |\beta_2|^2-|\beta_5|^2$$

so that

$$|\beta_3|^2+|\beta_5|^2 \geqslant |\beta_2|^2+|\beta_8|^2.$$

Again it can be seen that (11) is satisfied. Therefore in both cases

$$\lambda_5+\lambda_6 \geqslant \lambda_4.$$

Hence conditions (5) are both necessary and sufficient and provide a complete solution to the three-representability problem for the one-matrix of rank 6.

The results given above enable us to make an important general observation about the relative information content of a wavefunction and its density matrix. In the $N = 3$, $M = 6$ case, a real wavefunction contains four independent parameters (eight coefficients β_i, which are subject to three orthogonality conditions (10) and the normalization condition). On the other hand, a completely general N-representable one-matrix for this case, obeying the necessary and sufficient conditions (5), can be characterized in terms of just three independent parameters (four coefficients α_i, subject to a normalization condition). For the first time therefore, we have found an example of a one-body density matrix which can be specified more economically, in terms of independent parameters, than its corresponding wavefunction; or equivalently, we have shown that a *less than general* type of wavefunction, that is the four-configuration function introduced in § 2, can be used to generate a completely general N-representable one-matrix of rank 6.

It is the possibility of such a reduction in parametrization that has motivated research on N-representability. Although the main interest is of course in the two-body reduced density matrix for which such an information reduction is still an open question (Ruskai 1969), the results we have obtained have a practical application in atomic calculations. Whenever the one-matrix can be fully represented by a wavefunction of special form the use of that wavefunction may have advantages. It properly takes into account one-body contributions to the energy while at the same time giving an approximation to the two-body terms. Such a wavefunction can always be supplemented if desired by configurations which are thought to be of specific importance to the two-body contributions.

4. Extensions to further cases

By the use of ideas similar to those in § 2, it is possible to derive sufficient conditions for some other cases.

4.1. $N = 3$, $M = 7$

Consider a wavefunction consisting of the seven normalized determinants whose coefficients are A_{123}, A_{145}, A_{167}, A_{246}, A_{257}, A_{347} and A_{356}. We define the numbers γ_i, $i = 1, \ldots, 7$, by $\gamma_1 = |A_{123}|^2$ etc, and normalization requires that $\Sigma_{i=1}^{7} \gamma_i = 1$. Note that the one-matrix of this wavefunction is diagonal.

Solving for the γ_i in terms of the eigenvalues of the one matrix, λ_i, we obtain

$$2\gamma_1 = \lambda_1+\lambda_2+\lambda_3-1$$

$$2\gamma_2 = \lambda_1+\lambda_4+\lambda_5-1$$

$$2\gamma_3 = \lambda_1+\lambda_6+\lambda_7-1$$

$$2\gamma_4 = \lambda_2+\lambda_4+\lambda_6-1$$

$$2\gamma_5 = \lambda_2+\lambda_5+\lambda_7-1$$

$$2\gamma_6 = \lambda_3+\lambda_4+\lambda_7-1$$

$$2\gamma_7 = \lambda_3+\lambda_5+\lambda_6-1.$$

For the γ_i to be non-negative there are seven relations which the eigenvalues must satisfy. By insisting that the eigenvalues are ordered $\lambda_i \geqslant \lambda_{i+1}$ three of these relations are automatically obeyed when the other four are satisfied, and therefore only the following four relations are independent

$$\lambda_1+\lambda_6+\lambda_7 \geqslant 1 \qquad (16a)$$

$$\lambda_2+\lambda_5+\lambda_7 \geqslant 1 \qquad (16b)$$

$$\lambda_3+\lambda_4+\lambda_7 \geqslant 1 \qquad (16c)$$

$$\lambda_3+\lambda_5+\lambda_6 \geqslant 1. \qquad (16d)$$

When taken together with the condition

$$0 \leqslant \lambda_i \leqslant 1 \qquad (16e)$$

and

$$\sum \lambda_i = 3 \qquad (16f)$$

it is clear that conditions (16) are sufficient for N-representability in the $N = 3, M = 7$ case.

In an exactly analogous way the following sufficient conditions can be obtained for the $N = 4$, $M = 7$ case

$$\lambda_1+\lambda_2+\lambda_7 \leqslant 2 \tag{17a}$$

$$\lambda_1+\lambda_3+\lambda_6 \leqslant 2 \tag{17b}$$

$$\lambda_1+\lambda_4+\lambda_5 \leqslant 2 \tag{17c}$$

$$\lambda_2+\lambda_3+\lambda_5 \leqslant 2 \tag{17d}$$

$$0 \leqslant \lambda_i \leqslant 1 \tag{17e}$$

$$\sum \lambda_i = 4. \tag{17f}$$

4.2. $N = 4$, $M = 8$

Consider a wavefunction consisting of the 14 normalized determinants whose coefficients are A_{1234}, A_{1256}, A_{1357}, A_{1467}, A_{2367}, A_{2457}, A_{3456}, A_{5678}, A_{3478}, A_{2468}, A_{2358}, A_{1458}, A_{1368} and A_{1278}. We define the numbers θ_i and ϕ_i, $i = 1, \ldots, 7$, by $\theta_1 = |A_{1234}|^2$ etc, $\phi_1 = |A_{5678}|^2$ etc and normalization demands that

$$\sum_{i=1}^{7} (\theta_i+\phi_i) = 1. \tag{18}$$

The density matrix of this wavefunction is diagonal and using equation (18) its eigenvalues can be related to the coefficients by the matrix equation

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \\ \lambda_7 \\ \lambda_8 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ -1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\ -1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 \\ -1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} \theta_1-\phi_1 \\ \theta_2-\phi_2 \\ \theta_3-\phi_3 \\ \theta_4-\phi_4 \\ \theta_5-\phi_5 \\ \theta_6-\phi_6 \\ \theta_7-\phi_7 \\ 1 \end{pmatrix} \tag{19}$$

We can now invert equation (19) and obtain

$$\begin{pmatrix} \theta_1-\phi_1 \\ \theta_2-\phi_2 \\ \theta_3-\phi_3 \\ \theta_4-\phi_4 \\ \theta_5-\phi_5 \\ \theta_6-\phi_6 \\ \theta_7-\phi_7 \\ 1 \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & 1 & -1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 & -1 & 1 & -1 \\ -1 & -1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \\ \lambda_6 \\ \lambda_7 \\ \lambda_8 \end{pmatrix}. \tag{20}$$

It can be seen that for equation (20) to be consistent the eigenvalues must be normalized correctly $\Sigma\lambda_i = 4$.

Consider now the problem of sufficiency. Given a set of λ_i, under what conditions can we determine a set of the θ_i and ϕ_i that give rise to them?

From the given normalized λ_i we can use equation (20) to solve for the entities $\theta_i - \phi_i$. We can satisfy the condition that θ_i and ϕ_i are non-negative by choosing either ϕ_i or θ_i to be zero according to whether $\theta_i - \phi_i$ is greater than or less than zero. We have now obtained a set of θ_i and ϕ_i which will satisfy equations (19) and (20). However, equation (19) is a valid equation for the eigenvalues only if the normalization condition (18) is obeyed and we have not, as yet, imposed this condition on the coefficients. If $\Sigma_{i=1}^{7}(\theta_i+\phi_i) < 1$, where at least seven of these coefficients are zero as assigned above, then we are free to increase any pair of coefficients θ_i and ϕ_i simultaneously by the same amount until the normalization (18) is correct. Both equations (19) and (20) will still be consistent. If, however, $\Sigma_{i=1}^{7}(\theta_i+\phi_i) > 1$ then we cannot determine a set of θ_i and ϕ_i obeying normalization and also yielding the correct density matrix. This implies a sufficient condition which the λ_i must obey. The condition is

$$|x_1|+|x_2|+|x_3|+|x_4|+|x_5|+|x_6|+|x_7| \leqslant 4 \tag{21}$$

where

$$\begin{aligned}
x_1 &= \lambda_1+\lambda_2+\lambda_3+\lambda_4-\lambda_5-\lambda_6-\lambda_7-\lambda_8\\
x_2 &= \lambda_1+\lambda_2+\lambda_5+\lambda_6-\lambda_3-\lambda_4-\lambda_7-\lambda_8\\
x_3 &= \lambda_1+\lambda_3+\lambda_5+\lambda_7-\lambda_2-\lambda_4-\lambda_6-\lambda_8\\
x_4 &= \lambda_1+\lambda_4+\lambda_6+\lambda_7-\lambda_2-\lambda_3-\lambda_5-\lambda_8\\
x_5 &= \lambda_2+\lambda_3+\lambda_6+\lambda_7-\lambda_1-\lambda_4-\lambda_5-\lambda_8\\
x_6 &= \lambda_2+\lambda_4+\lambda_5+\lambda_7-\lambda_1-\lambda_3-\lambda_6-\lambda_8\\
x_7 &= \lambda_3+\lambda_4+\lambda_5+\lambda_6-\lambda_1-\lambda_2-\lambda_7-\lambda_8.
\end{aligned}$$

This condition supplemented with the conditions $0 \leqslant \lambda_i \leqslant 1$ and $\Sigma\lambda_i = 4$ is sufficient to ensure that a four-body wavefunction may be found which corresponds to a given density matrix of rank 8.

From these conditions we can obtain sufficient conditions for the $N = 4$, $M = 7$ case by putting $\lambda_8 = 0$. The conditions are

$$0 \leqslant \lambda_i \leqslant 1 \tag{22a}$$

$$\sum \lambda_i = 4 \tag{22b}$$

and

$$|y_1|+|y_2|+|y_3|+|y_4|+|y_5|+|y_6|+|y_7| \leqslant 4 \tag{22c}$$

where

$$\begin{aligned}
y_1 &= \lambda_1+\lambda_2+\lambda_3+\lambda_4-\lambda_5-\lambda_6-\lambda_7\\
y_2 &= \lambda_1+\lambda_2+\lambda_5+\lambda_6-\lambda_3-\lambda_4-\lambda_7\\
y_3 &= \lambda_1+\lambda_3+\lambda_5+\lambda_7-\lambda_2-\lambda_4-\lambda_6\\
y_4 &= \lambda_1+\lambda_4+\lambda_6+\lambda_7-\lambda_2-\lambda_3-\lambda_5
\end{aligned}$$

$$y_5 = \lambda_2+\lambda_3+\lambda_6+\lambda_7-\lambda_1-\lambda_4-\lambda_5$$
$$y_6 = \lambda_2+\lambda_4+\lambda_5+\lambda_7-\lambda_1-\lambda_3-\lambda_6$$
$$y_7 = \lambda_3+\lambda_4+\lambda_5+\lambda_6-\lambda_1-\lambda_2-\lambda_7.$$

It is possible to show that the inequality in equation (22*c*) is unnecessary; the expression must be equal to 4. It can also be demonstrated that these conditions (22) are equivalent to the conditions (17) already given.

For each of the above three cases it is to be noted that the relations obtained reduce correctly to the relations for a lower rank if $\lambda_M = 0$. For example $N = 4$, $M = 7$ conditions give $N = 4$, $M = 6$ conditions if $\lambda_7 = 0$.

Being unable to find an analytical proof that the sufficient conditions obtained above are also necessary, we decided to investigate this possibility numerically.

For each inequality we varied the wavefunction so as to minimize (maximize) the relevant eigenvalue expression, in an attempt to violate the inequality. However each minimum (maximum) obtained was as expected. For example in the $N = 3, M = 7$ case, the minimum of $\lambda_1+\lambda_6+\lambda_7$ was found to be one. We used different starting wavefunctions as well as two different minimization techniques for each inequality.

As a result of these numerical investigations we are led to believe that the sufficient conditions we have obtained are also necessary, and hence constitute a solution of the N-representability problem for the cases $N = 3$, $M = 7$; $N = 4$, $M = 7$ and $N = 4$, $M = 8$. The slight vestige of doubt that exists arises because the numerical minimization techniques cannot guarantee that a minimum obtained is the global minimum for the problem and not just a local minimum. For this reason and also for insight into more complicated cases it would be desirable to confirm these results analytically.

In a recent paper (Peltzer and Brandstatter 1971) a complete solution to the N-representability problem for one-body density matrices was presented (excluding the case $N = 3$, $M = 6$). It was claimed that for $N \geqslant 4$ and rank $M \geqslant N+3$ or for $N = 3$ and rank $M \geqslant N+4$, then every one-body density matrix is N-representable when each of its eigenvalues is strictly less than one and their sum is equal to N (using our normalization). Clearly if this solution is correct then the conditions we have presented in this paper are not necessary. For example, in the case $N = 3$, $M = 7$, a set of eigenvalues can be chosen which satisfy the Peltzer and Brandstatter conditions for N-representability but do not satisfy the condition $\lambda_1+\lambda_6+\lambda_7 \geqslant 1$, which our numerical studies have indicated is necessary. We therefore conclude that Peltzer and Brandstatter must be in error.

4.3. $N = 3$, $M = 8$

Using the minimization techniques mentioned above we have made a numerical investigation of this case. The results obtained indicated that the following are some of the necessary conditions.

$$\lambda_1+\lambda_6+\lambda_7+\lambda_8 \geqslant 1$$
$$\lambda_2+\lambda_5+\lambda_7+\lambda_8 \geqslant 1$$
$$\lambda_3+\lambda_4+\lambda_7+\lambda_8 \geqslant 1$$
$$\lambda_3+\lambda_5+\lambda_6+\lambda_8 \geqslant 1$$
$$\lambda_2+\lambda_4+\lambda_6 \geqslant 1.$$

There appears to be a discontinuity in the nature of the N-representability problem in going from the $N = 3, M = 7$ case to the $N = 3, M = 8$ case. One cannot for example take the seven configurations which are sufficient for the $M = 7$ case and add to them another configuration containing the 8th orbital in such a way that the one-matrix is automatically diagonal. It is possible on the other hand to generate a different set of eight configurations in the $M = 8$ case which do give rise to a diagonal one-matrix. But in this case the wavefunction only contains five configurations when $\lambda_8 = 0$. Consequently the conditions do not break down correctly into the $M = 7$ conditions. It is therefore to be expected that an understanding of the $N = 3$, $M = 8$ case, when it is obtained, should shed new light on the nature of the N-representability problem for the one-matrix.

5. Summary

We have solved the N-representability problem for the case $N = 3$, $M = 6$ and demonstrated explicitly the reduction of information possible using density matrices rather than wavefunctions.

We have good reason to believe that we have also found the necessary and sufficient conditions for the cases $N = 3$, $M = 7$; $N = 4$, $M = 7$; and $N = 4$, $M = 8$. The conditions are rigorously sufficient and extensive numerical work has provided strong evidence that they are necessary.

By the Carlson–Keller theorem (Carlson and Keller 1961) we know that the eigenvalues of the two-body reduced density matrix are identical to those of the one-body matrix for a three-particle system. Consequently the results in this paper also contribute in a small way towards an understanding of the N-representability problem for the two-body matrix.

The full set of conditions in the $N = 3, M = 8$ case is still obscure. We have reported some apparently necessary conditions in this paper. In addition we have accumulated more detailed numerical results on this case which are too disjointed to publish here. Certain conditions that one might be tempted to conjecture to be necessary are disproved by these results; we would be happy to supply details on request.

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