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FAST TRACK COMMUNICATION

Connecting N-representability to Weyl's problem: the one-particle density matrix for $N = 3$ and $R = 6$*

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Abstract
An analytic proof of the necessity of the Borland–Dennis conditions for 3-representability of a one-particle density matrix with rank 6 is given. This may shed some light on Klyachko's recent use of Schubert calculus to find general conditions for N-representability.

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1. Introduction

The recent announcement by Klyachko [8] of the solution of the pure state N-representability problem [3] for fermionic one-particle density matrix observes that this is the first new result since the work of Borland and Dennis [2] in the early 1970s. There may therefore be some historical value in unpublished work of the author from that time, which makes a connection between the Borland–Dennis conditions and Weyl's problem [11]. The latter asks for conditions on sequences $\{a_k\}$, $\{b_k\}$, $\{c_k\}$ which ensure that there exist self-adjoint matrices A, B, C with eigenvalues a_k, b_k, c_k, respectively, such that $A + B = C$. The first complete solution to Weyl's problem was given by Klyachko [7] in 1998.

Let γ be a density matrix normalized so that $\operatorname{tr}\gamma = N$. The pure state N-representability problem for fermions asks for necessary and sufficient conditions on γ for the existence of an antisymmetric N-particle state whose one-particle reduced density matrix is γ. Let R denote the rank of γ. For the case $N = 3$ and $R = 6$, Borland and Dennis [2] gave a pair of conditions on the eigenvalues λ_k of γ which can be written as follows under the assumption that they are arranged in non-increasing order:

$$\lambda_1 + \lambda_6 = 1, \qquad \lambda_2 + \lambda_5 = 1, \qquad \lambda_3 + \lambda_4 = 1 \tag{1}$$

$$\lambda_1 + \lambda_2 \leqslant \lambda_3 + 1. \tag{2}$$

Note that (1) can be written compactly as $\lambda_k + \lambda_{7-k} = 1$ for $k = 1, 2, 3$.

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Borland and Dennis [2] proposed their conditions on the basis of numerical studies and gave a proof of (2) under an assumption, which is equivalent to (1), about the pre-image of γ. In this communication, we show that (1) is a necessary condition for N-representability when $N = 3$ and $R = 6$, completing the analytic proof of Borland and Dennis. We begin with some background material in section 2. In section 3, we present a proof of the necessity of (1). In section 4 we give a different, independent proof of the necessity of the inequality (2) from Weyl's inequalities. For completeness, we include a proof of sufficiency of (1) and (2) in section 5. In sections 6 and 7, we present some partial results for the cases $N = 3$ and $R = N+3$ in the hope of providing some intuition behind the success of Klyachko's approach to a full solution.

2. Notation and background

In this communication, we write the eigenvectors of γ as $|\phi_k\rangle$ so that

$$\gamma = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|. \tag{3}$$

We will let $\mathcal{A}$ denote the anti-symmetrization operator and use the notation $[f_j, f_k, f_\ell] = \mathcal{A} f_j(x_1) f_k(x_2) f_\ell(x_3)$ to denote a Slater determinant. The notation $\langle , \rangle_m$ indicates a partial inner product on a tensor product of Hilbert spaces.

We need some results from section 10 of Coleman's fundamental paper [3]. The first is theorem 10.6 in [3].

Lemma 1 (Coleman)**.** *The one-particle density matrix γ is N-representable with pre-image $|\Psi\rangle = \sqrt{\lambda_1}\mathcal{A}|\phi_1\rangle \otimes |\Phi_1\rangle + \sqrt{1-\lambda_1}|\Phi_2\rangle$ if and only if it can be written in the form*

$$\gamma = \lambda_1 |\phi_1\rangle\langle\phi_1| + \lambda_1\gamma_1 + (1-\lambda_1)\gamma_2 \tag{4}$$

where γ_1 is the $(N-1)$-representable reduced density matrix of $|\Phi_1\rangle$ and γ_2 is N-representable with pre-image Φ_2 satisfying

$$\langle\phi_1, \Phi_2\rangle_1 = \langle\Phi_1, \Phi_2\rangle_{2,3,\ldots,N} = 0. \tag{5}$$

The next two results are theorems 10.2 and 10.4, respectively, in [3]. (See also [10].)

Theorem 2. *A one-particle density matrix γ is 2-representable if and only if all non-zero eigenvalues are doubly degenerate. If there are no other degeneracies and the eigenvalues are written in non-increasing order so that $\lambda_{2k-1} = \lambda_{2k} > \lambda_{2k+1}$, then the pre-image of γ must have the form*

$$|\Psi\rangle = \sum_k e^{i\theta_k}\sqrt{\lambda_{2k}}[\phi_{2k-1}, \phi_{2k}]. \tag{6}$$

Theorem 3. *When $N = 2n+1$ is odd and the one-particle density matrix γ has rank $R = N+2$, it is N-representable if and only if $\lambda_1 = 1$ and the remaining eigenvalues are doubly degenerate.*

3. Necessity of the condition $\lambda_k + \lambda_{7-k} = 1$

To show that (1) is a necessary condition for 3-representability when $R = 6$, observe that since $\lambda_1 = \langle\phi_1, \gamma\phi_1\rangle$ it follows from (4) that

$$\langle\phi_1, \gamma_1\phi_1\rangle = \langle\phi_1, \gamma_2\phi_1\rangle = 0.$$

Therefore, γ_1 and γ_2 have rank $\leqslant 5$. It then follows from theorem 3 that one can write

$$\gamma_2 = |g_1\rangle\langle g_1| + |a|^2|g_2\rangle\langle g_2| + |a|^2|g_3\rangle\langle g_3| + |b|^2|g_4\rangle\langle g_4| + |b|^2|g_5\rangle\langle g_5|$$

with $|a|^2 + |b|^2 = 1$ and $|\Phi_2\rangle = a[g_1, g_2, g_3] + b[g_1, g_4, g_5]$. There is no loss of generality in writing $\Phi_1 = \sum_{j<k} c_{jk}[g_j, g_k]$.

We first consider the case in which both $a, b \neq 0$. Then a simple computation shows that (5) implies

$$|\Phi_1\rangle = c_{24}[g_2, g_4] + c_{25}[g_2, g_5] + c_{34}[g_3, g_4] + c_{35}[g_3, g_5]$$

so that $\langle g_1, \Phi_1\rangle_1 = 0$. Defining $|\phi_6\rangle = |g_1\rangle$, gives $\lambda_6 = 1 - \lambda_1$ and one can rewrite (4) as

$$\gamma = \lambda_1|\phi_1\rangle\langle\phi_1| + (1-\lambda_1)|\phi_6\rangle\langle\phi_6| + \lambda_1\gamma_1 + (1-\lambda_1)\widetilde{\gamma}_2 \qquad (7)$$

where $\widetilde{\gamma}_2 = \gamma_2 - |g_1\rangle\langle g_1|$ is the reduced density matrix of $|G_1\rangle = \langle g_1, \Phi_2\rangle_3 = a[g_2, g_3] + b[g_4, g_5]$. Thus, in the orthonormal basis $\{g_2, g_3, g_4, g_5\}$ we find

$$\gamma_1 = \begin{pmatrix} |c_{24}|^2 + |c_{25}|^2 & \bar{c}_{24}c_{34} + \bar{c}_{25}c_{35} & 0 & 0 \\ c_{24}\bar{c}_{34} + c_{25}\bar{c}_{35} & |c_{34}|^2 + |c_{35}|^2 & 0 & 0 \\ 0 & 0 & |c_{24}|^2 + |c_{34}|^2 & \bar{c}_{24}c_{25} + \bar{c}_{34}c_{35} \\ 0 & 0 & c_{24}\bar{c}_{25} + c_{34}\bar{c}_{35} & |c_{25}|^2 + |c_{35}|^2 \end{pmatrix}.$$

The key point is that γ_1 is block diagonal and can be diagonalized by a block diagonal unitary transformation which mixes only within pairs g_2, g_3 and g_4, g_5 leaving the Slater determinants in G_1 unaffected (except possibly for a phase factor which can be absorbed into the new basis). Denoting the new basis as ϕ_k, we now have $|G_1\rangle = a[\phi_2, \phi_3] + b[\phi_4, \phi_5]$. Then either by explicit computation or from Coleman's proof [4] of theorem 2, one can write $|\Phi_1\rangle = s[\phi_2, \phi_4] + t[\phi_3, \phi_5]$ with $|s|^2 + |t|^2 = 1$. Thus, the eigenvalues of γ satisfy

$$\lambda_2 = \lambda_1|a|^2 + (1-\lambda_1)|s|^2 \qquad (8a)$$

$$\lambda_3 = \lambda_1|b|^2 + (1-\lambda_1)|s|^2 \qquad (8b)$$

$$\lambda_4 = \lambda_1|a|^2 + (1-\lambda_1)|t|^2 \qquad (8c)$$

$$\lambda_5 = \lambda_1|b|^2 + (1-\lambda_1)|t|^2 \qquad (8d)$$

which implies

$$\lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = \lambda_1 + (1-\lambda_1) = 1. \qquad (9)$$

We now consider the possibility that one of a, b is zero, in which case $|\Phi_2\rangle$ is a single Slater determinant and there is no loss of generality in writing $\Phi_2 = [g_1, g_2, g_3]$. Then, (5) implies that one can write

$$|\Phi_1\rangle = \sum_{j=1,2,3}\sum_{k=4,5} x_{jk}[g_j, g_k] + c[g_4, g_5]. \qquad (10)$$

Now regard x_{jk} as a 3×2 matrix and observe when U, V are 3×3 and 2×2 unitary matrices, $Y = UXV^\dagger$ corresponds to a basis change which mixes g_1, g_2, g_3 and g_4, g_5 among themselves. By the singular value decomposition we can find U, V such that only y_{24} and y_{35} are non-zero. Thus, in the new basis which we call ϕ_k

$$|\Phi_1\rangle = y_{24}[\phi_2, \phi_4] + y_{35}[\phi_3, \phi_5] + c[\phi_4, \phi_5]. \qquad (11)$$

Again writing $\phi_6 = g_1$, we find that the pre-image of γ has the form

$$|\Psi\rangle = a_{123}[\phi_1, \phi_2, \phi_3] + a_{246}[\phi_2, \phi_4, \phi_6] + a_{356}[\phi_3, \phi_5, \phi_6] + a_{456}[\phi_4, \phi_5, \phi_6] \qquad (12)$$

which implies (1).

4. Necessity of the inequality (2)

We now prove that the inequality (2) is necessary for N-representability. When γ has the form (3) and (1) holds, its pre-image can be written in the form

$$|\Psi\rangle = x_{000}[\phi_1,\phi_2,\phi_3] + x_{001}[\phi_1,\phi_2,\phi_4] + x_{010}[\phi_1,\phi_5,\phi_3] + x_{011}[\phi_1,\phi_5,\phi_4] + x_{100}[\phi_6,\phi_2,\phi_3] + x_{101}[\phi_6,\phi_2,\phi_4] + x_{110}[\phi_6,\phi_5,\phi_3] + x_{111}[\phi_6,\phi_5,\phi_4]. \qquad (13)$$

In this form, there is no loss of generality in assuming that λ_k are arranged in non-increasing order. If we now define

$$S = \begin{pmatrix} x_{000} & x_{001} \\ x_{010} & x_{011} \end{pmatrix} \qquad T = \begin{pmatrix} x_{100} & x_{101} \\ x_{110} & x_{111} \end{pmatrix} \qquad (14)$$

then the reduced density matrix of $|\Psi\rangle$ is (up to a permutation) $W_1 \oplus W_2 \oplus W_3$ with

$$W_1 = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_6 \end{pmatrix} = \begin{pmatrix} \operatorname{tr} SS^\dagger & \operatorname{tr} ST^\dagger \\ \operatorname{tr} TS^\dagger & \operatorname{tr} TT^\dagger \end{pmatrix} \qquad (15)$$

$$W_2 = \begin{pmatrix} \lambda_2 & 0 \\ 0 & \lambda_5 \end{pmatrix} = SS^\dagger + TT^\dagger \qquad (16)$$

$$W_3 = \begin{pmatrix} \lambda_3 & 0 \\ 0 & \lambda_4 \end{pmatrix} = S^\dagger S + T^\dagger T. \qquad (17)$$

It follows from (15) that the eigenvalues of $SS^\dagger$, which are the same as those of $S^\dagger S$, can be written as $\sigma, \lambda_1 - \sigma$ with $0 \leqslant \sigma \leqslant \lambda_1$; similarly those of $TT^\dagger$ and $T^\dagger T$ can be written as $\tau, \lambda_6 - \tau$ with $0 \leqslant \tau \leqslant \lambda_6$.

The form of (16) and (17) is suggestive of Weyl's problem with $A = SS^\dagger$, $B = TT^\dagger$, $C = W_2$ in the case of (16) and adjoints reversed for (17). Weyl [6, 11] used the max–min principle to find necessary conditions

$$a_1 + b_1 \geqslant c_1, \qquad a_2 + b_1 \geqslant c_2, \qquad a_1 + b_2 \geqslant c_2 \qquad (18)$$

(with all three sequences in non-increasing order). For 2×2 matrices satisfying $\operatorname{tr} A + \operatorname{tr} B = \operatorname{tr} C$, these are also sufficient. We apply Weyl's inequalities to (16) and (17) and retain the stronger in each pair to obtain

$$\sigma + \tau \geqslant \lambda_2 \qquad (19a)$$

$$\lambda_1 - \sigma + \tau \geqslant \lambda_4 \qquad (19b)$$

$$\sigma + \lambda_6 - \tau \geqslant \lambda_4. \qquad (19c)$$

Adding together the first two inequalities implies

$$2\tau \geqslant \lambda_2 + \lambda_4 - \lambda_1. \qquad (20)$$

Combining this with $2\lambda_6 \geqslant 2\tau$ and using (1) gives

$$2(1 - \lambda_1) = 2\lambda_6 \geqslant \lambda_2 + 1 - \lambda_3 - \lambda_1 \qquad (21)$$

which is equivalent to (2).

5. Sufficiency

To prove sufficiency, it suffices to consider a pre-image of the form

$$\Psi = \hat{a}[\phi_1, \phi_2, \phi_3] + \hat{b}[\phi_1, \phi_4, \phi_5] + \hat{s}[\phi_6, \phi_2, \phi_4] + \hat{t}[\phi_6, \phi_5, \phi_3] \tag{22}$$

and observe that its first-order reduced density matrix is diagonal in the basis ϕ_k with

$$|\hat{a}|^2 + |\hat{b}|^2 = \lambda_1 \qquad |\hat{s}|^2 + |\hat{t}|^2 = \lambda_6.$$

Under the assumption that (1) holds, the linear relation between the eigenvalues of γ and $|\hat{a}|^2, |\hat{b}|^2, |\hat{s}|^2, |\hat{t}|^2$ can be inverted to yield

$$|\hat{a}|^2 = \tfrac{1}{2}(\lambda_2 + \lambda_3 - \lambda_6) \qquad |\hat{b}|^2 = \tfrac{1}{2}(\lambda_1 - \lambda_2 + \lambda_4) \tag{23a}$$

$$|\hat{s}|^2 = \tfrac{1}{2}(\lambda_2 - \lambda_3 + \lambda_6) \qquad |\hat{t}|^2 = \tfrac{1}{2}(\lambda_6 - \lambda_2 + \lambda_3). \tag{23b}$$

With the ordering convention $\lambda_k \geqslant \lambda_{k+1}$, the expressions for $|\hat{a}|^2$, $|\hat{b}|^2$ and $|\hat{s}|^2$ are all positive; and $|\hat{t}|^2 \geqslant 0$ is equivalent to (2).

In section 3, we showed slightly more than that (1) holds. We also showed that the pre-image can always be written in a form in which only four of the coefficients in (13) are non-zero. However, neither of these forms is equivalent to (22) with λ_k decreasing. The equations for the coefficients in one of those forms might have solutions only when a stronger inequality than (2) holds. In particular, the form obtained from (7) in the paragraph before (8) has solutions only when $\lambda_1 + \lambda_2 \leqslant \lambda_4 + 1$.

6. General $R = N + 3$ with N odd

It is tempting to try to extend the argument in section 3 to the general case of $R = N+3$ when N is odd. Using (4) we can conclude as before that γ_2 must be N-representable with $R = N+2$ and thus has an eigenvector $|g_1\rangle$ with eigenvalue 1. We can write its pre-image as

$$\begin{aligned}|\Phi_2\rangle = a_m[g_1, g_2, g_3, \ldots, g_{N-1}, g_N] + \cdots + a_k[g_1, g_2, g_3, \ldots, g_{2k-1}g_{2k+2}, \ldots, g_{N-1}, g_N] \\ + \cdots + a_1[g_1, g_4, g_4, \ldots, g_{N+1}, g_{N+2}]\end{aligned} \tag{24}$$

where $m = \frac{1}{2}(N+1)$ and a_k is the coefficient of the Slater determinant which does *not* contain g_{2k} or g_{2k+1}. However, it is not evident that the strong orthogonality condition $\langle g_1, \Phi_1\rangle_1 = 0$ holds as was the case for $N = 3$. If we knew that

$$\lambda_1 + \langle g_1, \gamma g_1\rangle \leqslant 1, \tag{25}$$

strong orthogonality would follow, and we could again conclude that g_1 is an eigenvector of γ with eigenvalue $\langle g_1, \gamma g_1\rangle = 1 - \lambda_1$. However, we can only show that the assumption of strong orthogonality implies (25) with equality.

Proposition 4. *Let $R = N+3$ with N odd and consider the decomposition (4) of a one-particle density matrix γ under the assumption that λ_1 is the largest eigenvalue. Then $|\Phi_2\rangle$ has an eigenvector $|g_1\rangle$ with eigenvalue 1. If $\langle g_1, \Phi_1\rangle_1 = 0$, then $|g_1\rangle$ is an eigenvector of γ with eigenvalue $1 - \lambda_1$ and this is the smallest eigenvalue of γ.*

Proof. Let $|\phi_k\rangle$ denote an eigenvector of γ orthogonal to both $|\phi_1\rangle$ and $|g_1\rangle$ and write

$$|\Phi_1\rangle = a\mathcal{A}|\phi_k \otimes \chi_1\rangle + \sqrt{1 - a^2}|\psi_1\rangle$$
$$|\Phi_2\rangle = b\mathcal{A}|g_1 \otimes \phi_k \otimes \chi_2\rangle + \sqrt{1 - b^2}\mathcal{A}|g_1 \otimes \psi_2\rangle,$$

where we have absorbed any phases into ψ_j. Then $\lambda_k = \lambda_1 a^2 + (1-\lambda_1)b^2$. Since each $|\psi_j\rangle$ is strongly orthogonal to $|\phi_1\rangle, |g_1\rangle$ and $|\phi_k\rangle$, each $|\psi_j\rangle$ is an $(N-1)$-particle function with one rank at most N. It is well known [3, 5, 10] that this implies that $|\psi_j\rangle$ is a single Slater determinant. Since both $|\psi_1\rangle$ and $|\psi_2\rangle$ have one-particle density matrices in the same N-dimensional subspace, it follows that the ranges of these one-particle density matrices have a non-zero intersection. Let $|f\rangle$ be in this intersection. Then

$$\langle f, \gamma f\rangle = (1-a^2)\lambda_1 + (1-b^2)(1-\lambda_1) = 1 - \lambda_k. \tag{26}$$

Thus, if $\lambda_k < 1 - \lambda_1$, then $\langle f, \gamma f\rangle > \lambda_1$ contradicting the assumption that λ_1 is the largest eigenvalue. □

If the strong orthogonality assumption does not hold then (4) and (24) imply that $\lambda_1 + \langle g_1, \gamma g_1\rangle \geqslant 1$ which is the reverse of (25) and implies that $\lambda_1 + \lambda_k \geqslant 1$, for some $k \neq 1$. Altunbulak and Klyachko [1] have proved the stronger result that

$$\lambda_1 + \lambda_R \geqslant 1 \tag{27}$$

in this situation. Actually, they proved an equivalent dual condition, i.e., when $N = 3$ and R is even $\lambda_1 + \lambda_R \leqslant 1$. A condition of the form $\lambda_j + \lambda_{j'} \leqslant 1$ is sometimes called a 'strong Pauli condition'; for $N = 3$ and R even Altunbulak and Klyachko have shown the strong Pauli condition $\lambda_{1+k} + \lambda_{r-k} \leqslant 1$; combining this with the fact that particle–hole duality yields the reverse inequality, gives another proof of the necessity of (1) in the case $N = 3$, $R = 6$. The following conjecture would imply that *both* the strong Pauli condition and (27) hold. Although that might be too much too expect, it would be interesting to know under what circumstances it is valid.

Conjecture 5. *When N is odd and $R = N + 3$, a necessary condition for pure state N-representability of a one-particle density matrix is $\lambda_1 + \lambda_R = 1$, where we have assumed that the eigenvalues are in non-increasing order.*

7. Further connections with Weyl's problem

Now assume that g_1 is strongly orthogonal to Φ_1 and, as in (7), write

$$\gamma = \lambda_1|\phi_1\rangle\langle\phi_1| + (1-\lambda_1)|g_1\rangle\langle g_1| + \lambda_1\gamma_1 + (1-\lambda_1)\widetilde{\gamma}_2. \tag{28}$$

The N-representability problem in this situation is reduced to finding conditions which ensure that a density matrix is a convex combination of two $(N-1)$-representable density matrices of rank $N+1$ which satisfy an additional orthogonality constraint. Write

$$|\Phi_1\rangle = \sum_{k_1<k_2<\cdots k_{N-1}} x_{k_1k_2\ldots k_{N-1}}[g_1, g_2, \ldots, g_{N-1}]$$

$$|\Phi_2\rangle = \sum_{k_1<k_2<\cdots k_{N-1}} y_{k_1k_2\ldots k_{N-1}}.[g_1, g_2, \ldots, g_{N-1}].$$

Let X, Y be the corresponding anti-symmetric tensors, and let

$$XY^\dagger = \sum_{k_2,k_3,\ldots,k_M} x_{k_1,k_2,\ldots,k_M}\overline{y}_{k_1,k_2,\ldots,k_M} \tag{29}$$

denote contraction over $k_2 \ldots k_M$. Then, we can rewrite (7) as

$$\gamma - \lambda_1|\phi_1\rangle\langle\phi_1| - (1-\lambda_1)|g_1\rangle\langle g_1| = XX^\dagger + YY^\dagger \tag{30}$$

with the constraint $\langle\Phi_1, \Phi_2\rangle = \operatorname{tr} XY^\dagger = 0$. This is a constrained version of Weyl's problem. If the $R = N+3$ problem could be solved in this way, then by particle–hole duality, we would also have the solution to the 3-representability problem. Although we do not know if strongly orthogonality of g_1 to Φ_1 holds in general, this viewpoint provides a connection to Weyl's problem that is more general than the situation for which it was used in section 4.

For general R (or for $R = N + 3$ without the simplification that leads to (7)), Coleman's lemma 1 gives a constrained version of Weyl's problem with $\gamma_1 = XX^\dagger$ and $\gamma_2 = YY^\dagger$. But now γ_1 is $(N-1)$-representable and γ_2 is N-representable and the orthogonality condition (5) must be translated to tensors of different sizes. Nevertheless, it now seems clear that what Coleman referred to as a double induction lemma was a constrained version of Weyl's problem. The solution to Weyl's problem was given less than 10 years ago, with more recent refinements [9]. Thus, it is not surprising that the pure state N-representability problem also resisted solution and that Klyachko succeeded by using powerful techniques associated with Schubert calculus to solve both problems.

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