SEARCHING FOR NEW CONDITIONS FOR FERMION $N$-REPRESENTABILITY

Hubert Grudziński
Department of Physics, Academy of Bydgoszcz, 85-072 Bydgoszcz, pl. Weyssenhoffa 11, Poland
(e-mail: hubertg@ab-byd.edu.pl)

Jacek Hirsch
Institute of Physics, Nicholas Copernicus University, 87-100 Toruń, Poland
(e-mail: jacekh@phys.uni.torun.pl)

Abstract

New elements of the dual cone of the set of fermion $N$-representable 2-density operators are proposed. So far, the explicit form of the corresponding necessary conditions for $N$-representability is obtained for $N = 3$. In this case the new condition is stronger than the known B- and C-conditions for 3-representability. The results provide evidence that in the spectral decomposition of the $N$-representable 2-density operator there exists an intrinsic relation between the eigenvalue and the corresponding eigenfunction.

keywords: fermion $N$-representability problem, conditions for $N$-representability

1. Introduction

The $N$-representability problem [1, 5, 13, 18, 19, 23, 25] appears in non-relativistic quantum mechanics of $N$-fermion systems. The Hamiltonian $H^N$ for systems of $N$-fermions contain only operators with 1- and 2-body interactions:

$$H^N = \sum_{i=1}^{N} H^1(i) + \sum_{1 \leq i < j \leq N} H^2(i, j) = \sum_{1 \leq i < j \leq N} h^2(i, j).$$
The ground state energy of the system can be determined variationally by minimizing the $N$-particle functional
\[ E = \inf_{D^N \in \mathcal{P}_N} Tr(H^N D^N) \]
over the set $\mathcal{P}_N$ consisting of all fermion $N$-particle density operators. Instead, because of the appearance of at most 2-body interactions between the particles, the ground state energy of the system of $N$-fermions could be, in principle, determined variationally by minimizing the 2-particle functional
\[ E = \inf_{D^2 \in \mathcal{P}_N^2} \left( \begin{array}{c} N \\ 2 \end{array} \right) Tr(h^2 D^2) \]
over the set $\mathcal{P}_N^2$ consisting of all fermion 2-particle reduced density operators, i.e. such 2-particle density operators $D^2$ which possess an $N$-particle fermion preimage $D^N$:
\[ D^2 = L_N^2 D^N = Tr_{3,...,N} D^N. \]

It is known [1, 19] that the set $\mathcal{P}_N^2$ is a proper convex subset of $\mathcal{P}_N$, the set of all fermion 2-density operators. However, the complete characterization of $\mathcal{P}_N^2$ as a convex proper subset of $\mathcal{P}_N$ is not yet known. It has been shown [19] that a knowledge of all exposed points (which are extreme) of $\mathcal{P}_N^2$ is sufficient to characterize the closure of $\mathcal{P}_N^2$; only some of them are known. The dual characterization of $\mathcal{P}_N^2$ involves a determination of the dual (polar) cone $\mathcal{P}_N^2$ consisting of 2-particle self-adjoint operators $b^2$ for which $Tr(b^2 D^2) \geq 0$, $\forall D^2 \in \mathcal{P}_N^2$, that is equivalent to the positive-semidefiniteness of the $N$-particle operator $\Gamma^N b^2 = b^2 \wedge I^{(N-2)} = A^N b^2 \otimes I^{(N-2)} A^N \geq 0$. The dual cone $\mathcal{P}_N^2$ is a convex one. Any element of the dual cone $\mathcal{P}_N^2$ provides an $N$-representability condition. Those coming from the extreme elements of $\mathcal{P}_N^2$ are the strongest ones. They give the hyperplane characterization of $\mathcal{P}_N^2$ and thus the solution of the $N$-representability problem. Several necessary conditions for $N$-representability have been derived and some of their structural features and mutual interrelations are established [2, 3, 6, 7, 8, 9, 10, 11, 13, 14, 15, 16, 17, 19, 20, 21, 22, 24, 26, 27].

In this paper we find new elements of the dual cone $\mathcal{P}_N^2$, and thus define new necessary conditions for $N$-representability of a trial 2-particle density matrix $D^2$. In the case $N=3$, in which the new elements of the dual cone are given explicitly, they lead to necessary conditions for 3-representability of the trial $D^2$ which are stronger in comparison with the known $B$ and
The conditions [3, 4, 21]. The results show that in the spectral decomposition of a 2-particle fermion density operator $D^2$ there exists an intimate relation between the eigenvalue and the corresponding eigenfunction which has to be satisfied in order that $D^2$ can be 3-representable (in general $N$-representable). More precisely, the condition obtained for 3-representability says that the upper bound of the eigenvalue of $D^2$ is a functional of the corresponding eigenfunction. It is worthwhile to remember that for $N$-representability of a 1-particle density matrix $D^1$ the upper bound on the eigenvalues does not depend on the eigenfunctions. This explains why the $N$-representability problem for $D^2$ is so much harder than for $D^1$.

2. The dual P-condition.

In this paper the underlying 1-particle Hilbert space $\mathcal{H}^1$ is finite dimensional $\dim \mathcal{H}^1 = n$. $\mathcal{H}^\wedge 2$ is a 2-particle antisymmetric Hilbert space, the Grassmann product $\mathcal{H}^1 \wedge \mathcal{H}^1 = \mathcal{A}^2 \mathcal{H}^1 \otimes \mathcal{H}^1$. $P_g^2 = g^2 \otimes g^2$ is the projection operator onto a 2-particle antisymmetric function $g^2 \in \mathcal{H}^\wedge 2$. The operator $\binom{2}{N} P_g^2 \wedge I^{\wedge (N-2)} = \binom{2}{N} A^N P_g^2 \otimes I^{\otimes (N-2)} A^N = A^N \sum_{1 \leq i < j \leq N} P_g^2(i,j) \otimes I^{N-2}(1, \ldots, i-1, i+1, \ldots, j-1, j+1, \ldots, N) A^N$ is the simplest (elementary) antisymmetric operator with "2-body interactions" acting on $\mathcal{H}^\wedge N$. Because $\binom{2}{N} P_g^2 \wedge I^{\wedge (N-2)}$ is positive-semidefinite, $P_g^2$ belongs to the dual cone $\mathcal{P}_N^2$, and therefore $Tr(D^2 P_g^2) \geq 0$ is a necessary condition for $N$-representability of $D^2$ (the P-condition). Besides, there exists another element of $\mathcal{P}_N^2$ that is generated by the 2-particle antisymmetric function $g^2 \in \mathcal{H}^\wedge 2$. Let $\Lambda_{\max}(g^2)$ denote the maximal eigenvalue of $\binom{2}{N} P_g^2 \wedge I^{\wedge (N-2)}$, which in general depends on $g^2$, then the operator $\Lambda_{\max}(g^2) I^{\wedge N} - \binom{2}{N} P_g^2 \wedge I^{\wedge (N-2)} \geq 0$ (is positive-semidefinite), and therefore the 2-particle operator $\frac{\Lambda_{\max}(g^2)}{\binom{2}{N}} I^{\wedge 2} - P_g^2$ belongs to the dual cone $\mathcal{P}_N^2$. Thus, we have obtained

**Theorem 2.1:** For any $g^2 \in \mathcal{H}^\wedge 2$ the operator

$$\frac{\Lambda_{\max}(g^2)}{\binom{2}{N}} I^{\wedge 2} - P_g^2 \in \mathcal{P}_N^2,$$

and gives the following necessary condition for $N$-representability of a 2-particle fermion density matrix $D^2$: $Tr[\frac{\Lambda_{\max}(g^2)}{\binom{2}{N}} I^{\wedge 2} - P_g^2]D^2] \geq 0$, i.e.

$$Tr(D^2 P_g^2) \leq \frac{\Lambda_{\max}(g^2)}{\binom{2}{N}}, \quad \forall g^2 \in \mathcal{H}^\wedge 2.$$
Here, $\Lambda_{\text{max}}(g^2)$ is the maximal eigenvalue of the operator $\left(\begin{array}{c} N \\ 2 \end{array}\right)P^2_g \wedge I^{\wedge (N-2)}$.

We propose to call the new condition "the dual P-condition".

In particular, from the above theorem follows

**Theorem 2.2:** If $D^2 = \sum_{i=1}^{(N\choose 2)} \lambda_i P^2_{g_i}$ is the spectral decomposition of $D^2$, then it is a necessary condition for $N$-representability that the eigenvalues $\lambda_i$ must satisfy the inequalities $\lambda_i \leq \frac{\Lambda_{\text{max}}(g^2_1)}{(N\choose 2)}$. Here, $\Lambda_{\text{max}}(g^2_1)$ is the maximal eigenvalue of the operator $\left(\begin{array}{c} N \\ 2 \end{array}\right)P^2_{g_1} \wedge I^{\wedge (N-2)}$, where $g^2_1$ is the eigenfunction corresponding to the eigenvalue $\lambda_i$.

This theorem shows that the bound on the eigenvalue is a functional of the corresponding eigenfunction. For the $N$-fermion 1-body elementary operator $NP^1_g \wedge I^{\wedge (N-1)}$, $g^1 \in \mathcal{H}^1$, the maximal eigenvalue $\Lambda_{\text{max}}(g^1) = 1$ for any $g^1$, because $NP^1_g \wedge I^{\wedge (N-1)}$ is a projection operator. Hence, the equivalent of Theorem 2.1 says that $Tr(D^1P^1_g) \leq \frac{1}{N}$ for arbitrary $g^1 \in \mathcal{H}^{\wedge 1}$, which in particular means that the bound on an eigenvalue of an $N$-representable 1-density operator does not depend on the corresponding eigenfunction, contrary to the 2-density matrix case.

As seen from Theorem 2.1, the new necessary condition for $N$-representability of a 2-particle density matrix $D^2$ requires knowledge of the maximal eigenvalue $\Lambda_{\text{max}}(g^2)$ of the $N$-particle operator $\left(\begin{array}{c} N \\ 2 \end{array}\right)P^2_g \wedge I^{\wedge (N-2)}$. It is rather hopeless to find $\Lambda_{\text{max}}(g^2)$ for arbitrary $N$ and any $g^2 \in \mathcal{H}^{\wedge 2}$. But even the solution for some "simple" $g^2$ would contribute to knowledge of the structure of both the dual cone $P^2_N$ and the set $P^2_N$ of fermion $N$-representable 2-density operators. So far, we have results for $N = 3$, in which case it was possible to find the spectral decomposition of the elementary operator $3P^2_g \wedge I^1$ for arbitrary $g^2 \in \mathcal{H}^{\wedge 2}$. The details and proofs concerning this spectral decomposition and the reduced 2- and 1-particle density operators corresponding to the eigenstates of the operator $3P^2_g \wedge I^1$ will be published in a separate paper. In this paper we use only the following result which we formulate as

**Theorem 2.3:** Let $\mathcal{H}^1$ be a finite dimensional Hilbert space (dim $\mathcal{H}^1 = n$), and $\mathcal{H}^{\wedge 2} = \mathcal{H}^1 \wedge \mathcal{H}^1$ denotes the 2-particle antisymmetric space generated by $\mathcal{H}^1$ (the 2-fold Grassmann product of $\mathcal{H}^1$). Let $P^2_g$ denote the 1-dimensional projection operator onto a 2-particle antisymmetric function $g^2 \in \mathcal{H}^{\wedge 2}$ of 1-rank $r = 2s$ possessing the canonical decomposition $g^2 = \sum_{i=1}^{s} \xi_i | 2i - 1, 2i \rangle = \sqrt{2} \phi_{2i-1} \wedge \phi_{2i} = \frac{1}{\sqrt{2}} \det(\phi_{2i-1}, \phi_{2i})$ is the 2-particle normalized Slater determinant. Let the identity operator
on $H^1$ possess the decomposition $I^1 = \sum_{i=1}^{r=2s} P_i^1 + \sum_{i=r+1}^{n} P_i^1$, where $P_i^1 = |i\rangle\langle i| = \phi^1_i \otimes \tilde{\phi}^1_i$ (i = 1, ..., n) are 1-dimensional mutually orthogonal projection operators onto the functions $|i\rangle = \phi^1_i$. Then, the 3-particle operator $3P_g^2 \wedge I^1$ possesses the following spectral decomposition

$$3P_g^2 \wedge I^1 = \sum_{k=1}^{s=r/2} (1 - |\xi_k|^2)(P_{g_{2k-1}}^3 + P_{g_{2k}}^3) + \sum_{l=r+1}^{n} P_{g_l}^3 + 0 \cdot \text{Ker}(3P_g^2 \wedge I^1).$$

Here, $P_{g_{2k-1}}^3, P_{g_{2k}}^3 (k = 1, ..., s = r/2), P_{g_l}^3 (l = r+1, ..., n)$ are 1-dim projectors onto the following functions:

$$g_{2k-1}^3 = \frac{1}{\sqrt{1 - |\xi_k|^2}} \sum_{i=1}^{s} \xi_i |2i-1, 2i, 2k-1\rangle = \sqrt{3} \frac{1}{1 - |\xi_k|^2} g^2 \wedge |2k-1\rangle,$$

$$g_{2k}^3 = \frac{1}{\sqrt{1 - |\xi_k|^2}} \sum_{i=1}^{s} \xi_i |2i-1, 2i, 2k\rangle = \sqrt{3} \frac{1}{1 - |\xi_k|^2} g^2 \wedge |2k\rangle,$$

$$g_l^3 = \sum_{i=1}^{s} \xi_i |2i-1, 2i, l\rangle = \sqrt{3} g^2 \wedge |l\rangle,$$

$\text{Ker}(3P_g^2 \wedge I^1)$ denotes the projection operator onto the null-space of the operator $3P_g^2 \wedge I^1$, which is of dimension $(n^3) - n$. The symbols of the type $|2i-1, 2i, 2k-1\rangle$ denote the appropriate 3-particle Slater determinants.

Now, we can apply results of Theorem 2.3 to find new necessary conditions for 3-representability according to the formulae of Theorems 2.1 and 2.2. The required $\Lambda_{\text{max}}(g^2)$ is either $1 - |\xi|^2_{min}$, if the 1-rank of $g^2$ is equal to the dimension $n$ of the 1-particle Hilbert space $H^1$ ($r = 2s = n$), or $\Lambda_{\text{max}}(g^2) = 1$, if $r$ is less than $n (r < n)$. Hence, we have

**Theorem 2.4:** If $D^2$ ($TrD^2 = 1$) is a 2-fermion density matrix, then for 3-representability it must satisfy for any $g^2 \in H^{\wedge 2}$, with the canonical decomposition $g^2 = \sum_{i=1}^{r/2} \xi_i |2i-1, 2i\rangle$, the following inequality:

$$Tr(D^2P_g^2) \leq \frac{1}{3}(1 - |\xi|^2_{min}),$$

(2.3)
if the 1-rank of \( g^2 \) equals \( n = \dim \mathcal{H}^1 (r = n) \),

\[
Tr(D^2 P_{g}^2) \leq \frac{1}{3},
\]

(2.4)

if the 1-rank \( r \) of \( g^2 \) is less than \( \dim \mathcal{H}^1 (r < n) \).

In particular, if we take as \( g^2 \) the eigenfunctions \( g^2_i \) of \( D^2 \), we get

**Theorem 2.5:** If \( D^2 \) has the spectral decomposition \( D^2 = \sum_{i=1}^{(n^2)} \lambda_i P^2_{g_i} \) with \( g^2_i = \sum_{j=1}^{\lambda_i} \xi_{ij} \mid 2j - 1, 2j \), then \( \lambda_i \leq \frac{1}{3}(1 - \mid \xi_{ij} \mid^2_{\min j}) \), if the eigenfunction \( g^2_i \) has 1-rank \( r_i = 2s_i = n \), and \( \lambda_i \leq \frac{1}{3} \), if the eigenfunction belonging to \( \lambda_i \) has 1-rank \( r_i < n = \dim \mathcal{H}^1 \).

It is worthwhile to observe that the eigenfunctions belonging to the maximal eigenvalue \( \lambda = \frac{1}{3} \) cannot have full 1-rank (\( r = n = \dim \mathcal{H}^1 \)) if \( D^2 \) is 3-representable, and on the other hand, the eigenvalues corresponding to the eigenfunctions with full 1-rank must be strictly less than \( \frac{1}{3} \).

3. **Strength of the dual P-condition for fermion 3-representability**

It is important to compare the new condition with the already known conditions for 3-representability because the effort to find \( \Lambda_{max}(g^2) \) for at least some \( g^2 \) in the general case (arbitrary \( N \)) might not pay off. Since the new condition is an estimation from the above on the expectation value of \( D^2 \) in any state \( g^2 \in \mathcal{H}^\wedge 2 \), it can be compared with the \( B \)- and \( C \)- conditions for \( N \)-representability of \( D^2 \) [2, 3, 21]:

\[
Tr[B_N^2(g^2)D^2] \geq 0, \quad Tr[C_N^2(g^2)D^2] \geq 0, \quad \forall g^2 \in \mathcal{H}^\wedge 2,
\]

(3.1)

where

\[
B_N^2(g^2) = I^\wedge 2 - (N - 2)L_2^1 P^2_g \wedge I^1 - (N - 1)P^2_g \in \tilde{\mathcal{P}}_N^2,
\]

\[
C_N^2(g^2) = (n - N + 2)L_2^1 P^2_g \wedge I^1 - (N - 1)P^2_g \in \tilde{\mathcal{P}}_N^2.
\]

In the case \( N = 3 \), conditions (3.1) take the form:

\[
Tr(D^2 P_{g}^2) \leq \frac{1}{2} [1 - Tr(L_2^1 D^2 L_2^1 P_{g}^2)], \quad \forall g^2 \in \mathcal{H}^\wedge 2
\]

(3.2)
\[ \text{Tr}(D^2P^2_g) \leq \frac{n-1}{2} \text{Tr}(L_2^1D^2L_1^1P^2_g), \quad \forall g^2 \in \mathcal{H}^{\wedge 2}. \quad (3.3) \]

In order to compare the inequalities (2.2), (3.2), (3.3), we choose as \( g^2 \) the so called "extreme geminal" [2] \( g^2_{\text{extr}} \) of 1-rank \( r=2s=n=\dim \mathcal{H}^1 \) possessing the following canonical decomposition:

\[ g^2_{\text{extr}} = \sum_{i=1}^{n/2} \frac{\sqrt{2}}{n} |2i-1, 2i\rangle. \]

The required by inequality (2.3) \( |\xi|^{2 \text{min}} = \frac{2}{n} \), and therefore the new condition gives

\[ \text{Tr}(D^2P^2_{g_{\text{extr}}}) \leq \frac{1}{3} (1 - \frac{2}{n}). \quad (3.4) \]

On the other hand, since \( L_2^1P^2_{g_{\text{extr}}} = \sum_{i=1}^{n} \frac{1}{n} P^1_i \), \( P^1_i = |i\rangle\langle i| \), \( \sum_{i=1}^{n} P^1_i = I^1 \), we have from both (3.2) and (3.3) the same result

\[ \text{Tr}(D^2P^2_{g_{\text{extr}}}) \leq \frac{1}{2} (1 - \frac{1}{n}). \quad (3.5) \]

Comparing (3.4) with (3.5), we see that the new condition is stronger than the B and C ones. So far, we were unable to establish the relation between the new condition (2.3) and the G-condition [13] for 3-representability. This would be important because it is known [11, 20] that the G-condition implies the B- and C- ones.

4. The strengthened B-condition

While comparing the new condition with the B-condition we found out that the B-condition could in principle be improved for \( N \) odd. \( B^2_{N}(g^2) \in \mathcal{P}^2_N \), \( \forall g^2 \in \mathcal{H}^{\wedge 2} \) means that the operator \( \binom{N}{2} B^2_N(g^2) \wedge I^{\wedge (N-2)} \geq 0, \forall g^2 \in \mathcal{H}^{\wedge 2}. \) If \( \Lambda_{\text{min}}^{B(g)} \) is the minimal eigenvalue of the operator \( \binom{N}{2} B^2_N(g^2) \wedge I^{\wedge (N-2)} \), then the operator \( \binom{N}{2} B^2_N(g^2) \wedge I^{\wedge (N-2)} - \Lambda_{\text{min}}^{B(g)} I^{\wedge N} \) is positive-semidefinite and therefore

\[ \binom{N}{2} B^2_N(g^2) - \Lambda_{\text{min}}^{B(g)} I^{\wedge 2} \in \mathcal{P}^2_N, \quad (4.1) \]

giving a necessary condition for \( N \)-representability (the strengthened B-condition). It is known [3] that for \( N \) even \( \Lambda_{\text{min}}^{B(g)} = 0, \forall g^2 \in \mathcal{H}^{\wedge 2}. \) For
$N = 3$ and $g_{extr}^2$, the eigenvalue $\Lambda_{min}^{B(g_{extr})}$ is greater than zero, and can be found explicitly. The operator

\[ 3B_3^2(g_{extr}^2) \wedge I^1 = 3\left(1 - \frac{1}{n}\right)I^3 - 2(3P_2^2 g_{extr}^2 \wedge I^1) \]

possesses the following minimal eigenvalue

\[ \Lambda_{min}^{B(g_{extr})} = 3\left(1 - \frac{1}{n}\right) - 2\left(1 - \frac{2}{n}\right) = 1 + \frac{1}{n}, \]

where Theorem 2.3 has been used. Hence, the strengthened B-condition in this case is

\[ 3B_3^2(g_{extr}^2) - \Lambda_{min}^{B(g_{extr})} I^\wedge 2 = \frac{2(n - 2)}{n} I^\wedge 2 - 2(3P_2^2 g_{extr}^2) \in \tilde{P}_N^2, \quad (4.2) \]

and therefore

\[ Tr(D^2 P_2^2 g_{extr}^2) \leq \frac{1}{3}(1 - \frac{2}{n}). \quad (4.3) \]

Comparing inequalities (3.4) and (4.3) we see that both the new conditions for 3-representability in the case under consideration ($g^2 = g_{extr}^2$) give the same bound from above on the expectation value $Tr(D^2 P_2^2 g_{extr}^2)$.

It seems that the above results suggest, it would be worthwhile to make an effort to extend the new conditions to arbitrary $N$ for at least some $g^2$ for which the maximum eigenvalue $\Lambda_{max}(g^2)$ of the operator $\binom{N}{2} P_g^2 \wedge I^{\wedge (N-2)}$ can be found, e.g. the extreme geminal $g_{extr}^2$. So far, we have obtained only partial information about the spectral decomposition of the operator $\binom{N}{2} P_2^2 g_{extr}^2 \wedge I^{\wedge (N-2)}$ for arbitrary $N$. However, at least in this case it is realistic to succeed. The other known conditions for $N$-representability could be treated in a similar way as the P- and B- conditions considered in this paper, provided the maximal and minimal eigenvalues of the appropriate operators were known. The obtained results concerning arbitrary $N$ will be published later.

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