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Sufficient conditions for pure state N-representability

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Abstract. A simple scheme is presented allowing the construction of most of the known and a wide variety of new sufficient conditions for pure state N-representability of reduced one-electron density operators.

1. Introduction

The purpose of this paper is to gain new insights into the complicated nature of reduced one-electron density operators. Most research has concentrated on discovering the necessary or sufficient conditions for ensemble N-representability, since the publications by Coleman [1] on the problem. Often, the dual-cone approach was employed due to the conic properties of the reduced density operator set. A complete solution for reduced one-electron density operators was evaluated by Kuhn [3], but only limited success was demonstrated with the general N-representability problem.

The apparently related problem of *pure state* N-representability turned out to be significantly more complicated, and in the decade after statement of the problem [2], only a limited number of partial solutions were published [5–7]. Later, the pure state N-representability problem was conjectured contentless for large particle numbers or high-rank cases [8, 9], erroneously, as was marked by [10]. In spite of being regarded as one of the ten most prominent research challenges for theoretical and computational chemistry [11], little or no progress in this field has been made in recent years.

In the following paper, a simple and unified scheme is presented for the construction of nearly all the known sufficient conditions for pure state N-representability of reduced one-electron density operators. Moreover, this scheme opens a route for constructing a wide variety of new sufficient conditions.

2. Notation and definitions

With a finite orthonormal basis $\{e_i, i = 1, 2, \ldots, r\}$ of one-electron state vectors (orbitals), every N-electron state vector can be expanded into configurations:

$$\Psi = \sum_{(i_1, i_2, \ldots, i_N)} c_{i_1, i_2, \ldots, i_N} \qquad (e_{i_1} \wedge e_{i_2} \wedge \cdots \wedge e_{i_N}). \tag{1}$$

The configurations are written here using the antisymmetric wedge product '$\wedge$'. The sum in (1) runs over all sets $(i_1, i_2, \ldots, i_N)$ of indices satisfying $1 \leqslant i_1 \leqslant i_2 \leqslant \cdots \leqslant i_N \leqslant r$.

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By change of the orbital basis it is always possible to write Ψ in its polar Schmidt form [12]:

$$\Psi = \sum_{i=1}^{r} \sqrt{|\lambda_i|} \qquad \phi_i \wedge \chi_i \tag{2}$$

$\{\phi_i\}$ are the new one-electron states, called natural states, and χ_i are some proper choosen $(N-1)$-electron state vectors. The Schmidt form has the feature that on contraction the N-electron density operator $\rho_\Psi := |\Psi\rangle\langle\Psi|$ results in the diagonal $(N-1)$- respective one-electron reduced density operators:

$$\mu = \mathrm{tr}_{1,2,\ldots,N-1}\, |\Psi\rangle\langle\Psi| = \sum_{i=1}^{r} \lambda_i |\phi_i\rangle\langle\phi_i| \tag{3}$$

$$\Gamma_{N-1} = \mathrm{tr}_1\, |\Psi\rangle\langle\Psi| = \sum_{i=1}^{r} \lambda_i |\chi_i\rangle\langle\chi_i|. \tag{4}$$

The non-zero eigenvalues λ_i of μ and Γ_{N-1} are identical.

2.1. The N-vector-representability problem

The *N-representability problem by pure states* was stated by Coleman [2] as follows.

> For a given p-electron operator Γ_p, give the (necessary and/or sufficient) conditions that Γ_p is the image of *some* pure state N-electron density operator $\rho_\Psi = |\Psi\rangle\langle\Psi|$ on contraction:

$$\Gamma_p = \mathrm{tr}_{1,2,\ldots,N-p}\, \rho_\Psi. \tag{5}$$

For simplicity, hereafter we use the shorter term *N-vector representability* instead of 'N-representability by pure states'.

Asking for N-vector representability is therefore a sharpened version of the ensemble N-representability problem, where the preimage in equation (5) is allowed to be an ensemble N-electron density operator ρ, i.e. a convex combination of projectors ρ_Ψ. The ensemble N-representability problem was solved for reduced one-electron density operators, where a necessary and sufficient condition was given entirely in terms of the spectrum [1, 3]: $\mu \geqslant 0$, $(1-\mu) \geqslant 0$, $\mathrm{tr}\,\mu = N$. However, the problem deciding N-vector representability could only be solved for special cases and, in general, remained unsolved. Unless otherwise stated, we are only concerned with N-vector representability in this paper.

3. Polytopes

In this section, a short survey on polytopes is given. Though a lot of useful ideas in polytope theory are developed from our geometric intuition in $\mathbb{R}^3$, they often fail in higher dimensions. Easily answerable questions in low dimensions often reveal themselves to be difficult problems in higher dimensions. For a more complete and recent overview on polytope theory, we refer to [14].

In order to fix the notation and language, some definitions are given here. A point set $K \in \mathbb{R}^d$ is *convex* if with any two points $\boldsymbol{x}, \boldsymbol{y} \in K$, the straight line segment $\{c\boldsymbol{x} + (1-c)\boldsymbol{y} : 0 \leqslant c \leqslant 1\}$ also belongs to K. The *convex hull* of a point set $K \in \mathbb{R}^d$ is the smallest convex set containing K. If $K = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ is a finite point set in some $\mathbb{R}^d$, its convex hull is called a *V-polytope*:

$$P = \left\{ \beta_1\boldsymbol{x}_1 + \beta_2\boldsymbol{x}_2 + \cdots + \beta_n\boldsymbol{x}_n : \beta_i \geqslant 0, \sum_{i=1}^{n} \beta_i = 1 \right\} \tag{6}$$

A convex combination may be distinguished from an ordinary linear combination through the requirements that the numbers β_i be non-negative and sum to unity. The dimension of a polytope is the affine rank of its points.

There is a complementary representation of a V-polytope, called a *H-polytope*, where the polytope is described as the bounded intersection of a finite number of closed halfspaces in some $\mathbb{R}^d$:

$$P = \{\boldsymbol{x} : \boldsymbol{A}\boldsymbol{x} \leqslant 1\} \tag{7}$$

where $\boldsymbol{A}$ is a matrix. A H-polytope is bounded in the sense that it does not contain any ray $\boldsymbol{x} + c\boldsymbol{y} : c \geqslant 0, \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^d\}$ with $\boldsymbol{y} \neq 0$.

The intersection of some hyperplane $\{\boldsymbol{x} : \boldsymbol{c}\boldsymbol{x} = 1\}$ with a polytope is called a *face*. Faces of dimension 0, 1, $d-1$ are called *vertices*, *edges* and *facets*, respectively. The vertices of a polytope P are the only points which cannot be represented as convex combinations of two other points in P. They therefore provide the most compact point set describing P. The supporting hyperplanes of facets fix the halfspaces of a H-polytope.

The complementary representations V-polytopes and H-polytopes are mathematically but not algorithmically equivalent. For example, it is algorithmically difficult to decide, whether a given point $\boldsymbol{x}$ is contained in a V-polytope, but easy to decide for a H-polytope. One method to change from one polytope representation to the other is the Fourier–Motzkin elimination (we refer to [14] for further details). The program `PORTA` [15] was used here for the tedious computation of the Fourier–Motzkin elimination.

4. Sets of independent binary words

Consider the subset of vertices of the r-dimensional unit cube, where exactly w coordinates are ones and the other $r-w$ coordinates are zeros. r and w are kept arbitrary but fixed in the following. There is a natural homomorphism between the vertices of the unit cube and binary words of size r and weight w by identifying the vector coordinates with the word bits. In the following, we therefore use both the terms *word* and *vector* interchangeably.

Two words are *adjacent*, if there are exactly $w-1$ one-bits common in both words. A set of words is called *independent*, if there is no pair of adjacent words therein. By connecting all adjacent words, the Johnson graph $J(r, w)$ is formed [4].

The Johnson graphs are invariant under bit permutation of the words, i.e. adjacent words remain adjacent. Two sets of words are called equivalent, if there is a permutation of bits acting as homomorphism between the two sets. A set of independent words is called *maximal*, if there does not exist any other word non-adjacent to the words of the set.

4.1. Construction of maximal independent sets

Classifying the maximal independent sets for a given pair (r, w) is of no theoretical difficulty, though in practice the only known general method is an exhaustive search over the whole graph. Unfortunately, algorithms inplementing this search have a high demand on computational time of non-polynomial order.

In table 1, a complete classification of inequivalent maximal independent sets for some small word sizes r is presented. Since the number of classes grows rapidly with increasing r and w as shown in table 2, a summary is only given here, but we can provide a long listing on request.

Starting from known independent sets, other (not necessarily maximal) independent sets can be constructed by a number of different methods as listed below.

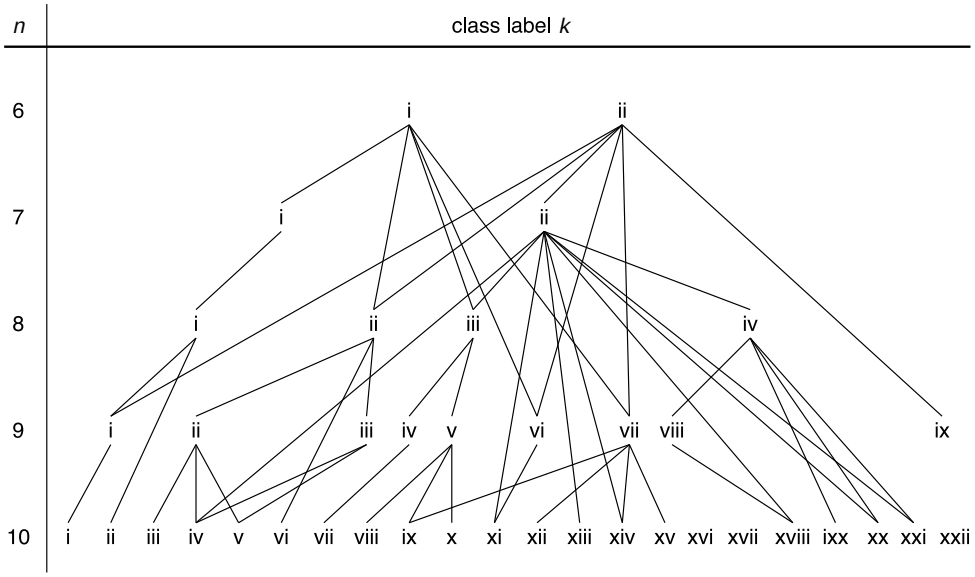

Figure 1. The genealogical relation between equivalence classes of maximal independent sets with same weight three but different size n. The classes are labelled as in table 1, i.e. by sorting lexicographically. A line connecting two equivalence classes indicates that the members of the class with smaller word size are subsets of the class with bigger word size. For readability, the lines connecting the $n = 10$ and $n = 6$ classes are omitted. Note that the $n = 10$ equivalence classes xvi, xvii and xxii do not have any maximal independent subset with smaller word size.

Juxtaposition. Let $\{\boldsymbol{a}_i\}$ and $\{\boldsymbol{b}_j\}$ be two independent sets. By juxtaposing the two sets—placing all possible pairs of words side by side—a new independent set $\{\boldsymbol{a}_i\boldsymbol{b}_j\}$ is obtained.

Example: placing the words of the sets {0011, 1100} and {000111, 111000} side by side yields the independent set {0011000111, 1100000111, 0011111000, 1100111000}.

Adding constant bits. Placing in front of a set of independent words $\{\boldsymbol{b}_i\}$ another word $\boldsymbol{x}$, we get the independent set $\{\boldsymbol{x}\boldsymbol{b}_i\}$. This is a special case of the juxtaposition above.

Example: $\boldsymbol{x} = 111$ and {0011, 1100} result in the independent set {1110011, 1111100}.

Inversion. Given a set of independent words $\{\boldsymbol{b}_i\}$, another independent set can be constructed by bitwise inversion.

Example: the set {00000111, 00011001} is mapped to {11111000, 11100110}.

Action of the permutation group. The orbit under the action of a nontrivial permutation group may be an independent set, if a clever start word or a group of words and the appropriate permutation group is choosen.

Example: with the start word 00001011 and the subgroup of the full permutation group S_8 generated by the cycle (12345678), one gets an independent set, which is maximal and belongs to the equivalence class $I(8, 3, \text{iv})$ in table 1.

4.2. Bounds on the size of maximal independent sets

For given word size r and weight w, the number $A(r, w)$ of words of the biggest possible independent set is of much interest in coding theory (cf [13] and references therein). The *Johnson bound* provides an upper bound to $A(r, w)$. It is usually very close to the exact value $A(r, w)$. Although there is no closed formula for the Johnson bound, it may be calculated by

Table 1. Complete list of equivalence classes $I(r, w, k)$ of maximal independent sets sorted by word size r, weight w and a label k. For each equivalence class, the representative coming lexicographically is given first. The sets are also sorted lexicographic.

r	w	k	Class representative
r	2	i	...0000011, ...0001100, ...0110000, ...
6	3	i	000111, 011001, 101010, 110100
		ii	000111, 111000
7	3	i	0000111, 0011001, 0101010, 0110100, 1001100, 1010010, 1100001
		ii	0000111, 0011001, 0101010, 1001100, 1110000
8	3	i	00000111, 00011001, 00101010, 00110100, 01001100, 01010010, 01100001
		ii	00000111, 00011001, 00101010, 00110100, 01001100, 01010010, 10100001
		iii	00000111, 00011001, 00101010, 00110100, 01001100, 10010010, 11000001
		iv	00000111, 00011001, 00101010, 01001100, 01110000, 10010010, 10100100, 11000001
8	4	i	00001111, 00110011, 00111100, 01010101, 01011010, 01100110, 01101001, 10010110, 10011001, 10100101, 10101010, 11000011, 11001100, 11110000
		ii	00001111, 00110011, 00111100, 01010101, 01011010, 01100110, 10010110, 10011001, 10100101, 11000011, 11101000
		iii	00001111, 00110011, 00111100, 01010101, 01011010, 10010110, 10100101, 11001001, 11100010
		iv	00001111, 00110011, 00111100, 01010101, 01011010, 10100101, 10101010, 11000110, 11001001, 11110000
		v	00001111, 00110011, 00111100, 01010101, 01011010, 10100110, 11001001, 11110000
		vi	00001111, 00110011, 00111100, 01010101, 01101010, 10010110, 10101001, 11000011, 11011000, 11100100
		vii	00001111, 00110011, 00111100, 01010101, 01101010, 10010110, 11001001, 11100100
		viii	00001111, 00110011, 00111100, 01010101, 01101010, 11000110, 11011000, 11100001
		ix	00001111, 00110011, 00111100, 01010101, 10101010, 11000110, 11011000, 11100001
		x	00001111, 00110011, 01010101, 01101001, 10011010, 10101100, 11100010
		xi	00001111, 00110011, 01010101, 01101010, 10010110, 10101100, 11011000, 11100001
9	3	i	000000111, 000011001, 000101010, 000110100, 001001100, 001010010, 001100001, 110000001
		ii	000000111, 000011001, 000101010, 000110100, 001001100, 001010010, 010100001, 101000001, 110000010
		iii	000000111, 000011001, 000101010, 000110100, 001001100, 001010010, 010100001, 111000000
		iv	000000111, 000011001, 000101010, 000110100, 001001100, 010010010, 011000001, 100100001, 101000010, 110000100
		v	000000111, 000011001, 000101010, 000110100, 001001100, 010010010, 011000001, 101000010, 110100000
		vi	000000111, 000011001, 000101010, 000110100, 001001100, 010010010, 100100001, 111000000
		vii	000000111, 000011001, 000101010, 000110100, 001001100, 010010010, 101000001, 110100000
		viii	000000111, 000011001, 000101010, 001001100, 001110000, 010010010, 010100100, 011000001, 100010100, 100100001, 101000010, 110001000
		ix	000000111, 000011001, 000101010, 001001100, 010010010, 011100000, 100100100, 101010000, 110000001

repeated application of the inequalities

$$A(r, w) \leqslant \left\lfloor \frac{r}{w} A(r-1, w-1) \right\rfloor \qquad A(r, w) \leqslant \left\lfloor \frac{r}{r-w} A(r-1, w) \right\rfloor \quad (8)$$

using the symmetry $A(r, r-w) = A(r, w)$ until $A(r, 2) = \lfloor r/2 \rfloor$ is reached.

Table 2. The number of equivalence classes of maximal independent sets sorted by word size r and weight w. In the fourth coloumn, the number of classes sorted by the set size (in brackets) is given.

r	w	Total	Sorted by set size
r	2	1	1($\lfloor r/2 \rfloor$)
8	3	4	3(7), 1(8)
9	3	9	4(8), 3(9), 1(10), 1(12)
10	3	22	1(8), 5(10), 7(11), 8(12), 1(13)
11	3	85	2(11), 7(12), 38(13), 28(14), 8(15), 1(16), 1(17)
12	3	411	8(13), 13(14), 84(15), 187(16), 92(17), 20(18), 6(19), 1(20)
8	4	11	1(7), 5(8), 1(9), 2(10), 1(11), 1(14)
9	4	537	1(9), 27(11), 110(12), 161(13), 200(14), 35(15), 2(16), 1(18)

A lower bound to $A(r, w)$ is given by

$$A(r, w) \geqslant \frac{1}{r}\binom{r}{w}. \tag{9}$$

The exact values of $A(r, w)$ are usually found by explicit construction of the maximal independent sets. A huge table of values $A(r, w)$ is collected in [13].

The upper and lower bounds are of importance here because they present a reasonable guess at how good the sufficient conditions below will be.

5. Sufficient conditions for N-representability

With an arbitrary but fixed set of orthonormal one-electron states ϕ_i, natural labels for N-electron configurations are binary words $\boldsymbol{b}$ of size r and weight N

$$\boldsymbol{b} \mapsto \Phi_{\boldsymbol{b}} := \bigwedge_{i:\boldsymbol{b}_i=1} \phi_i. \tag{10}$$

The wedge product runs over all one-bits in $\boldsymbol{b}$.
Example: the binary number 01001100 labels the configuration $\Phi_{01001100} = \phi_3 \wedge \phi_4 \wedge \phi_7$.

Definition 1. *A one-electron operator of finite rank r has property $\mathcal{C}(N)$ iff the eigenvalues are equal to the coordinates of a vector $\boldsymbol{d}$ in some V-polytope defined by a set of independent vectors $\boldsymbol{b}_1, \boldsymbol{b}_2, \ldots, \boldsymbol{b}_k$ of size r and weight N.*

The main link between independent sets of words and the N-representability problem is noted in the following theorem.

Theorem 1. *Every one-electron operator of finite rank r with property $\mathcal{C}(N)$ is N-vector representable.*

Proof. With appropriate non-negative coefficients, β_i, summing to unity, every point in the polytope of a set of independent vectors $\boldsymbol{b}_i$ has at least one decomposition

$$\boldsymbol{d} = \sum_i \beta_i \boldsymbol{b}_i \qquad \sum_i \beta_i = 1 \qquad \beta_i \geqslant 0. \tag{11}$$

Then construct N-electron state vectors

$$\Psi = \sum_i \mathrm{e}^{\mathrm{i}\alpha_i} \sqrt{\beta_i}\, \Phi_{\boldsymbol{b}_i} \tag{12}$$

with arbitrary phase factors $e^{i\alpha_i}$. Because all configurations $\Phi_{\boldsymbol{b}_i}$ in equation (12) differ by at least two orbitals, all outer diagonal terms $|\Phi_{\boldsymbol{b}_k}\rangle\langle\Phi_{\boldsymbol{b}_l}|$ with $k \neq l$ of the N-electron density operator ρ_Ψ vanish by contraction to the reduced one-electron density operator

$$\mu = \mathrm{tr}_{1,2,\ldots,N-1}\,\rho_\Psi = \sum_i \sum_{j:(\boldsymbol{b}_i)_j=1} \beta_i |\phi_j\rangle\langle\phi_j| = \sum_{i=1}^{r} \boldsymbol{d}_i |\phi_i\rangle\langle\phi_i|. \tag{13}$$

By equality of the coordinates $\boldsymbol{d}_i$ and the eigenvalues λ_i of μ as assumed, the theorem is proved. □

We are now able to compare this simple *independent set construction* with previously known sufficient conditions for N-vector representability.

Corollary 1. *A one-electron operator μ is N-vector representable if all eigenvalues have multiplicity divisible by N (theorem 5 in [5]).*

Proof. Take the N-clique of words of weight N

$$00\ldots0\underbrace{11\ldots1}_{N}, \quad 00\ldots0\underbrace{11\ldots1}_{N}\underbrace{00\ldots0}_{N}, \quad \ldots$$

which is a not maximal set of independent words. Every convex combination of these words is a vector with coordinates degenerate by multiples of N. □

Corollary 2. *μ is two-vector representable iff all eigenvalues have multiplicity divisible by two (theorem 6 in [5]).*

Proof. Sufficiency follows from corollary 1. Though there is only one equivalence class of maximal independent sets with weight two (cf table 1), necessity does not follow from theorem 1 but may be deduced using the polar Schmidt form [5]. □

Corollary 3. *μ of rank $N + 2$ is N-vector representable if all eigenvalues have multiplicity divisible by two for N even and one additional eigenvalue is one if N is odd (cf theorem 8 in [5]).*

Proof. Use the one and only equivalence class of independent sets with word size $N + 2$ and weight two. Every convex combination of these words is a vector with coordinates degenerate by multiples of two. □

Corollary 4. *μ is N-vector representable if the first m eigenvalues are equal to unity and the other $(N - m)$ eigenvalues have property $\mathcal{C}(N - m)$ i.e. form a vector inside some polytope of an independent set with word size $r - m$ and weight $N - m$ (cf theorem 9 in [5]).*

Proof. Let the vector formed by the $r - m$ eigenvalues of μ smaller than unity have a decomposition (11) with some independent words $\boldsymbol{b}_i$. By attaching m one-bits to the words $\boldsymbol{b}_i$, another independent set arises, whose convex combination are also N-vector representable. □

Corollary 5. *Let $(N_1, N_2, \ldots, N_m)$ be a partition of N with $N_k \geqslant 2$. μ is N-vector representable if the eigenvalues may be divided into m groups and the kth group of eigenvalues has property $\mathcal{C}(N_k)$.*

Proof. The corollary follows immediately by the independent set construction *juxtaposition*. □

Corollary 6. *μ of rank six is three-vector representable iff the ordered eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_6$ of μ solve the following system of (in)equalities [7]:*

$$\begin{aligned} &\lambda_1 + \lambda_6 = 1 \qquad \lambda_2 + \lambda_5 = 1 \\ &\lambda_3 + \lambda_4 = 1 \qquad \lambda_5 + \lambda_6 \geqslant \lambda_4. \end{aligned} \tag{14}$$

Proof. For size $r = 6$ and weight $w = 3$, there are exactly two equivalence classes of maximal independent sets (cf table 1). Take the V-polytope defined by the independent set

$$\{001011, 010101, 100110, 111000\} \tag{15}$$

belonging to the equivalence class $I(6, 3, \mathrm{i})$. Then generate a complete system of facet-defining inequalities of the H-polytope from the vertex list of the V-polytope by Fourier–Motzkin elimination:

$$\begin{aligned} &\lambda_1 + \lambda_4 = 1 \qquad \lambda_2 + \lambda_5 = 1 \qquad \lambda_3 + \lambda_6 = 1 \\ &\lambda_3 + \lambda_4 \geqslant \lambda_2 \qquad \lambda_5 + \lambda_6 \geqslant \lambda_4 \qquad \lambda_1 + \lambda_2 \geqslant \lambda_6 \\ &\lambda_2 + \lambda_4 + \lambda_6 \geqslant 1. \end{aligned} \tag{16}$$

Now assume the eigenvalues, λ_i, to be ordered non-increasing, then the only non-redundant inequality is the one in system (14). All other independent sets and also the sets belonging to the class $I(6, 3, \mathrm{ii})$ give rise to (in)equality systems weaker than (14).

For the necessity part of the proof, we refer to [7]. □

It is a very special situation here that different pairs of eigenvalues sum up to unity due to the low polytope dimensionality. In general, this cannot be expected and the conjecture in section 8 in [5] is clearly false.

Corollary 7. *μ of rank seven is three-vector representable if the ordered eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_7$ of μ solve the following system of inequalities [7]:*

$$\begin{aligned} &\lambda_1 + \lambda_6 + \lambda_7 \geqslant 1 \qquad \lambda_2 + \lambda_5 + \lambda_7 \geqslant 1 \\ &\lambda_3 + \lambda_4 + \lambda_7 \geqslant 1 \qquad \lambda_3 + \lambda_5 + \lambda_6 \geqslant 1. \end{aligned} \tag{17}$$

Proof. Take the V-polytope defining maximal independent set

$$\{0010110, 0011001, 0100101, 0101010, 1000011, 1001100, 1110000\} \tag{18}$$

belonging to the equivalence class $I(7, 3, \mathrm{i})$ (cf table 1). Fourier–Motzkin elimination yields the H-polytope description

$$\begin{aligned} &\lambda_3 + \lambda_4 + \lambda_7 \geqslant 1 \qquad \lambda_2 + \lambda_4 + \lambda_6 \geqslant 1 \qquad \lambda_2 + \lambda_5 + \lambda_7 \geqslant 1 \\ &\lambda_3 + \lambda_5 + \lambda_6 \geqslant 1 \qquad \lambda_1 + \lambda_2 + \lambda_3 \geqslant 1 \qquad \lambda_1 + \lambda_4 + \lambda_5 \geqslant 1 \\ &\lambda_1 + \lambda_6 + \lambda_7 \geqslant 1. \end{aligned} \tag{19}$$

Due to the ordering of the eigenvalues, this system is equivalent to the system (17). □

Other independent sets do not necessarily result in the same system of inequalities. For example, the representative of the equivalence class $I(7, 3, \mathrm{i})$ leads to a single inequality

$$\lambda_5 + \lambda_6 + \lambda_7 \geqslant 1 \tag{20}$$

which is clearly more restrictive than system (17).

In order to find the strongest system of inequalties, one has to check every independent set of a given equivalence class and there is no guarantee that one resulting system of inequalities covers all the others.

The assumption of ordered eigenvalues can be translated into the V-polytope picture. The H-polytope defined by the chain of inequalities $1 \geqslant \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_7 \geqslant 0$ and the equality $\lambda_1 + \lambda_2 + \cdots + \lambda_7 = 3$ correspond to the V-polytope with vertices

$$\begin{aligned}
\boldsymbol{x}_1 &= (1, 1, 1, 0, 0, 0, 0)\\
\boldsymbol{x}_2 &= (1, 1, \tfrac{1}{2}, \tfrac{1}{2}, 0, 0, 0)\\
\boldsymbol{x}_3 &= (1, 1, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, 0, 0)\\
\boldsymbol{x}_4 &= (1, 1, \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{4}, 0)\\
\boldsymbol{x}_5 &= (1, 1, \tfrac{1}{5}, \tfrac{1}{5}, \tfrac{1}{5}, \tfrac{1}{5}, \tfrac{1}{5})\\
\boldsymbol{x}_6 &= (1, \tfrac{2}{3}, \tfrac{2}{3}, \tfrac{2}{3}, 0, 0, 0)\\
\boldsymbol{x}_7 &= (1, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, 0, 0)\\
\boldsymbol{x}_8 &= (1, \tfrac{2}{5}, \tfrac{2}{5}, \tfrac{2}{5}, \tfrac{2}{5}, \tfrac{2}{5}, 0)\\
\boldsymbol{x}_9 &= (1, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3})\\
\boldsymbol{x}_{10} &= (\tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{4}, 0, 0, 0)\\
\boldsymbol{x}_{11} &= (\tfrac{3}{5}, \tfrac{3}{5}, \tfrac{3}{5}, \tfrac{3}{5}, \tfrac{3}{5}, 0, 0)\\
\boldsymbol{x}_{12} &= (\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2}, 0)\\
\boldsymbol{x}_{13} &= (\tfrac{3}{7}, \tfrac{3}{7}, \tfrac{3}{7}, \tfrac{3}{7}, \tfrac{3}{7}, \tfrac{3}{7}, \tfrac{3}{7}).
\end{aligned} \tag{21}$$

We can now reformulate corollary 7 in the following new corollary.

Corollary 8. *μ of rank seven is three-vector representable if the vector formed from the eigenvalues of μ is contained in both V-polytopes (18) and (21).*

In general, sets of eigenvalues ordered non-increasing $1 \geqslant \lambda_1 \geqslant \cdots \geqslant \lambda_r \geqslant 0$ and satisfying $\sum_i \lambda_i = N$, considered as coordinates of polytope vectors, correspond to a V-polytope with $1 + N(r - N)$ vertices. The H-polytope description is therefore more compact.

Corollary 9. *μ of rank nine is three-vector representable if the ordered eigenvalues $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_9$ of μ solve the following system of (in)equalities:*

$$\begin{aligned}
&\sum_{i=1}^{9} \lambda_i = 3\\
&\lambda_1 - \lambda_3 + \lambda_4 - \lambda_6 - \lambda_7 - 2\lambda_9 \leqslant 0\\
&\lambda_1 + \lambda_3 - \lambda_5 - \lambda_6 - 2\lambda_8 - \lambda_9 \leqslant 0\\
&\lambda_1 + \lambda_2 - 2\lambda_6 - \lambda_7 - \lambda_8 - \lambda_9 \leqslant 0\\
&\lambda_1 - \lambda_2 + \lambda_4 - \lambda_5 - \lambda_8 - 2\lambda_9 \leqslant 0.
\end{aligned} \tag{22}$$

Proof. Take the V-polytope defined by the maximal independent set

$$\{000000111, 000011001, 000101010, 001001100, 001110000, 010010010,$$
$$010100100, 011000001, 100010100, 100100001, 101000010, 110001000\}$$

belonging to the equivalence class $I(9, 3, \text{viii})$ in table 1. Though there are 81 facet defining inequalities for the corresponding H-polytope, only the four in (22) are non-redundant, if the eigenvalues are ordered non-increasing. □

From the standpoint of the independent set construction of sufficiency conditions, it is very unlikely that the N-representability problem becomes contentless for large one-electron rank

r or particle number n, as convex combinations of adjacent words do not generally have the property $\mathcal{C}(n)$. On the other hand, there seem to be only a few N-representable one-electron operators not covered by the sufficient conditions above, as the number $A(r, N)$ is at most $1/r$ smaller than the number of possible configurations for given r and N.

6. Conclusion

We have shown how sufficient conditions for N-representability by pure states of one-electron operators may be found with help of independent sets of binary words. By this construction, every one-electron operator with eigenvalues identical to the coordinates of a vector inside a certain type of polytope is N-representable by pure states. The polytopes are completely defined by a set of vertices of the r-dimensional unit cube, where each pair of vertices differs in more than one coordinate. The N-representability problem is thereby converted into a geometric problem, providing a visual interpretation. Most of the previously known and a wide varity of new sufficient conditions for N-representability by pure states are obtained in a unified approach.

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