Commun. Math. Phys. 282, 287–322 (2008)
Digital Object Identifier (DOI) 10.1007/s00220-008-0552-z

Communications in
Mathematical Physics

The Pauli Principle Revisited

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Received: 22 November 2006 / Accepted: 25 February 2008
Published online: 4 July 2008 – © Springer-Verlag 2008

Abstract: By the Pauli exclusion principle, no quantum state can be occupied by more than one electron. One can state this as a constraint on the one electron density matrix that bounds its eigenvalues by 1. Shortly after its discovery, the Pauli principle was replaced by anti-symmetry of the multi-electron wave function. In this paper we solve a longstanding problem about the impact of this replacement on the one electron density matrix, that goes far beyond the original Pauli principle. Our approach uses Berenstein and Sjamaar's theorem on the restriction of an adjoint orbit onto a subgroup, and allows us to treat any type of permutational symmetry.

Electronic Supplementary Material: The online version of this article (doi:10.1007/s00220-008-0552-z) contains supplementary material, which is available to authorized users.

Contents

1. Introduction

The Pauli exclusion principle, discovered in 1925, claims that no quantum state can be occupied by more than one electron. In terms of the electron density matrix[1] ρ

[1] There is no agreement on a proper normalization of the one-electron matrix. To avoid confusion we call it *electron density matrix* for Dirac's normalization to the number of particles $\operatorname{Tr}\rho = N$, and reserve the term *reduced state* for the probability normalization $\operatorname{Tr}\rho = 1$.

this amounts to the inequality $\langle\psi|\rho|\psi\rangle \leq 1$, that bounds its eigenvalues by one. The following year Heisenberg and Dirac replaced the Pauli principle by skew symmetry of a multi-electron wave function [11, Ch. 4].

The subject of this study is the impact of this replacement on the electron density matrix. The latter determines the light scattering and therefore quite literally represents a visible state of the electron system. The impact goes far beyond the original Pauli principle. As an example, consider a three electron system $\wedge^3\mathcal{H}_6$ with one-electron space $\mathcal{H}_6$ of dimension 6. Then the spectrum λ of the electron density matrix, arranged in non-increasing order, is bounded by the following (in)equalities discovered by Borland and Dennis [3]:

$$\lambda_1 + \lambda_6 = \lambda_2 + \lambda_5 = \lambda_3 + \lambda_4 = 1, \quad \lambda_4 \leq \lambda_5 + \lambda_6. \tag{1}$$

The authors established the sufficiency of these constraints and refer for a complete proof to M.B. Ruskai and R.L. Kingsley.[2] It worth reading their comment:

> *We have no apology for consideration of such a special case. The general N-representability problem is so difficult and yet so fundamental for many branches of science that each concrete result is useful in shedding light on the nature of general solution.*

In spite of some bogus claims [29], refuted in [32], this result had stood for more than three decades as the only known solution of the N-representability problem beyond two electrons $\wedge^2\mathcal{H}_r$ and two holes $\wedge^{r-2}\mathcal{H}_r$. For the latter systems the problem is easy and the constraints amount to double degeneracy of the spectrum, starting from the head $\lambda_{2i-1} = \lambda_{2i}$ for two electrons and from the tail $\lambda_{r-2i} = \lambda_{r-2i-1}$ for two holes [5], where we set $\lambda_i = 0$ for $i > r$, and $\lambda_i = 1$ for $i < 1$.

Here we solve this longstanding problem. The content of the paper is as follows.

In Sect. 2 we recast the Berenstein-Sjamaar theorem [1, Thm 3.2.1] into a usable form (Theorem 1). This provides a theoretical basis for our study.

We start Sect. 3 by a variation of the above problem, called *ν-representability*, that takes into account both spin and orbital occupation numbers. Mathematically this amounts to replacing the exterior power $\wedge^N\mathcal{H}$ by a representation $\mathcal{H}^\nu$ defined by a Young diagram ν of order N. Theorem 2 gives a formal solution of the ν-representability problem. We derive from it the majorization inequality $\lambda \preceq \nu$, that plays the rôle of the Pauli principle. This inequality is necessary and sufficient for λ to be occupation numbers of an unspecified *mixed* state (Theorem 3). Theorem 4 deals with a class of systems where the majorization inequality alone provides a criterion for *pure* ν-representability. This includes the so-called *closed shell*, meaning a system of electrons of total spin zero. The corresponding Young diagram ν consists of two columns of equal length. For this system all constraints on the occupation numbers are given by the Pauli type inequality $\lambda \leq 2$. Next in Theorem 5 we calculate the topological coefficients $c_w^v(a)$ that governed the constraints on the occupation numbers in Theorem 2. This gives it the full strength we need in the next section.

Section 4 starts with analysis of pure ν-representability for a toy example of two-row diagrams, that allows us to illustrate the basic technique (Theorem 6). These are exceptional systems where the constraints on the occupation numbers are given by a *finite* set

[2] Recently M.B. Ruskai published the proof [33] derived from known constraints on the spectra of Hermitian matrices A, B, and $C = A + B$. Conceptually the N-representability problem is close to the Hermitian spectral problem [15,16], but a direct connection between them, beyond sporadic coincidences, is unlikely. R.L. Kingsley's independent solution apparently has never been published.

of inequalities independent of the rank. Then we return to the original N-representability problem, that appears to be the most difficult one. For example, in contrast to Theorem 6, no finite system of inequalities can describe N-representability for a fixed $N > 1$ and arbitrary big rank (Corollary 3 to Proposition 5). This forces us to restrict either the rank, as we do in the last section, or the type of the inequalities. Here we focus on the inequalities with 0/1 coefficients. It turns out that under some natural conditions such an inequality should be either of the form

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_{N-1}} \leq N - 2, \tag{2}$$

with $\sum_k (i_k - k) = r - N + 1$, or of the form

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_p} \leq N - 1, \tag{3}$$

with $p \geq N$ and $\sum_k (i_k - k) = \binom{p}{N}$. We call them *Grassmann inequalities* of the first and second kind respectively. A surprising result is that these inequalities actually hold true with very few exceptions (Theorems 7 and 8).

In the simplest case $N = 3$ we get from (2) inequalities

$$\lambda_{k+1} + \lambda_{r-k} \leq 1, \quad 0 \leq k < (r-1)/2$$

that hold for any even rank $r \geq 6$. This constraint prohibits more than one electron to occupy *two* symmetric orbitals and supersedes the original Pauli principle. For $r = 6$, due to the normalization $\sum_i \lambda_i = 3$, the inequalities degenerate into Borland-Dennis *equalities* (1). For odd rank the first inequality $k = 0$ should be either skipped or replaced by the weaker one $\lambda_1 + \lambda_r \leq 1 + \frac{2}{r-1}$.

We treat Grassmann inequalities of the second kind (3) only for lowest levels $p = N, N + 1$. For $N = 3$ and $p = N + 1$ they amount to four inequalities:

$$\begin{array}{ll} \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2, & \lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2, \\ \lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2, & \lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2, \end{array} \tag{4}$$

that hold for arbitrary rank r and give all the constraints for $r \leq 7$. For $r = 6$ they turn into Borland-Dennis conditions (1).

In Sect. 5 we briefly discuss a connection of the ν-representability with representation theory, that provides information complementary to Theorem 2. A combination of the two approaches leads to an algorithm for solution of the problem for any fixed rank. The algorithm, along with other tools, has been used in calculations reported in the last Sect. 6. Eventually this led to a complete solution of the N-representability problem for rank $r \leq 10$. However, we provide a rigorous justification only for $r \leq 8$. We also give an example of constraints on the spin and orbital occupation numbers for a system of three electrons of total spin $1/2$.

The first sections may be mathematically more demanding than the rest of the paper. We recommend books [7–9] as general references on Schubert calculus, Lie algebra, and representation theory.

The theoretical results of the paper belong to the second author. They were often inspired by calculations, that at this stage couldn't be accomplished by a computer without intelligent human assistance and insight.

2. A Review of the Berenstein-Sjamaar Paper

Let M be a compact connected Lie group with the Lie algebra $\mathfrak{m}$ and its dual coadjoint representation $\mathfrak{m}^*$. For coadjoint orbit $\mathcal{O} \subset \mathfrak{m}^*$ of group M and a Cartan subalgebra $\mathfrak{t} \subset \mathfrak{m}$ consider the composition $\Delta : \mathcal{O} \hookrightarrow \mathfrak{m}^* \to \mathfrak{t}^*$ known as the *moment map*. By Kostant's theorem its image is a convex polytope spanned by the W-orbit of some weight $\mu \in \mathfrak{t}^*$ which can be taken from a fixed positive Weyl chamber $\mathfrak{t}^*_+$. Here $W = N(\mathfrak{t})/Z(\mathfrak{t})$ is the Weyl group of M. This gives a parameterization of the coadjoint orbits $\mathcal{O}_\mu$ by the dominant weights $\mu \in \mathfrak{t}^*_+$.

Example 1. In this paper we will mostly deal with the unitary group $\mathrm{U}(n)$ whose Lie algebra $\mathfrak{u}(n)$ consists of all Hermitian[3] $n \times n$ matrices. Let us identify $\mathfrak{u}(n)$ with its dual via the invariant trace form $(A, B) = \mathrm{Tr}(AB)$. Then the (co)adjoint orbit $\mathcal{O}_\mu$ consists of all Hermitian matrices A of spectrum $\mu : \mu_1 \geq \mu_2 \geq \cdots \geq \mu_n$ and the moment map $\Delta : \mathcal{O}_\mu \to \mathfrak{t}$ is given by orthogonal projection into the Cartan subalgebra of diagonal matrices $\mathfrak{t}$. Kostant's theorem in this case amounts to Horn's observation that the diagonal entries of Hermitian matrices of spectrum μ form a convex polytope with vertices $w\mu$ obtained from μ by permutations of the coordinates μ_i. This is equivalent to the *majorization inequalities*

$$\begin{aligned} d_1 &\leq \mu_1, \\ d_1 + d_2 &\leq \mu_1 + \mu_2, \\ d_1 + d_2 + d_3 &\leq \mu_1 + \mu_2 + \mu_3, \\ &\cdots\cdots\cdots \\ d_1 + d_2 + \cdots + d_n &= \mu_1 + \mu_2 + \cdots + \mu_n \end{aligned} \tag{5}$$

for the diagonal entries $d : d_1 \geq d_2 \geq \cdots \geq d_n$ of matrix A. We will use for them a shortcut $d \preceq \mu$.

Consider now an immersion $f : L \to M$ of another compact Lie group L and the induced morphisms $f_* : \mathfrak{l} \hookrightarrow \mathfrak{m}$ and $f^* : \mathfrak{m}^* \to \mathfrak{l}^*$ of the Lie algebras and their duals. In the paper [1] Berenstein and Sjamaar found a decomposition of the projection $f^*(\mathcal{O}_\mu) \subset \mathfrak{l}^*$ of an M-orbit $\mathcal{O}_\mu \subset \mathfrak{m}^*$ into L-orbits $\mathcal{O}_\lambda \subset f^*(\mathcal{O}_\mu)$. Here we paraphrase their main result in a form suitable for the intended applications.

Fix Cartan subalgebras $\mathfrak{t}_L \hookrightarrow \mathfrak{t}_M$, and for every *test spectrum* $a \in \mathfrak{t}_L$ consider the inclusion of the adjoint orbits of groups L and M,

$$\varphi_a : \mathcal{O}_a \hookrightarrow \mathcal{O}_{f_*(a)}, \tag{6}$$

through a and $f_*(a)$ respectively. Topologically the orbits are (generalized) *flag varieties*. They carry a hidden complex structure coming from the representation

$$\mathcal{O}_a = L/Z_L(a) = L^{\mathbb{C}}/P_a, \tag{7}$$

where $P_a \subset L^{\mathbb{C}}$ is a parabolic subgroup of the complexified group $L^{\mathbb{C}}$ whose Lie algebra $\mathfrak{p}_a$ is spanned by $\mathfrak{t}_L$ and the root vectors X_α such that $\langle \alpha, a \rangle \geq 0$. One can say this in another way:

$$P_a = \{g \in L^{\mathbb{C}} \mid \lim_{t \to -\infty} e^{ta} g e^{-ta} \text{ exists}\},$$

which makes it clear that $f : P_a \to P_{f_*(a)}$.

[3] Hereafter we treat $\mathfrak{u}(n)$ as the algebra of Hermitian, rather than skew-Hermitian, operators at the expense of a modified Lie bracket $[X, Y] = i(XY - YX)$.

We will use the parabolic subgroups to construct *canonical bases* in cohomologies $H^*(\mathcal{O}_a)$ and $H^*(\mathcal{O}_{f_*(a)})$. Let $T_L \subset B \subset P_a$ be a Borel subgroup containing a maximal torus T_L with Lie algebra $\mathfrak{t}_L$. The flag variety $\mathcal{O}_a = L^{\mathbb{C}}/P_a$ splits into a disjoint union of *Schubert cells* BvP_a/P_a, parameterized by the left cosets $v \in W_L/W_{Z_L(a)}$ or in practice by representatives of minimal length $\ell = \ell(v)$ in these cosets. We actually prefer to deal with shifted cells $v^{-1}BvP_a/P_a = B^vP_a/P_a$ depending on the Borel subgroups $B^v \supset T_L$ modulo conjugation by the Weyl group of the centralizer $W(Z_L(a))$. The closure of B^vP_a/P_a is known as the *Schubert variety*, and its cohomology class $\sigma_v \in H^{2\ell(v)}(\mathcal{O}_a)$ is called the *Schubert cocycle*. These cocycles form the *canonical basis* of the cohomology ring $H^*(\mathcal{O}_a)$.

Inclusion (6) induces a morphism of the cohomologies

$$\varphi_a^* : H^*(\mathcal{O}_{f_*(a)}) \to H^*(\mathcal{O}_a), \tag{8}$$

given in the canonical bases by the coefficients $c_w^v(a)$ of the decomposition

$$\varphi_a^* : \sigma_w \mapsto \sum_v c_w^v(a)\sigma_v. \tag{9}$$

They play a crucial rôle in the next theorem. We extend them by zeros if either $v \in W_L$ or $w \in W_M$ is not the minimal representative of a coset in $W_L/W_{Z_L(a)}$ or $W_M/W_{Z_M(f_*(a))}$ respectively.

Theorem 1. *In the above notations the inclusion $\mathcal{O}_\lambda \subset f^*(\mathcal{O}_\mu)$ is equivalent to the following system of linear inequalities*

$$\langle\lambda, va\rangle \le \langle\mu, wf_*(a)\rangle \tag{a, v, w}$$

for all $a \in \mathfrak{t}_L$, $v \in W_L$, $w \in W_M$ such that $c_w^v(a) \neq 0$.

Proof. This is not the way Berenstein and Sjamaar stated their result. Instead, for some generic $a_0 \in \mathfrak{t}_L$ they fix positive Weyl chambers $\mathfrak{t}_L^+ \ni a_0$ and $\mathfrak{t}_M^+ \ni f_*(a_0)$ and use them to define Schubert cocycles $\sigma_v \in H^*(\mathcal{O}_a)$ and $\sigma_w \in H^*(\mathcal{O}_{f_*(a)})$ for all other $a \in \mathfrak{t}_L^+$. Hence their Schubert cocycles σ_w are canonical in the above sense iff $f_*(a)$ and $f_*(a_0)$ are in the same Weyl chamber. The set of such $a \in \mathfrak{t}_L^+$ form a convex polyhedral cone called the *principle cubicle*. It is determined by a_0, and different choices of a_0 produce a polyhedral decomposition of the positive Weyl chamber $\mathfrak{t}_L^+$ into cubicles.

For every cubicle Berenstein and Sjamaar gave a system of linear constraints on the dominant weights λ, μ, so that all together they provide a criterion for the inclusion $\mathcal{O}_\lambda \subset f^*(\mathcal{O}_\mu)$. For the principal cubicle the constraints are simplest and are as follows [1, Thm 3.2.1]:

$$v^{-1}\lambda \in f^*(w^{-1}\mu - \mathcal{C}), \quad \text{for} \quad c_w^v(a_0) \neq 0, \tag{10}$$

where $\mathcal{C}$ is a cone spanned by the positive roots in $\mathfrak{t}_M^*$. Note that $f^*(\mathcal{C})$ is the cone dual to the principal cubicle and therefore the above condition can be recast into the inequalities

$$\langle v^{-1}\lambda, a\rangle \le \langle f^*(w^{-1}\mu), a\rangle \Longleftrightarrow \langle\lambda, va\rangle \le \langle\mu, wf_*(a)\rangle, \tag{11}$$

that hold for all a from the principle cubicle *provided* that $c_w^v(a_0) \neq 0$. The coefficients $c_w^v(a)$ are actually constant inside the cubicle, and therefore the last condition can be changed to $c_w^v(a) \neq 0$. Thus we arrive at the inequalities (a, v, w) for the principle cubicle. Other inequalities (a, v, w) follow by choosing another cubicle as the principle one. They are equivalent to the remaining more complicated inequalities in [1, Thm 3.2.1], but look different since Berenstein and Sjamaar use other non-canonical Schubert cocycles. □

Example 2. Quantum marginal problem [17]. Let's illustrate the above theorem with immersion of unitary groups

$$f : \mathrm{U}(\mathcal{H}_A) \times \mathrm{U}(\mathcal{H}_B) \to \mathrm{U}(\mathcal{H}_{AB}), \qquad g_A \times g_B \mapsto g_A \otimes g_B,$$

where $\mathcal{H}_{AB} = \mathcal{H}_A \otimes \mathcal{H}_B$. As we have seen in Example 1 the coadjoint orbit of $\mathrm{U}(\mathcal{H}_{AB})$ consists of the isospectral Hermitian operators $\rho_{AB} : \mathcal{H}_{AB}$ understood here as *mixed states*. The projection

$$f^*(\rho_{AB}) = \rho_A \otimes 1 + 1 \otimes \rho_B$$

amounts to *reduced operators* $\rho_A : \mathcal{H}_A$ and $\rho_B : \mathcal{H}_B$ implicitly defined by the equations

$$\mathrm{Tr}_{\mathcal{H}_A}(\rho_A X_A) = \mathrm{Tr}_{\mathcal{H}_{AB}}(\rho_{AB} X_A), \qquad \mathrm{Tr}_{\mathcal{H}_B}(\rho_A X_B) = \mathrm{Tr}_{\mathcal{H}_{AB}}(\rho_{AB} X_B) \tag{12}$$

for all Hermitian operators $X_A : \mathcal{H}_A$ and $X_B : \mathcal{H}_B$. This means that ρ_A, ρ_B are just the visible states of the subsystems $\mathcal{H}_A$, $\mathcal{H}_B$. In this setting Theorem 1 tells us that all constraints on the decreasing spectra $\lambda^{AB} = \mathrm{Spec}(\rho^{AB})$, $\lambda^A = \mathrm{Spec}(\rho^A)$, and $\lambda^B = \mathrm{Spec}(\rho^B)$ are given by the inequalities

$$\sum_i a_i \lambda^A_{u(i)} + \sum_j b_j \lambda^B_{v(j)} \le \sum_k (a+b)^{\downarrow}_k \lambda^{AB}_{w(k)}, \tag{13}$$

for all test spectra $a : a_1 \ge a_2 \ge \cdots \ge a_n$, $b : b_1 \ge b_2 \ge \cdots \ge b_m$ from the Cartan subalgebras $\mathfrak{t}_A$, $\mathfrak{t}_B$ and permutations u, v, w such that $c^{uv}_w(a, b) \neq 0$. Here $(a+b)^{\downarrow}$ denotes the sequence $a_i + b_j$ arranged in decreasing order. The order determines the canonical Weyl chamber containing $f_*(a, b)$. The pairs (a, b) with fixed order of terms $a_i + b_j$ in $(a+b)^{\downarrow}$ form a cubicle.

The adjoint orbit $\mathcal{O}_a \subset \mathfrak{u}(\mathcal{H}_A)$ is a classical flag variety understood as the set of Hermitian operators $X_A : \mathcal{H}_A$ of spectrum $a = \mathrm{Spec}\, X_A$. Denote it by $\mathcal{F}_a(\mathcal{H}_A)$. Then the morphism (6) is given by the equation

$$\varphi_{ab} : \mathcal{F}_a(\mathcal{H}_A) \times \mathcal{F}_b(\mathcal{H}_B) \to \mathcal{F}_{a+b}(\mathcal{H}_{AB}), \quad (X_A, X_B) \mapsto X_A \otimes 1 + 1 \otimes X_B, \tag{14}$$

and the coefficients $c^{uv}_w(a, b)$ are determined by the induced morphism of the cohomologies

$$\begin{aligned} \varphi^*_{ab} : H^*(\mathcal{F}_{a+b}(\mathcal{H}_{AB})) &\to H^*(\mathcal{F}_a(\mathcal{H}_A)) \otimes H^*(\mathcal{F}_b(\mathcal{H}_B)) \\ \sigma_w \quad &\mapsto \sum_{u,v} c^{uv}_w(a, b) \cdot \sigma_u \otimes \sigma_v. \end{aligned} \tag{15}$$

One can find the details of their calculation in [17]. Note that $c^{uv}_w(a, b) = 1$ for identical permutations u, v, w. Hence we get for free the following *basic inequality*:

$$\sum_i a_i \lambda^A_i + \sum_j b_j \lambda^B_j \le \sum_k (a+b)^{\downarrow}_k \lambda^{AB}_k, \tag{16}$$

valid for all test spectra a, b.

3. One Point ν-Representability

In this section we apply the above results to the morphism $f : \mathrm{U}(\mathcal{H}) \to \mathrm{U}(\mathcal{H}^\nu)$ given by an irreducible representation $\mathcal{H}^\nu$ of group $\mathrm{U}(\mathcal{H})$ with a Young diagram ν of order $N = |\nu|$. For a column diagram we return to the N-fermion system $\wedge^N\mathcal{H}$, while a row diagram corresponds to the N-boson space $S^N\mathcal{H}$. However, the main reason to consider the general *para-statistical* representations $\mathcal{H}^\nu$ is not a uniform treatment of fermions and bosons, but taking into account spin. Observe that the state space of a single particle with spin splits into the tensor product $\mathcal{H} = \mathcal{H}_r \otimes \mathcal{H}_s$ of the orbital $\mathcal{H}_r$ and the spin $\mathcal{H}_s$ degrees of freedom. The total N-fermion space decomposes into spin-orbital components as follows [35]:

$$\wedge^N (\mathcal{H}_r \otimes \mathcal{H}_s) = \sum_{|\nu|=N} \mathcal{H}_r^\nu \otimes \mathcal{H}_s^{\nu^t}, \tag{17}$$

where ν^t stands for the transpose diagram. In many physical systems, like electrons in an atom or a molecule, the total spin is a well defined quantity that singles out a specific component of this decomposition. Theorem 1 applied to the component gives all constraints on the possible spin and orbital occupation numbers, see the details in n° 3.1.1 below.

3.1. Physical interpretation. Let's now relate Theorem 1 to the N-representability problem and its ramifications indicated above. We'll refer to the latter as the ν-*representability* problem.

It is instructive to think about $X \in \mathfrak{u}(\mathcal{H})$ as an *observable* and treat $\rho \in \mathfrak{u}(\mathcal{H})^*$ as a *mixed state* with the duality pairing given by the expectation value of X in state ρ,

$$\langle X, \rho\rangle = \mathrm{Tr}_{\mathcal{H}}\, X\rho \tag{18}$$

(forget for a while about the positivity $\rho \geq 0$ and normalization $\mathrm{Tr}\,\rho = 1$).

We want to elucidate the physical meaning of the projection $f^* : \mathfrak{u}(\mathcal{H}^\nu)^* \to \mathfrak{u}(\mathcal{H})^*$ uniquely determined by the equation

$$\langle f_*(X), \rho^\nu\rangle = \langle X, f^*(\rho^\nu)\rangle, \qquad X \in \mathfrak{u}(\mathcal{H}), \qquad \rho^\nu \in \mathfrak{u}(\mathcal{H}^\nu)^*.$$

In the above setting (18) it reads as follows:

$$\mathrm{Tr}_{\mathcal{H}^\nu}(X\rho^\nu) = \mathrm{Tr}_{\mathcal{H}}(Xf^*(\rho^\nu)), \qquad \forall X \in \mathfrak{u}(\mathcal{H}). \tag{19}$$

A good point to start with is *Schur's duality* between irreducible representations of the unitary $\mathrm{U}(\mathcal{H})$ and the symmetric S_N groups,

$$\mathcal{H}^{\otimes N} = \sum_{|\nu|=N} \mathcal{H}^\nu \otimes \mathcal{S}^\nu. \tag{20}$$

The latter group acts on $\mathcal{H}^{\otimes N}$ by permutations of the tensor factors, and its irreducible representations $\mathcal{S}^\nu$ show up in the right-hand side. One can treat $\mathcal{H}^{\otimes N}$ as a state space of N-particles, and for identical particles all physical quantities should commute with S_N. Looking into the right-hand side of (20) we see that such quantities are linear combinations of operators $\rho^\nu \otimes 1$ acting in the component $\mathcal{H}^\nu \otimes \mathcal{S}^\nu$ and equal to zero elsewhere. In the case of a genuine mixed state ρ^ν, i.e. a nonnegative operator of trace

1, one can treat $(\rho^\nu \otimes 1)/\dim \mathcal{S}^\nu$ as a mixed state of N identical particles obeying some para-statistics of type ν. Let $\rho_i : \mathcal{H}$ be its i^{th} *reduced state*. Since $\rho^\nu \otimes 1$ commutes with S_N, the reduced state $\rho = \rho_i$ is actually independent of i. However, occasionally we retain the index i just to indicate the tensor component where it operates.

Proposition 1. *In the above notations*

$$f^*(\rho^\nu) = N\rho. \tag{21}$$

Proof. We have to check that (21) fits Eq. (19):

$$\operatorname{Tr}_{\mathcal{H}^\nu}(X\rho^\nu) = \operatorname{Tr}_{\mathcal{H}^\nu\otimes\mathcal{S}^\nu} X\frac{\rho^\nu\otimes 1}{\dim\mathcal{S}^\nu} = \operatorname{Tr}_{\mathcal{H}^{\otimes N}} X\frac{\rho^\nu\otimes 1}{\dim\mathcal{S}^\nu} = \sum_i \operatorname{Tr}_{\mathcal{H}} X_i\rho_i = N\operatorname{Tr}_{\mathcal{H}} X\rho,$$

where X_i is a copy of X acting in the i^{th} component of $\mathcal{H}^{\otimes N}$, so that

$$\operatorname{Tr}_{\mathcal{H}^{\otimes N}} X_i\frac{\rho^\nu\otimes 1}{\dim\mathcal{S}^\nu} = \operatorname{Tr}_{\mathcal{H}} X_i\rho_i$$

by definition (12) of the reduced state. □

A general ν-*representability problem* concerns the relationship between the spectrum μ of a mixed state ρ^ν and spectrum λ of its *particle density matrix* $N\rho$. The latter spectrum is known as the *occupation numbers*[4] of the system in state ρ^ν. Formally the constraints on the spectra are given by Theorem 1.

Remark 1. The above construction allows for a given mixed state ρ^ν to define the higher order reduced matrices. Their characterization would have almost unlimited applications. Indeed, behavior of most systems of physical interest is governed by two-particle interaction. As a result, the energy of a state becomes a linear functional of its two-point reduced matrix. To minimize the energy and to find the correlation matrix of the ground state one has to elucidate all the constraints that a two-point reduced matrix should satisfy. This problem and the whole program are known as the *Coulson challenge*[5] [6]. In the form just described it may be unfeasible even for quantum computers [23]. For other approaches and the current state of the art see [26]. This problem is far beyond the scope of our paper. Nevertheless, the characterization of one point reduced matrices given below imposes also new constraints on the higher reduced states.

3.1.1. Constraints on spin and orbital occupation numbers Let's return to a system of N fermions, this time of smallest possible spin $s = 1/2$, $\dim\mathcal{H}_s = 2$. In this case spin-orbital decomposition (17) involves only terms

$$\mathcal{H}_r^\nu \otimes \mathcal{H}_s^{\nu^t} \tag{22}$$

with at most a two-column diagram ν. The sizes of the columns $\alpha \geq \beta$ are determined by equations

$$\alpha + \beta = N, \qquad \alpha - \beta = 2J, \tag{23}$$

[4] More precisely, the occupation numbers of *natural orbitals*. The latter are defined as eigenvectors of the particle density matrix.

[5] Also known as two-particle N-representability or, following D. Herschbach, a holy grail of theoretical chemistry.

where J is the total spin of the system, so that $\mathcal{H}_s^{\nu^t} = \mathcal{H}_J$ is just the spin J representation of the group $\mathrm{SU}(\mathcal{H}_s) = \mathrm{SU}(2)$.

Consider now a pure N-fermion state of total spin J

$$\psi \in \mathcal{H}_r^\nu \otimes \mathcal{H}_J,$$

where the diagram ν is determined by Eqs. (23). Let ρ^ν and ρ^J be its reduced states in the orbital and spin components respectively. The basic fact is that the reduced states are isospectral Spec $\rho^\nu =$ Spec ρ^J. Hence Spec ρ^ν can be identified with the *spin occupation numbers*. On the other hand Theorem 1, in view of Proposition 1, relates Spec ρ^ν with the *orbital occupation numbers* given by the spectrum of the particle density matrix $N\rho$. In this way one can produce all constraints on allowed spin and orbital occupation numbers, *provided* that a solution of the ν-representability problem is known for two-column diagrams. We address this issue in Sects. 3.2 and 3.3. See also Corollary 1 in Sect. 3.2.

3.2. Formal solution of the ν-representability problem. Henceforth we treat the lower index r as the rank of the Hilbert space $\mathcal{H}_r$. Recall that the character of the representation $\mathcal{H}_r^\nu$, i.e. the trace of a diagonal operator

$$z = \mathrm{diag}(z_1, z_2, \ldots, z_r) \in \mathrm{U}(\mathcal{H}_r), \tag{24}$$

in some orthonormal basis e of $\mathcal{H}_r$, is given by *Schur's function* $S_\nu(z_1, z_2, \ldots, z_r)$. It has a purely combinatorial description in terms of the so called *semistandard tableaux* T of shape ν. The latter are obtained from the diagram ν by filling it with numbers $1, 2, \ldots, r$ strictly increasing in columns and weakly in rows. Then the Schur function can be written as a sum of monomials $z^T = \prod_{i\in T} z_i$,

$$S_\nu(z) = \sum_T z^T,$$

corresponding to all semistandard tableaux T of shape ν. The monomials are actually the *weights* of representation $\mathcal{H}_r^\nu$, meaning that

$$z \cdot e_T = z^T e_T \tag{25}$$

for some basis e_T of $\mathcal{H}_r^\nu$ parameterized by the semistandard tableaux. Denote by $\mathfrak{t} \subset \mathfrak{u}(\mathcal{H}_r)$ and $\mathfrak{t}_\nu \subset \mathfrak{u}(\mathcal{H}_r^\nu)$ the Cartan subalgebras of real diagonal operators in the bases e and e_T respectively, so that the *differential* of the above group action $z : e_T \mapsto z^T e_T$ gives the morphism

$$f_* : \mathfrak{t} \to \mathfrak{t}_\nu, \qquad f_*(a) : e_T \mapsto a_T e_T, \tag{26}$$

where $a_T := \sum_{i\in T} a_i$. As in Example 2 we treat the orbits $\mathcal{O}_a$ and $\mathcal{O}_{f_*(a)}$ as flag varieties $\mathcal{F}_a(\mathcal{H}_r)$ and $\mathcal{F}_{a^\nu}(\mathcal{H}_r^\nu)$ consisting of Hermitian operators of spectra $a : a_1 \geq a_2 \geq \cdots \geq a_r$ and a^ν respectively. Here a^ν consists of the quantities a_T arranged in the non-increasing order

$$a^\nu := \{a_T \mid T = \text{semistandard tableau of shape } \nu\}^\downarrow. \tag{27}$$

Finally, we need the morphism

$$\varphi_a : \mathcal{F}_a(\mathcal{H}_r) \to \mathcal{F}_{a^\nu}(\mathcal{H}_r^\nu), \qquad X \mapsto f_*(X), \tag{28}$$

together with its cohomological version

$$\varphi_a^* : H^*(\mathcal{F}_{a^\nu}(\mathcal{H}_r^\nu)) \to H^*(\mathcal{F}_a(\mathcal{H}_r)), \tag{29}$$

given in the canonical bases by coefficients $c_w^v(a)$:

$$\varphi_a^* : \sigma_w \mapsto \sum_v c_w^v(a)\sigma_v. \tag{30}$$

Theorem 2. *In the above notations all constraints on the occupation numbers λ of the system $\mathcal{H}_r^\nu$ in a state ρ^ν of spectrum μ are given by the inequalities*

$$\sum_i a_i \lambda_{v(i)} \le \sum_k a_k^\nu \mu_{w(k)} \tag{31}$$

for all test spectra a and permutations v, w such that $c_w^v(a) \neq 0$.

Proof. In view of Proposition 1, this is what Theorem 1 tells. One has to remember that the left action of a permutation on "places" is inverse to its right action on indices. That is why the permutations v and w, acting on a and $f_*(a) = a^\nu$ in Theorem 1, move to the indices of λ and μ in the inequality (31). □

The coefficient $c_w^v(a)$ depends only on the order in which quantities a_T appear in the spectrum a^ν. The order changes when the test spectrum a crosses a hyperplane

$$H_{T|T'} : \sum_{i \in T} a_i = \sum_{j \in T'} a_j.$$

The hyperplanes cut the set of all test spectra into a finite number of polyhedral cones called *cubicles*. For each cubicle one has to check the inequality (31) only for its *extremal edges*. As a result, the ν-representability amounts to a *finite system* of linear inequalities.

Remark 2. Let's emphasize once again the difference between the Berenstein-Sjamaar Theorem [1, Thm 3.2.1] and its version used in this paper. In the settings of Theorem 2 it manifests itself in the way the quantities a_T are ordered in the spectrum a^ν, or which parabolic subgroup is used for definition of Schubert cocycles. Berenstein and Sjamaar choose a specific order of tableaux T, while we rely on the natural order of the quantities $a_T = \sum_{i \in T} a_i$. The latter choice allows to treat the inequalities uniformly, and to avoid a rather cumbersome transformation every time the test spectrum passes from one cubicle to another.

Recall from Sect. 3.1.1 that the theorem also describes a relationship between the spin and orbital occupation numbers. We keep for them the above notations μ and λ respectively.

Corollary 1. *All constraints on spin and orbital occupation numbers of N-electron system in a pure state of total spin J are given by the inequalities (31), applied to two column diagram ν determined by Eqs. (23), and bounded to mixed states ρ^ν of rank not exceeding dimensionality $2J + 1$ of the spin space.*

We postpone the calculation of the coefficients $c_w^v(a)$ to Sect. 3.3 and focus instead on some general results that can be deduced from the theorem as it stands.

3.2.1. Basic inequalities Being a ring homomorphism, φ_a^* maps unit into unit $\varphi_a^*(1) = 1$, that is $c_w^v(a) = 1$ for identical permutations v, w. Hence the following *basic inequality*

$$\sum_i a_i \lambda_i \leq \sum_k a_k^\nu \mu_k$$

holds for all test spectra a. Let's look at it more closely for a *pure state* $\rho^\nu = |\psi\rangle\langle\psi|$ in which case the right-hand side is maximal and the inequality takes the form

$$\sum_i a_i \lambda_i \leq a_1^\nu = \max_T \sum_{i\in T} a_i = \sum_i a_i \nu_i, \tag{32}$$

where $\nu_1 \geq \nu_2 \geq \cdots \geq 0$ are rows of ν. The maximum in the right-hand side is attained for the tableau T of shape ν whose i-row is filled by i.

The normalization $\sum_i \lambda_i = N = \sum_j \nu_j$ allows to shift the test spectra into the positive domain $a_1 \geq a_2 \geq \cdots \geq 0$, so that they become nonnegative linear combinations of the fundamental weights

$$\omega_k = (\underbrace{1, 1, \ldots, 1}_{k}, 0, 0, \ldots, 0). \tag{33}$$

Hence it is enough to check (32) for $a = \omega_k$, that gives the *majorization inequality* $\lambda \preceq \nu$, cf. Example 1. Thus we arrive at the first claim of the following result that characterizes occupation numbers of system $\mathcal{H}^\nu$ in an unspecified mixed state.

Theorem 3. *The occupation numbers of the system $\mathcal{H}^\nu$ in an arbitrary mixed state satisfy the majorization inequality*

$$\lambda \preceq \nu, \tag{34}$$

and any such λ can be realized as the occupation numbers of some mixed state.

Proof. The second claim follows from two observations:

1. *The occupation numbers of a coherent state $\psi \in \mathcal{H}^\nu$, that is a highest vector of the representation, are equal to ν.*
2. *The set of allowed occupation numbers, written in any order, form a convex set.*

Indeed, the polytope given by the majorization inequality (34) is just a convex hull of vectors obtained from ν by permutations of coordinates, cf. Example 1. Hence by 1 and 2 it consists of legitimate occupation numbers.

Proof of 1. Consider a decomposition of the complexified Lie algebra

$$\mathfrak{u}(\mathcal{H}) \otimes \mathbb{C} = \mathfrak{gl}(\mathcal{H}) = \mathfrak{n}_- + \mathfrak{h} + \mathfrak{n}_+,$$

into a diagonal Cartan subalgebra $\mathfrak{h} = \mathfrak{t} \otimes \mathbb{C}$ accompanied with lower- and upper-triangular nilpotent subalgebras $\mathfrak{n}_\mp$. By definition $\mathfrak{n}_+$ annihilates the highest vector $\psi \in \mathcal{H}^\nu$ of weight ν. Hence $\langle\psi|X^\pm|\psi\rangle = \langle X^\mp\psi|\psi\rangle = 0$ for all $X^\pm \in \mathfrak{n}_\pm$. Then by Eq. (19)

$$\langle\psi|X^\pm|\psi\rangle = \mathrm{Tr}_{\mathcal{H}^\nu}(X^\pm|\psi\rangle\langle\psi|) = \mathrm{Tr}_{\mathcal{H}}(X^\pm f^*(|\psi\rangle\langle\psi|)) = 0, \qquad \forall X^\pm \in \mathfrak{n}_\pm.$$

This means that $\rho = f^*(|\psi\rangle\langle\psi|)$ is a diagonal matrix. On the other hand $t\psi = \langle t, \nu\rangle\psi$ for $t \in \mathfrak{t}$, hence as above

$$\langle t, \nu\rangle = \langle\psi|t|\psi\rangle = \mathrm{Tr}_{\mathcal{H}^\nu}(t|\psi\rangle\langle\psi|) = \mathrm{Tr}_{\mathcal{H}}(tf^*(|\psi\rangle\langle\psi|)) = \mathrm{Tr}_{\mathcal{H}}(t\rho) = \langle t, \rho\rangle,$$

that is $\mathrm{Spec}\,\rho = \nu$.

Proof of 2. Let ρ_1^ν, ρ_2^ν be mixed states, with the particle densities ρ_1, ρ_2, and the occupation numbers λ_1, λ_2. We apply to ρ_1, ρ_1^ν a unitary rotation $\rho_1 \mapsto U\rho_1 U^*, \rho_1^\nu \mapsto U\rho_1^\nu U^*$ that transforms orthonormal eigenvectors of ρ_1 into that of ρ_2 in a prescribed order. The resulting new operators ρ_1, ρ_2 commute and have the original spectra λ_1, λ_2. Then the particle density matrix $\rho = p_1\rho_1 + p_2\rho_2$ of the convex combination $\rho^\nu = p_1\rho_1^\nu + p_2\rho_2^\nu$ has spectrum $\lambda = p_1\lambda_1 + p_2\lambda_2$. □

For a column diagram ν the majorization inequality $\lambda \preceq \nu$ amounts to the *Pauli exclusion principle* $\lambda_i \leq 1$. In general, we refer to it as the *Pauli constraint*. Note that the above proof shows that equality in (34) is attained for coherent states only. The second part of Theorem 3 extends Coleman's result [5] for $\wedge^N\mathcal{H}$.

Recall, that the theorem solves the ν-representability problem for unspecified mixed states. We will see later that for pure states the answer in general is much more complicated. Nevertheless, there are surprisingly many systems for which the majorization inequality alone is sufficient for pure ν-representability. We address them in the next item.

3.2.2. Pure moment polytope One of the most striking features of Theorem 2 is the linearity of the constraints (31). As a result, the allowed spectra (λ, μ) form a convex polytope, called (noncommutative) *moment polytope*. The convexity still holds for any fixed $\mu = \operatorname{Spec}\rho^\nu$, and in particular for the occupation numbers λ of all *pure* states. We refer to the latter case as the *pure moment polytope*. It sits inside the positive Weyl chamber, and its multiple kaleidoscopic reflections in the walls of the chamber generally form a *nonconvex* rosette, consisting of all legitimate occupation numbers written in an arbitrary order. It can be convex only if all constraints on the occupation numbers are given by the majorization inequality $\lambda \preceq \nu$ alone. Here we describe a class of representations $\mathcal{H}^\nu$ with this property.

This happens, for example, for a system of $N \geq 2$ bosons. In this case ν is a row diagram and the majorization inequality imposes no constraints on λ. By Theorem 3 this means that every nonnegative spectrum λ of trace N represents occupation numbers of some *mixed* state. However for bosons one can easily find a *pure* state that does the job:

$$\psi = \sum_i \sqrt{\lambda_i}\, e_i^{\otimes N} \in S^N\mathcal{H},$$

where e_i is an orthonormal basis of $\mathcal{H}$. This makes the bosonic N-representability problem trivial.

A more interesting physical example constitutes the so-called *closed shell*, meaning a system of electrons of total spin zero. The corresponding diagram ν consists of two columns of equal length. We will see shortly that in this case the Pauli constraint $\lambda \leq 2$ shapes the pure moment polytope.

Observe that it is enough to construct pure states whose occupation numbers are generators of the cone cut out of the Weyl chamber by the majorization inequality $\lambda \preceq \nu$. Then the convexity does the rest.

Recall that in the proof of Theorem 3 we have already identified ν with the occupation numbers of a *coherent state*. Due to the majorization inequality $\lambda \preceq \nu$, the entropy of its reduced state is minimal possible. For that reason coherent states are generally considered closest to classical ones [30]. At the other extreme one finds the so-called *completely entangled* states $\psi \in \mathcal{H}^\nu$ whose particle density matrix $\rho = f^*(|\psi\rangle\langle\psi|)$ is scalar and the reduced entropy is maximal [19]. By definition (19) we have

$\mathrm{Tr}_{\mathcal{H}}(X\rho) = \mathrm{Tr}_{\mathcal{H}^\nu}(X|\psi\rangle\langle\psi|) = \langle\psi|X|\psi\rangle$, so that the completely entangled states can be described by the equation

$$\langle\psi|X|\psi\rangle = 0, \qquad \forall\, X \in \mathfrak{su}(\mathcal{H}). \tag{35}$$

Let's call a system $\mathcal{H}_r^\nu$ *exceptional* if the $\mathrm{SU}(\mathcal{H}_r)$-representation $\mathcal{H}_r^\nu$ is equivalent to one of the following: $\mathcal{H}_r$, its dual $\mathcal{H}_r^*$, and, for odd rank r, $\wedge^2\mathcal{H}_r$, $\wedge^2\mathcal{H}_r^*$. The Young diagram ν of an exceptional system can be obtained from an $r \times m$ rectangle by adding an extra column of length $1, r-1, 2, r-2$ respectively.

One readily realizes that the exceptional systems contain no completely entangled states, say because the reduced matrix of $\psi \in \wedge^2\mathcal{H}_r$ has an even rank.

Proposition 2. *In every non-exceptional system $\mathcal{H}^\nu$ there exists a completely entangled state.*

Proof. The result is actually well known, but in a different context. The entanglement equation (35) is nothing but the stationarity condition for the length of vector $\langle\psi|\psi\rangle$ with respect to the action of the *complexified* group $\mathrm{SL}(\mathcal{H})$. It is known [34] that every stationary point is actually a minimum, and an $\mathrm{SL}(\mathcal{H})$-orbit contains a minimal vector if and only if the orbit is closed. As a result, we end up with the problem of existence of a nonzero closed orbit, or, what is the same, the existence of a nonconstant polynomial invariant. The proposition just reproduces a known answer to the latter question [34]. □

By admitting other simple Lie groups we find only two more exceptional representations: the standard representation of the symplectic group $\mathrm{Sp}(n)$ and a halfspinor representation of $\mathrm{Spin}(10)$.

Now we can solve the pure ν-representability problem for a wide class of systems, including the above mentioned closed shell.

Theorem 4. *Suppose that all columns of Young diagram ν are multiple, meaning that every number in the sequence of column lengths $\nu_1^t \geq \nu_2^t \geq \nu_3^t \geq \cdots$ appears at least twice. Then all constraints on the occupation numbers of the system $\mathcal{H}^\nu$ in a pure state are given by the majorization inequality $\lambda \preceq \nu$ alone.*

Proof. We'll proceed by induction on the height of the diagram ν. The triviality of the bosonic N-representability problem provides a starting point for the induction.

Let now λ be a vertex of the polytope cut out of the positive Weyl chamber by the majorization inequality $\lambda \preceq \nu$. Note that the latter includes the equation $\mathrm{Tr}\,\lambda = \mathrm{Tr}\,\nu$. Then the following alternative holds:

1. *Either all nonzero components of λ are equal,*
2. *Or one can split λ and ν into two parts $\lambda = \lambda'|\lambda''$, $\nu = \nu'|\nu''$ containing the first p components and the remaining ones, both satisfying the inequalities $\lambda' \preceq \nu'$, $\lambda'' \preceq \nu''$.*

Indeed, the second claim states that the p^{th} majorization inequality in (5) turns into an equation. On the other hand, if all the majorization inequalities are strict, and λ contains different nonzero entries, then one can linearly vary these entries preserving the non-increasing order of λ and the majorization $\lambda \preceq \nu$. As result we get a line segment in the polytope containing λ, which is impossible for a vertex.

We have to prove that every vertex λ represents occupation numbers of some pure state. Consider the above two cases separately.

Case 1. Let λ contain r equal nonzero entries and $\mathcal{H}_r \subset \mathcal{H}$ be a subspace of dimension r. The conditions of the theorem ensure that the system $\mathcal{H}_r^\nu$ is non-exceptional, hence by Proposition 2 it contains a state $\psi \in \mathcal{H}_r^\nu$ with occupation numbers equal to the nonzero part of λ. In the bigger system $\mathcal{H}^\nu \supset \mathcal{H}_r^\nu$ its occupation numbers will be extended by zeros.

Case 2. Let the system have rank $r = p + q$. Choose a decomposition $\mathcal{H}_r = \mathcal{H}_p \oplus \mathcal{H}_q$ and consider a restriction of the representation $\mathcal{H}_r^\nu$ onto subgroup $\mathrm{U}(\mathcal{H}_p) \times \mathrm{U}(\mathcal{H}_q)$

$$\mathcal{H}_r^\nu = \sum_{\mu,\pi} c_{\mu\pi}^\nu \mathcal{H}_p^\mu \otimes \mathcal{H}_q^\pi, \tag{36}$$

where $c_{\mu\pi}^\nu$ are the omnipresent Littlewood-Richardson coefficients. Observe that $c_{\nu'\nu''}^\nu = 1$, and therefore $\mathcal{H}_p^{\nu'} \otimes \mathcal{H}_q^{\nu''} \subset \mathcal{H}_r^\nu$. By the induction hypothesis there exist states $\psi' \in \mathcal{H}_p^{\nu'}$ and $\psi'' \in \mathcal{H}_q^{\nu''}$ with occupation numbers λ', λ'' and particle densities ρ', ρ'' respectively. Then decomposable state $\psi = \psi' \otimes \psi''$ has particle density $\rho' \oplus \rho''$, and its occupation numbers are equal to $\lambda = \lambda'|\lambda''$. □

Let's extract for reference a useful corollary from the last part of the proof.

Corollary 2. *Suppose that the Littlewood-Richardson coefficient $c_{\mu\pi}^\nu$ is nonzero. Then merging the occupation numbers λ', λ'' of the systems $\mathcal{H}_p^\mu$, $\mathcal{H}_q^\pi$ form legitimate occupation numbers of the system $\mathcal{H}_{p+q}^\nu$.*

Remark 3. The restriction on the column's multiplicities of diagram ν is needed only to ensure that the components of any splitting $\nu = \nu'|\nu''|\nu'''|\ldots$ are non-exceptional. The latter condition holds for any two-row diagram $[\alpha, \beta]$, $\beta \neq 1$ for $\dim \mathcal{H} \geq 3$. This gives examples of systems beyond Theorem 4, say for $\nu = [3, 2]$, whose pure moment polytope is given by the majorization inequality alone. More such diagrams can be produced as follows: take ν as in Theorem 4 and remove one cell from its last row. This works when the last row contains at least three cells and the rank of the system is bigger than the height of ν. A complete classification of all such systems is still missing.

3.2.3. Dadok-Kac construction In the last two theorems we encounter the problem of constructing a pure state with given occupation numbers. The problem lies at the very heart of the ν-representability and one shouldn't expect an easy solution. Nevertheless, there is a combinatorial construction that produces a state with *diagonal* density matrix, whose spectrum can be easily controlled. It has been used first by Borland and Dennis [3] to forecast the structure of the moment polytope for small fermionic systems. Later on Müller [27] formalized and advanced their approach to the limit. It fits into a general Dadok-Kac construction [10] that works for any representation.

Below we follow the notations introduced at the beginning of Sect. 3.2. Let $x = \mathrm{diag}(x_1, x_2, \ldots, x_r)$ be a typical element from the Cartan subalgebra $\mathfrak{t} \subset \mathfrak{u}(\mathcal{H}_r)$. For a given semi-standard tableau T call the linear form $\omega_T : x \mapsto x_T = \sum_{i \in T} x_i$ the *weight* of the basic vector $e_T \in \mathcal{H}_r^\nu$. We also need nonzero weights of the adjoint representation $\alpha_{ij} : x \mapsto x_i - x_j$, $i \neq j$ called *roots*. Let's turn the set of semi-standard tableaux of shape ν into a graph by connecting T and T' each time $\omega_T - \omega_{T'}$ is a root, i.e. the contents of T and T', considered as multi-sets, differ by exactly one element.

Proposition 3. *Let* $\mathbf{T}$ *be a set of semi-standard tableaux of shape* ν *containing no connected pairs. Then every state* $\psi = \sum_{T\in\mathbf{T}} c_T e_T \in \mathcal{H}^\nu$ *with support* $\mathbf{T}$ *has a diagonal particle density matrix with entries*

$$\lambda_i = \sum_{T\ni i} |c_T|^2, \tag{37}$$

where every tableau T *is counted as many times as the index* i *appears in it.*

Proof. The proof refines the arguments used in Claim 1 of Theorem 3, from which we borrow the notation. As in the above theorem we have to prove $\langle\psi|X|\psi\rangle = 0$ for every $X \in \mathfrak{n}_+ + \mathfrak{n}_-$. It is enough to consider root vectors X_α that form a basis of $\mathfrak{n}_+ + \mathfrak{n}_-$. Then

$$\langle\psi|X_\alpha|\psi\rangle = \sum_{T,T'\in\mathbf{T}} \overline{c}_{T'} c_T \langle e_{T'}|X_\alpha|e_T\rangle.$$

Since $X_\alpha e_T$ has weight $\alpha + \omega_T$, it is orthogonal to $e_{T'}$, except for $\omega_{T'} = \omega_T + \alpha$. The latter is impossible for $T, T' \in \mathbf{T}$, and therefore the reduced state of ψ is diagonal. A straightforward calculation gives the diagonal entries (37). □

We'll have a chance to use this construction in Sect. 4.1.

Note that for a fixed support $\mathbf{T}$ the set of unordered spectra (37) form a convex polytope. It is not known when this approach exhausts the whole moment polytope. The smallest fermionic system where it fails is $\wedge^3\mathcal{H}_8$, see Sect. 6.

3.3. Calculation of the coefficients $c_w^\nu(a)$. To progress further and to give Theorem 1 full strength one has to calculate the coefficients $c_w^\nu(a)$. Berenstein and Sjamaar left this problem mostly untouched. However, in the ν-representability settings, highlighted in Theorem 2, this can be done very explicitly.

3.3.1. Canonical generators To proceed we first need an alternative description of the cohomology of the flag variety $\mathcal{F}_a(\mathcal{H}_r)$ [2]. Recall that the latter is understood here as the set of Hermitian operators in $\mathcal{H}_r$ of given spectrum a. To avoid technicalities, we assume the spectrum to be simple, $a_1 > a_2 > \cdots > a_r$. Let $\mathcal{E}_i$ be the *eigenbundle* on $\mathcal{F}_a(\mathcal{H}_r)$ whose fiber at $X \in \mathcal{F}_a(\mathcal{H}_r)$ is the eigenspace of operator X with eigenvalue a_i. Their Chern classes $x_i = c_1(\mathcal{E}_i)$ generate the cohomology ring $H^*(\mathcal{F}_a(\mathcal{H}_r))$ and we refer to them as the *canonical generators*. The elementary symmetric functions $\sigma_i(x)$ of the canonical generators are the characteristic classes of the trivial bundle $\mathcal{H}_r$ and thus vanish. This identifies the cohomology with the *ring of coinvariants*

$$H^*(\mathcal{F}_a(\mathcal{H}_r)) = \mathbb{Z}[x_1, x_2, \ldots, x_r]/(\sigma_1, \sigma_2, \ldots, \sigma_r). \tag{38}$$

This approach to the cohomology is more functorial and for that reason leads to an easy calculation of the morphism (29),

$$\varphi_a^* : H^*(\mathcal{F}_{a^\nu}(\mathcal{H}^\nu)) \to H^*(\mathcal{F}_a(\mathcal{H})).$$

Recall that the spectrum a^ν consists of the quantities $a_T = \sum_{i\in T} a_i$ arranged in decreasing order, where T runs over all semi-standard tableaux of shape ν. We define $x_T = \sum_{i\in T} x_i$ in a similar way.

Proposition 4. *Let x_i and x_k^ν be the canonical generators of $H^*(\mathcal{F}_a(\mathcal{H}))$ and $H^*(\mathcal{F}_{a^\nu}(\mathcal{H}^\nu))$ respectively. Then*

$$\varphi_a^*(x_k^\nu) = x_T, \quad \textit{when} \quad a_k^\nu = a_T. \tag{39}$$

In other words, $\varphi_a^*(x_k^\nu)$ is obtained from a_k^ν by the substitution $a_i \mapsto x_i$.

Proof. The eigenbundle $\mathcal{E}_i$ is equivariant with respect to the adjoint action $X \mapsto uXu^*$ of the unitary group $\mathrm{U}(\mathcal{H})$. Therefore it is uniquely determined by the linear representation of the centralizer $D = Z(X)$ in a fixed fiber $\mathcal{E}_i(X)$ or by its character $\varepsilon_i : D \to \mathbb{S}^1 = \{z \in \mathbb{C}^* \mid |z| = 1\}$. In the eigenbasis e of the operator X the centralizer becomes a diagonal torus with typical element $z = \mathrm{diag}(z_1, z_2, \dots, z_r)$ and the character $\varepsilon_i : z \mapsto z_i$.

Let now $X^\nu = \varphi_a(X)$, $D^\nu = Z(X^\nu)$, and e_T be the weight basis of $\mathcal{H}^\nu$, introduced in Sect. 3.2, parameterized by the semi-standard tableaux T of shape ν and arranged in the order of eigenvalues a^ν. Then the character of the pull-back $\varphi_a^{-1}(\mathcal{E}_k^\nu)$ is just the weight $\prod_{i\in T} \varepsilon_i$ of the k^{th} vector e_T, where the tableau T is determined from the equation $a_k^\nu = a_T$, cf. (25). Thus $\varphi_a^{-1}(\mathcal{E}_k^\nu) = \bigotimes_{i\in T} \mathcal{E}_i$, and we finally get

$$\varphi_a^*(x_k^\nu) = \varphi_a^*(c_1(\mathcal{E}_k^\nu)) = c_1(\varphi_a^{-1}(\mathcal{E}_k^\nu)) = c_1\Big(\bigotimes_{i\in T} \mathcal{E}_i\Big) = \sum_{i\in T} x_i = x_T.$$

□

Remark 4. Formula (39) may look ambiguous for a degenerate spectrum a, while in fact it is perfectly self-consistent. Indeed, consider a small perturbation $\tilde{a}$, resolving multiple components of a, and the natural projection

$$\pi : \mathcal{F}_{\tilde{a}}(\mathcal{H}) \to \mathcal{F}_a(\mathcal{H})$$

that maps $\widetilde{X} = \sum_i \tilde{a}_i |e_i\rangle\langle e_i|$ into $X = \sum_i a_i |e_i\rangle\langle e_i|$, where e_i is an orthonormal eigenbasis of $\widetilde{X}$. It is known [2] that π induces the isomorphism

$$\pi^* : H^*(\mathcal{F}_a(\mathcal{H})) \simeq H^*(\mathcal{F}_{\tilde{a}}(\mathcal{H}))^{W(D)}, \tag{40}$$

where the right-hand side denotes the algebra of invariants with respect to permutations of the canonical generators $\tilde{x}_i$ with the same unperturbed eigenvalue $a_i = \alpha$. Such permutations form the Weyl group $W(D)$ of the maximal torus $\widetilde{D} = Z(\widetilde{X})$ in $D = Z(X)$. For example, characteristic classes of the eigenbundle $\mathcal{E}_\alpha$ with the multiple eigenvalue $\alpha = a_i$ correspond to elementary symmetric functions of the respective variables $\tilde{x}_i$.

Equation (39), as it stands, depends on a specific ordering of the unresolved spectral values a_i and a_k^ν. However, when φ_a^* is applied to invariant elements with respect to the above Weyl group, the ambiguity vanishes.

Note also that the Schubert cocycle $\sigma_w \in H^*(\mathcal{F}_{\tilde{a}}(\mathcal{H}))$ is invariant with respect to $W(D)$ if and only if w is the shortest representative in its left coset modulo $W(D)$. Such cocycles form the canonical basis of cohomology $H^*(\mathcal{F}_a(\mathcal{H}))$.

3.3.2. Schubert polynomials To calculate the coefficients $c_w^v(a)$ we have to return to the Schubert cocycles σ_w and express them via the canonical generators x_i. This can be accomplished by the *divided difference operators*

$$\partial_i : f(x_1, x_2, \dots, x_n) \mapsto \frac{f(\dots, x_i, x_{i+1}, \dots) - f(\dots, x_{i+1}, x_i, \dots)}{x_i - x_{i+1}} \tag{41}$$

as follows. Write a permutation $w \in S_n$ as a product of the minimal number of transpositions $s_i = (i, i+1)$,

$$w = s_{i_1} s_{i_2} \cdots s_{i_\ell}. \tag{42}$$

The number of factors $\ell(w) = \#\{i < j \mid w(i) > w(j)\}$ is called the *length* of the permutation w. The product

$$\partial_w := \partial_{i_1} \partial_{i_2} \cdots \partial_{i_\ell}$$

is independent of the reduced decomposition and in terms of these operators the Schubert cocycle σ_w is given by the equation

$$\sigma_w = \partial_{w^{-1}w_0}(x_1^{n-1} x_2^{n-2} \cdots x_{n-1}), \tag{43}$$

where $w_0 = (n, n-1, \dots, 2, 1)$ is the unique permutation of maximal length.

The right-hand side of Eq. (43) makes sense for independent variables x_i and in this setting it is called the *Schubert polynomial* $S_w(x_1, x_2, \dots, x_n)$, $\deg S_w = \ell(w)$. They were first introduced by Lascoux and Schützenberger [21,22] who studied them in a series of papers. See [24] for further references and a concise exposition of the theory. We borrow from [21] the following table, in which x, y, z stand for x_1, x_2, x_3:

w	S_w	w	S_w	w	S_w	w	S_w
3210	x^3y^2z	2301	x^2y^2	2031	$x^2y + x^2z$	1203	xy
2310	x^2y^2z	3021	$x^3y + x^3z$	2103	x^2y	2013	x^2
3120	x^3yz	3102	x^3y	3012	x^3	0132	$x + y + z$
3201	x^3y^2	1230	xyz	0231	$xy + yz + zx$	0213	$x + y$
1320	$x^2yz + xy^2z$	0321	$x^2y + x^2z + xy^2$	0312	$x^2 + xy + y^2$	1023	x
2130	x^2yz	1302	$x^2y + xy^2$	1032	$x^2 + xy + xz$	0123	1

Extra variables $x_{n+1}, x_{n+2}, \dots$ added to (43) leave the Schubert polynomials unaltered. For that reason they are usually treated as polynomials in an infinite ordered alphabet $x = (x_1, x_2, \dots)$. With this understanding every homogeneous polynomial can be decomposed into Schubert components as follows:

$$f(x) = \sum_{\ell(w)=\deg(f)} \partial_w f \cdot S_w(x).$$

Applying this to the polynomial

$$\varphi_a^*(S_w(x^\nu)) = S_w(\varphi_a^*(x^\nu)) = \sum_{\ell(v)=\ell(w)} c_w^v(a) \cdot S_v(x),$$

and using Proposition 4 we finally arrive at the following result.

Theorem 5. *For the* ν*-representability problem the coefficients of the decomposition* $\varphi_a^*(\sigma_w) = \sum_v c_w^v(a)\sigma_v$ *are given by the formula*

$$c_w^v(a) = \partial_v S_w(x^\nu) \mid_{x_k^\nu \mapsto x_T}, \tag{44}$$

where the tableau T *is derived from equation* $a_k^\nu = a_T$*, and the operator* ∂_v *acts on the variables* x_i*, replacing* x_k^ν *via specialization* $x_k^\nu \mapsto x_T = \sum_{i\in T} x_i$.

Note that this equation is independent of an ordering of the unresolved spectral values a_k^ν. Indeed, the Schubert polynomial $S_w(x^\nu)$ is symmetric in the respective variables x_k^ν, *provided* that w is the minimal representative in its left coset modulo the centralizer of the spectrum a^ν in the symmetric group. Only such permutations correspond to the Schubert cocycles $\sigma_w \in H^*(\mathcal{F}_{a^\nu}(\mathcal{H}^\nu))$, cf. Remark 4.

4. Beyond the Basic Constraints

Here we use the above results to derive some general inequalities for the pure ν-representability problem beyond the Pauli constraint $\lambda \preceq \nu$. We start with a complete solution of the problem for two-row diagrams, and then turn to the initial N-representability problem that appears to be the most difficult one.

4.1. Two-row diagrams. For the two-row diagram $\nu = [\alpha, \beta]$ the majorization inequality $\lambda \preceq \nu$ just tells us that $\lambda_1 \le \alpha$. As we know, for $\beta \ne 1$ it shapes the whole moment polytope, see Remark 3 to Theorem 4. Here we elucidate the remaining case $\nu = [N-1, 1]$, and thus solve the pure ν-representability problem for all two-row diagrams. The result can not be extended to three-row diagrams, nor even to three fermion systems, where the number of independent inequalities *increases* with the rank, see Corollary 3 below. For convenience and future reference we collect all known facts in the next theorem.

Theorem 6. *For a system* $\mathcal{H}_r^\nu$ *of rank* $r \ge 3$ *with the two-row diagram* $\nu = [\alpha, \beta]$, $\alpha + \beta = N$*, all constraints on the occupation numbers of a pure state are given by the following conditions:*

1. *Basic inequality:* $\lambda_1 \le \alpha$ *for* $\beta \ne 1$.
2. *Inequality:* $\lambda_1 - \lambda_2 \le N - 2$ *for* $\nu = [N-1, 1]$, $N > 3$.
3. *Inequalities:* $\lambda_1 - \lambda_2 \le 1$, $\lambda_2 - \lambda_3 \le 1$ *for* $\nu = [2, 1]$.
4. *Even degeneracy:* $\lambda_{2i-1} = \lambda_{2i}$ *for* $\nu = [1, 1]$.

Proof. We have already addressed Cases 1 and 4 in Remark 3 and the Introduction respectively.
Case 2. Necessity. To prove the inequality $\lambda_1 - \lambda_2 \le N - 2$ we have to put it into the form of Theorem 2:

$$\sum_i a_i \lambda_{v(i)} \le \sum_k a_k^\nu \mu_{w(k)}. \tag{45}$$

This suggests the test spectrum $a = (1, 0, 0, \dots, 0, -1)$ and the shortest permutation v that transforms it into $(1, -1, 0, 0, \dots, 0)$, which is the cyclic one $v = (2, 3, 4, \dots, r)$.

Thus we get the left-hand side of the inequality. To interpret its right-hand side $N-2$, notice that the spectrum a^ν starts with the terms

$$a^\nu = (\underbrace{N-1, N-1, \ldots, N-1}_{r-2}, N-2, \ldots),$$

corresponding to semi-standard tableaux T with first row of ones and the indices $2, 3, \ldots, r$ filling a unique place in the second row. Since for pure state $\mu = (1, 0, 0, \ldots, 0)$, then the shortest permutation w that produces $N-2$ in the right-hand side of (45) is also cyclic, $w = (1, 2, 3, \ldots, r-1)$. The corresponding Schubert polynomial is just the monomial

$$S_w(x^\nu) = x_1^\nu x_2^\nu \cdots x_{r-2}^\nu.$$

This is a special case of Grassmann permutations discussed in the next Sect. 4.2. Specialization $x_k^\nu \mapsto x_T$ of Theorem 5 transforms it into the product

$$P(x) = \prod_{i=2}^{r-1} [(N-1)x_1 + x_i].$$

Taking the reduced decomposition $v = s_2 s_3 \cdots s_{r-1}$ we infer

$$c_w^v(a) = \partial_v P(x) = \partial_2 \partial_3 \cdots \partial_{r-1} P(x).$$

The right-hand side is a constant, and the operators ∂_i do not touch x_1. Hence we can put $x_1 = 0$, that gives

$$c_w^v(a) = \partial_2 \partial_3 \cdots \partial_{r-1} (x_2 x_3 \cdots x_{r-1}) = 1.$$

Since $c_w^v(a) \neq 0$, the inequality follows from Theorem 2.

Case 2. Sufficiency. By the convexity it is enough to construct *extremal states* whose occupation numbers are vertices of the polytope cut out of the Weyl chamber by the inequality $\lambda_1 - \lambda_2 \leq N-2$ and the normalization $\operatorname{Tr} \lambda = N$. The vertices are given first of all by the fundamental weights normalized to trace N

$$\omega_k = (\underbrace{N/k, N/k, \ldots, N/k}_{k}, 0, 0, \ldots, 0)$$

that generate the edges of the Weyl chamber, except for ω_1 forbidden by the constraint $\lambda_1 - \lambda_2 \leq N-2$. The latter is replaced by the intersections τ_k of segments $[\omega_1, \omega_k]$ with the hyperplane $\lambda_1 - \lambda_2 = N-2$,

$$\tau_k = (\underbrace{N-2+2/k, 2/k, \ldots, 2/k}_{k}, 0, 0, \ldots, 0).$$

Here we tacitly assume that $N > 3$, since otherwise ω_2 would be also forbidden. The same condition ensures that the system $\mathcal{H}_k^\nu$ is non-exceptional for $k \geq 2$, hence ω_k are occupation numbers of some pure states by Proposition 2.

To deal with the remaining vertices τ_k we invoke the Dadok-Kac construction, Sect. 3.2.3 and observe that the state

$$\psi_k = \begin{array}{|c|c|c|c|c|c|c|}\hline 1 & k & k & \cdot & \cdot & \cdot & k \\ \hline k \\ \cline{1-1}\end{array} + \frac{1}{\sqrt{2}} \sum_{2 \leq i < k} \begin{array}{|c|c|c|c|c|c|c|}\hline i & i & k & \cdot & \cdot & \cdot & k \\ \hline k \\ \cline{1-1}\end{array}$$

has disconnected support and the occupation numbers τ_k, $k \geq 2$. Here for clarity we write tableau T instead of the weight vector e_T and skip an overall normalization factor.

Case 3. Here we only briefly sketch the proof which follows a similar scheme. The second inequality in the form $\lambda_2 - \lambda_3 \leq N-2$ holds for all N, but it becomes redundant for $N > 3$. It can be deduced from Theorem 2 by calculation of the coefficient $c_w^v(a)$ for the same a and w as above, but with another permutation $v = (1,2)(3,4,\ldots,r)$. Then, keeping the notations of Case 2, we get

$$\begin{aligned} c_w^v(a) &= \partial_3\partial_4\cdots\partial_{r-1}\partial_1 P(x_1,x_2,\ldots,x_{r-1}) \\ &= \partial_3\partial_4\cdots\partial_{r-1}\frac{P(x_1,x_2,\ldots,x_{r-1})-P(x_2,x_1,\ldots,x_{r-1})}{x_1-x_2}. \end{aligned}$$

The operators ∂_k, $k \geq 3$ do not affect the variables x_1, x_2. Therefore in the fraction we can pass to the limit $x_1, x_2 \to 0$ equal to $(N-2)x_3x_4\cdots x_{r-1}$, which gives $c_w^v(a) = N-2 \neq 0$.

To prove sufficiency of the above inequalities we again have to look at the vertices of a polytope cut out of the Weyl chamber by the constraints $\lambda_1 - \lambda_2 \leq 1$, $\lambda_2 - \lambda_3 \leq 1$, $\operatorname{Tr}\lambda = 3$. This time, along with ω_k, $k \geq 3$ and τ_k, $k \geq 2$, there are vertices of another type

$$\eta_k = (\underbrace{1+1/k, 1+1/k, 1/k, 1/k, \ldots, 1/k}_{k}, 0, 0, \ldots, 0)$$

for $k \geq 3$. They represent occupation numbers of the following states with disconnected support:

$$\psi_k = \sqrt{k+1}\,\begin{array}{|c|c|}\hline 1&1\\\hline 2\\\cline{1-1}\end{array} + \sqrt{2}\,\begin{array}{|c|c|}\hline 2&2\\\hline 3\\\cline{1-1}\end{array} + \sum_{3<i\leq k}\begin{array}{|c|c|}\hline 2&i\\\hline i\\\cline{1-1}\end{array}.$$

□

Remark 5. Two-row diagrams naturally appear in the description of bosonic systems, like photons where polarization plays the rôle of spin. Representation with diagram $\begin{array}{|c|c|}\hline \ & \ \\\hline \ \\\cline{1-1}\end{array}$ can be applied both for bosons and fermions. In this case we calculated all constraints on the spin and orbital occupation numbers for small ranks, see Sect. 6.1. It appears that the constraints are stable and independent of the rank.

4.2. Grassmann inequalities. Let's return to the initial pure N-representability problem for system $\wedge^N\mathcal{H}_r$ and consider a constraint on its occupation numbers with 0/1 coefficients,

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_p} \leq b, \tag{46}$$

called the *Grassmann inequality*. For example, all constraints (4) for the system $\wedge^3\mathcal{H}_7$ are Grassmannian. We assume that the Grassmann inequality is *essential*, meaning that it defines a facet of the moment polytope. Then it should fit into the form of Theorem 2 with

$$a = (\underbrace{1, 1, \ldots, 1}_{p}, 0, 0, \ldots, 0)$$

and the *Grassmann permutation* or *shuffle*

$$v = [i_1, i_2, \dots, i_p, j_1, j_2, \dots, j_q] := [I, J], \tag{47}$$

where I and J are increasing sequences of lengths p and q, $p + q = r$. This is the shortest permutation that produces the left-hand side of inequality (46). Our terminology stems from the observation that for the test spectrum a the flag variety $\mathcal{F}_a(\mathcal{H})$ reduces to the *Grassmannian* $\mathrm{Gr}_p^q(\mathcal{H})$ consisting of all subspaces in $\mathcal{H}$ of dimension p and codimension q.

It is instructive to think about the Grassmann permutation $v = [I, J]$ geometrically as a path Γ connecting the SW and NE corners of the $p \times q$ rectangle, with the k^{th} unit step running to the North for $k \in I$ and to the East for $k \in J$. The path cuts out of the rectangle a Young diagram γ at its NW corner. We'll refer to I and J as the *vertical* and *horizontal* sequences of the diagram $\gamma \subset p \times q$ and denote the corresponding shuffle by $v_\gamma = [I, J]$. The length of the shuffle v_γ is equal to the size $|\gamma|$ of the diagram γ and its Schubert polynomial reduces to the much better understood Schur function

$$S_{v_\gamma}(x) = S_\gamma(x_1, x_2, \dots, x_p).$$

Observe that $\gamma_{p-k+1} = i_k - k$, and the size of the Young diagram γ is related to its vertical sequence by the equation

$$|\gamma| = \sum_{1 \le k \le p} (i_k - k). \tag{48}$$

To get the strongest inequality (46) we choose w to be a cyclic[6] permutation

$$w = (1, 2, \dots, \ell + 1) = [2, 3, \dots, \ell + 1, 1, \ell + 2, \ell + 3 \dots, r]$$

of length $\ell = \ell(v) = |\gamma|$ for which the right-hand side $b = (\wedge^N a)_{\ell+1}$ of (45) is minimal and equal to the $(\ell + 1)^{\text{st}}$ term of the non-increasing sequence

$$\wedge^N a = \{a_K := a_{k_1} + a_{k_2} + \cdots + a_{k_N} \mid 1 \le k_1 < k_2 < \cdots < k_N \le r\}^\downarrow.$$

The sequence consists of nonnegative numbers m, each taken with multiplicity

$$\binom{p}{m}\binom{q}{N - m}.$$

Recall that w also should be the minimal representative in its left coset modulo the stabilizer of $\wedge^N a$. For the cyclic permutation this amounts to the inequality $(\wedge^N a)_\ell > (\wedge^N a)_{\ell+1} = b$, which tells us that the first ℓ terms of $\wedge^N a$ contain all the components bigger than b. The number of such terms is bounded by the inequality

$$\sum_{m > b} \binom{p}{m}\binom{q}{N - m} = \ell = |\gamma| \le pq. \tag{49}$$

To avoid sporadic constraints, assume that the inequality we are looking for is *stable*, i.e. remains valid for an arbitrary big rank r. Then the left-hand side should be linear in $q = r - p$ and the sum contains at most two terms: $m = N$ and $m = N - 1$. Thus we end up with two possibilities:

[6] Actually w is always cyclic for an essential pure ν-representability inequality. We'll address this issue elsewhere.

1. $b = N - 2$, $p = N - 1$, $\ell = r - p$, that gives the inequality

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_{N-1}} \leq N - 2, \tag{50}$$

with $\sum_k (i_k - k) = r - p$.

2. $b = N - 1$, $p \geq N$, $\ell = \binom{p}{N}$, that gives the inequality

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_p} \leq N - 1, \tag{51}$$

with $\sum_k (i_k - k) = \binom{p}{N}$.

We will refer to them as the Grassmann inequalities of the first and second kind respectively. For the inequalities of the first kind the sum $\sum_k (i_k - k) = r - p$ increases with the rank, and therefore some of the involved occupation numbers should move away from the head of the spectrum. In contrast, the constraints of the second kind deal only with a few leading occupation numbers that are independent of the rank. We analyze them below for $p = N + 1$ and postpone the more peculiar first kind to the next section. The final result is that these inequalities actually hold true with very few exceptions.

The cyclic permutation w is a special type of shuffle with the column Young diagram of height ℓ. The corresponding Schur function is just the monomial

$$S_w(y) = y_1 y_2 \dots y_\ell.$$

Applying to S_w the specialization of Theorem 5 we arrive at the product

$$P(x) = \prod_{1 \leq k_1 < k_2 < \cdots < k_N \leq p} (x_{k_1} + x_{k_2} + \cdots + x_{k_N}) = \sum_\gamma c_\gamma S_\gamma(x_1, x_2, \dots, x_p). \tag{52}$$

Being symmetric, it can be expressed via Schur functions and, by Theorem 2, each time $S_\gamma(x)$ enters into the decomposition with nonzero coefficient $c_\gamma \neq 0$ we get inequality

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_p} \leq N - 1, \tag{53}$$

where $i_1 < i_2 < \cdots < i_p$ is the vertical sequence of Young diagram $\gamma \subset p \times q$, $|\gamma| = \binom{p}{N}$.

The product $P(x)$ represents the top Chern class of the exterior power $\wedge^N \mathcal{E}_p$ of the tautological bundle $\mathcal{E}_p$ on the Grassmannian Gr_p^q and the decomposition (52) has been discussed in this context [20]. However, known results are very limited.

Example 3. For $N = 2$ and any $p \geq N$ the product

$$P(x) = \prod_{1 \leq i < j \leq p} (x_i + x_j) = S_\delta(x_1, x_2, \dots, x_p)$$

is just the Schur function with a triangular Young diagram $\delta = [p - 1, p - 2, \dots, 0]$, see [25]. This gives for the two fermion system $\wedge^2 \mathcal{H}$ the inequality

$$\lambda_1 + \lambda_3 + \lambda_5 + \lambda_7 \cdots \leq 1, \tag{54}$$

that, due to the normalization $\sum_i \lambda_i = 2$, degenerates into equality and implies even the degeneracy $\lambda_{2i-1} = \lambda_{2i}$ of the occupation numbers.

On the other hand, for arbitrary N and minimal value $p = N$ we get

$$P(x) = x_1 + x_2 + \cdots + x_N = S_\square(x).$$

The vertical sequence of the one-box diagram $\square$ gives a nontrivial inequality

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{N-1} + \lambda_{N+1} \leq N - 1 \tag{55}$$

that forces the N^{th} electron into the N^{th} orbital, when the preceding orbitals are fully occupied. We improve it below.

In the rest of this section we focus upon the next case $p = N + 1$ that provides an infinite series of inequalities. Observe that in this setting a row diagram γ of length $N + 1 = \binom{p}{N}$ produces a *false* inequality

$$\lambda_1 + \lambda_2 + \cdots + \lambda_N + \lambda_{2N+2} \leq N - 1, \tag{56}$$

that fails for a coherent state given by one Slater determinant $e_1 \wedge e_2 \wedge \ldots \wedge e_N$. Similarly, the column inequality

$$\lambda_2 + \lambda_3 + \ldots + \lambda_{N+2} \leq N - 1 \tag{57}$$

fails for even N. Indeed, in this case the system $\wedge^N \mathcal{H}_{N+2} \subset \wedge^N \mathcal{H}_r$ is non-exceptional and hence, by Proposition 2, the spectrum

$$\lambda = \frac{1}{N+2}(\underbrace{N, N, \ldots, N}_{N+2}, 0, 0 \ldots, 0)$$

represents legitimate occupation numbers violating the inequality.

Quite unexpectedly, all the other diagrams produce a valid constraint. In plain language the result can be stated as follows:

Theorem 7. *The occupation numbers of the* N*-fermion system* $\wedge^N \mathcal{H}$ *in a pure state satisfy the following constraint:*

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_{N+1}} \leq N - 1$$

each time $\sum_k (i_k - k) = N + 1$, *except for inequality* (56) *and, for even* N, *inequality* (57).

Proof. For $p = N + 1$ the decomposition (52) takes the form

$$\begin{aligned} P(x) &= \prod_{1 \leq i \leq N+1} (x_1 + x_2 + \cdots + \widehat{x_i} + \cdots + x_{N+1}) = \prod_{1 \leq i \leq N+1} (\sigma_1 - x_i) \\ &= \sum_{0 \leq k \leq N+1} (-1)^k \sigma_1^{N+1-k} \sigma_k = \sum_{\gamma} c_\gamma S_\gamma(x_1, x_2, \ldots, x_{N+1}), \end{aligned}$$

where $\sigma_k(x) = S_{[1^k]}(x)$ are elementary symmetric functions, or what is the same Schur functions for the column diagram $[1^k]$.

For Young diagrams $\tau \subset \gamma$ denote by $t(\gamma/\tau)$ the number of standard tableaux of skew shape γ/τ. Then

$$c_\gamma = \sum_{k \geq 0} (-1)^k t(\gamma/[1^k]). \tag{58}$$

Indeed, the coefficient at S_γ in $\sigma_1^{N+1-k}\sigma_k = S_{[1]}^{N+1-k} S_{[1^k]}$ is equal to the number of ways to build γ from the column diagram $[1^k]$ by adding cells one at a time. Numbering the cells in the order of their appearance gives a standard tableaux of shape $\gamma/[1^k]$ that encodes the whole building process. Thus the coefficient is $t(\gamma/[1^k])$ and Eq. (58) follows.

For a column diagram γ we infer from the last equation

$$c_\gamma = \sum_{k=0}^{N+1}(-1)^k = \begin{cases} 0, & N \equiv 0 \mod 2, \\ 1, & N \equiv 1 \mod 2. \end{cases}$$

Henceforth we assume that γ is not a column. Let's combine successive even and odd terms of the sum (58)

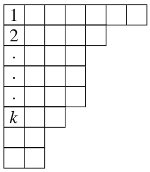
$$c_\gamma = \sum_{i\geq 0}[t(\gamma/[1^{2i}]) - t(\gamma/[1^{2i+1}])]. \tag{59}$$

We claim that

$$t(\gamma/[1^k]) - t(\gamma/[1^{k+1}]) = t(\gamma/[2, 1^{k-1}]), \tag{60}$$

where meaningless terms understood as zeros, e.g. the right-hand side for $k = 0$.

Indeed, the building process can be described as an extension of the partially filled tableau



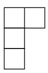
to a full standard tableau of shape γ. One can put the number $k+1$ either just below k or next to 1. For the first choice the number of ways to complete the tableau is $t(\gamma/[1^{k+1}])$, while for another one the number is $t(\gamma/[2, 1^{k-1}])$. Hence $t(\gamma/[1^k]) = t(\gamma/[1^{k+1}]) + t(\gamma/[2, 1^{k-1}])$.

Combining the last two equations we arrive at the following representation of the coefficient c_γ as a sum of nonnegative terms

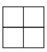
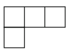
$$c_\gamma = \sum_{i>0} t(\gamma/[2, 1^{2i-1}]). \tag{61}$$

For a row diagram all terms vanish, while otherwise $t(\gamma/[2, 1]) \neq 0$. Hence $c_\gamma > 0$ if the diagram is neither a row nor a column. The result now follows from Theorem 2. □

Example 4. For $N = 3$ the theorem gives four inequalities listed below together with the corresponding diagrams

 : $\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2,$  : $\lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2,$

(62)

 : $\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2,$  : $\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2.$

They are valid for arbitrary rank r and give all constraints on the occupation numbers for $r \leq 7$. Observe also an improved version of the inequality (55)

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{N-1} + \lambda_{N+1} + \lambda_{2N+1} \leq N - 1, \tag{63}$$

coming from the diagram $[N, 1]$, and another inequality

$$\lambda_2 + \lambda_3 + \cdots + \lambda_{N+2} \leq N - 1,$$

originated from a column diagram and valid only for *odd* N.

Remark 6. We have considered above only Grassmann inequalities of the lowest levels $p = N, N + 1$. The higher levels provide further improvements. For example, the inequalities (55) and (63) are just the first terms of an infinite series corresponding to increasing values of p,

$$\lambda_{i_1} + \lambda_{i_2} + \lambda_{i_3} + \cdots + \lambda_{i_p} \leq N - 1, \tag{64}$$

where $i_k = k + \binom{k-1}{N-1}$. For $N = 2$ this gives the inequality (54) and the double degeneracy of the occupation numbers, while for $N = 3$ we get the inequality

$$\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 + \lambda_{11} + \lambda_{16} + \cdots \leq 2,$$

where the differences between the successive indices are natural numbers $1, 2, 3, 4, \ldots$. The details will be given elsewhere.

4.3. Grassmann inequalities of the first kind. Formally we have such an inequality

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_{N-1}} \leq N - 2 \tag{65}$$

each time the Schur function $S_\gamma = S_{v_\gamma}$ enters into the decomposition

$$P(x) = \prod_{N \leq j \leq r} (x_1 + x_2 + \cdots + x_{N-1} + x_j) = \sum_{\ell(v)=\ell} c_v S_v(x). \tag{66}$$

Here γ is a Young diagram of size $\ell = r - N + 1$ with the vertical sequence formed by the indices in the above inequality, and v_γ is the corresponding shuffle. In contrast to the previous case, the product is *not* a symmetric function and its decomposition into Schubert polynomials is a challenge.

Let's try a simple case of a row diagram that produces the inequality

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{N-2} + \lambda_r \leq N - 2. \tag{67}$$

A close look shows that it *fails* for odd $\ell = r - N + 1 = 2m - 1$ for the spectrum

$$\lambda = (\underbrace{1, 1, \ldots, 1}_{N-2}, \underbrace{1/m, 1/m, \ldots, 1/m}_{2m})$$

obtained by merging the occupation numbers of the systems $\wedge^{N-2}\mathcal{H}_{N-2}$ and $\wedge^2\mathcal{H}_{2m}$, see Corollary 2 of Theorem 4. Nevertheless

Proposition 5. *The inequality (67) holds for even $\ell = r - N + 1$. In this case the Schur function with a row diagram enters into the decomposition (66) with unit coefficient.*

Proof. The row diagram γ corresponds to the cyclic permutation

$$v = v_\gamma = (r, r-1, \dots, N, N-1) = s_{r-1}s_{r-2}\cdots s_{N-1},$$

where $s_i = (i, i+1)$ are transpositions. We have to calculate the coefficient c_v of the decomposition (66) given by the equation

$$c_v = \partial_v P(x) = \partial_{r-1}\partial_{r-2}\cdots\partial_{N-1}P(x).$$

The operator ∂_v does not affect the variables x_i, $i < N-1$, so we can set them to zero and deal with the polynomial

$$P_0(x) = \prod_{N\le i\le r}(x_{N-1}+x_i) = \sum_{N\le i_1<i_2<\cdots<i_k\le r} x_{N-1}^{\ell-k}x_{i_1}x_{i_2}\cdots x_{i_k}.$$

We claim that

$$\partial_v x_{N-1}^{\ell-k}x_{i_1}x_{i_2}\cdots x_{i_k} = \begin{cases}(-1)^k & \text{for } i_s = r-k+s,\\ 0 & \text{otherwise.}\end{cases} \tag{68}$$

Let's start with the second case $i_1 \le r-k = \ell+N-k-1$. In the following calculation we set to zero all variables that are not affected by the subsequent operators ∂_j. With this convention we get

$$\partial_{i_1-2}\partial_{i_1-3}\cdots\partial_{N-1}x_{N-1}^{\ell-k}x_{i_1}x_{i_2}\cdots x_{i_k} = x_{i_1-1}^{\ell+N-k-i_1}x_{i_1}x_{i_2}\cdots x_{i_k}. \tag{69}$$

The resulting monomial is divisible by an s_{i_1-1}-invariant factor $x_{i_1-1}x_{i_1}$ that commutes with the operator ∂_{i_1-1}. Hence everything vanishes in the next step as a result of the action ∂_{i_1-1} and setting $x_{i_1-1} = 0$.

In the case $i_1 = r-k+1 = \ell+N-k$ the right-hand side of (69) is just the product of the last k variables $x_{r-k+1}x_{r-k+2}\cdots x_r$ and application of the remaining operators ∂_j, $r-k\le j\le r-1$ gives $(-1)^k$.

Finally, from Eq. (68) we infer

$$c_v = \sum_{0\le k\le \ell}(-1)^k = \begin{cases}1, & \ell \text{ is even},\\ 0, & \ell \text{ is odd},\end{cases} \tag{70}$$

and the result follows from Theorem 2. □

Remark 7. The inequality (67) is most appealing for $N = 3$,

$$\lambda_1 + \lambda_r \le 1, \tag{71}$$

where it supersedes the Pauli principle $\lambda_1 \le 1$ for even r. Note that for the three electron system one- and two-point density matrices are isospectral and therefore the above inequality holds for both of them. We first came across this result reading paper [14], where the authors observed that if the 2-point density matrix of a three fermion system in state $\psi \in \wedge^3\mathcal{H}_r$ has an eigenvalue equal to one, then the corresponding eigenform $\omega \in \wedge^2\mathcal{H}_r$ can't have the full rank r. This is trivial for odd r, since rank of ω is always even. For even rank this follows from (71). Moreover, in the latter case the state $\psi \in \wedge^3\mathcal{H}_r$ itself has rank less than r. M.B. Ruskai also conjectured inequality (71) in her analysis of three fermion and three hole systems [33].

Observe the following result, anticipated by many experts. It may appear not so trivial if compared with Theorems 4 and 6.

Corollary 3. *No finite set of inequalities gives all constraints on occupation numbers of N-fermion system $\wedge^N\mathcal{H}$, $N > 1$ of arbitrary big rank.*

Proof. Indeed, a finite set Q of linear inequalities $L_\alpha(\lambda) \le b_\alpha$ includes only finitely many occupation numbers λ_i, $i < M$. Every inequality that follows from Q is a nonnegative combination of the inequalities from Q, the ordering conditions $\lambda_i - \lambda_{i-1} \le 0$, and a multiple of the normalization equation $\sum_{i=1}^{r} \lambda_i = N$.

Suppose now that the inequality of Proposition 5,

$$\lambda_1 + \lambda_2 + \cdots + \lambda_{N-2} + \lambda_r \le N - 2, \tag{72}$$

can be deduced from the system Q for some $r \gg M$ and even $\ell = r - N + 1$. The coefficients at λ_i in the left side for $i \ge M$ should come from the following linear combination with non-negative coefficients a_i,

$$\begin{aligned} &a_1(\lambda_2 - \lambda_1) + a_2(\lambda_3 - \lambda_2) + \cdots + a_{r-1}(\lambda_r - \lambda_{r-1}) - a_r\lambda_r = \\ &-\lambda_1 a_1 + \lambda_2(a_1 - a_2) + \cdots + \lambda_{r-1}(a_{r-2} - a_{r-1}) + \lambda_r(a_{r-1} - a_r), \end{aligned}$$

amended with a multiple of the normalization equation. The Abel transformation shown in the second line implies that the coefficients a_i should form an arithmetical progression $a_i = ai + b$ for $M \le i < r$, while $a_r = ar + b - 1 \ge 0$.

Suppose now that $a \ge 0$. Then the same combination of inequalities from Q that produces (72) and the same coefficients a_i for $i < r$ together with $a_r = ar + b \ge 0$, $a_{r+1} = a(r+1) + b - 1 \ge 0$ would give a *false* inequality of rank $r+1$ obtained from (72) by replacing $r \mapsto r + 1$. Recall that the inequality (72) *fails* for odd $\ell = r - N + 1$. For $a \le 0$ a similar consideration gives a false inequality of rank $r - 1$. □

Proposition 5 can be extended to two-row diagrams $\gamma = [\ell - k, k]$. For three fermions this leads to the constraints

$$\lambda_{k+1} + \lambda_{r-k} \le 1, \quad \text{for} \quad k + 1 < r - k, \tag{73}$$

that prohibit more than one electron to occupy *two* complementary orbitals. It holds both for even and odd r for $k > 0$. The corresponding coefficients $c_\gamma = c(\ell, k)$ of the decomposition (66) satisfy the recurrence relation $c(\ell, k) = c(\ell - 1, k) + c(\ell - 1, k - 1)$ and form the left half of the Pascal triangle

$$\begin{array}{c}
0\\
1 \quad -1\\
0 \quad 0 \quad 0\\
1 \quad 0 \quad 0 \quad -1\\
0 \quad 1 \quad 0 \quad -1 \quad 0\\
1 \quad 1 \quad 1 \quad -1 \quad -1 \quad -1\\
0 \quad 2 \quad 2 \quad 0 \quad -2 \quad -2 \quad 0\\
1 \quad 2 \quad 4 \quad 2 \quad -2 \quad -4 \quad -2 \quad -1\\
0 \quad 3 \quad 6 \quad 6 \quad 0 \quad -6 \quad -6 \quad -3 \quad 0\\
1 \quad 3 \quad 9 \quad 12 \quad 6 \quad -6 \quad -12 \quad -9 \quad -3 \quad -1
\end{array}$$

with apex at $\ell = -1$, and the 0/1 boundary condition for $k = 0$ set by Eq. (70). We return to the Pascal recurrence relation in a more general framework below, see Eq. (79).

Observe a zero in the forth line of the Pascal triangle, corresponding to diagram . In general, a column diagram should have zero coefficient, because it produces inequality

$$\lambda_1 + \lambda_2 + \cdots + \widehat{\lambda_{N-\ell}} + \cdots + \lambda_N \leq N - 2 \tag{74}$$

that *fails* for a coherent state given by one Slater determinant.

It turns out that the Grassmann inequality of the first kind (65) holds for all diagrams, except for a column and an odd row. To wit

Theorem 8. *The occupation numbers of N-fermion system $\wedge^N \mathcal{H}_r$ in a pure state satisfy the following constraint:*

$$\lambda_{i_1} + \lambda_{i_2} + \cdots + \lambda_{i_{N-1}} \leq N - 2 \tag{75}$$

each time $\sum_k (i_k - k) = r - N + 1$, except for inequality (74) and, for odd $\ell = r - N + 1$, inequality (67).

Proof. We have to show that the Schur function $S_\gamma(x) = S_{v_\gamma}(x)$ enters into the decomposition

$$P_r(x) = \prod_{N \leq j \leq r} (x_1 + x_2 + \cdots + x_{N-1} + x_j) = \sum_{\ell(v)=\ell} c_v S_v(x), \tag{76}$$

provided that $\gamma \subset p \times q$ is neither a column nor an odd row. Here $p = N - 1$, $q = \ell = |\gamma| = r - p$.

Note first of all, that the coefficients of this decomposition are nonnegative for $v \in S_r$ and can be positive only for shuffles $v = v_\gamma$. The first claim holds in general for the coefficients $c_v^w(a)$ of Theorem 2,

$$\varphi_a^*(\sigma_w) = \sum_v c_w^v(a)\sigma_v,$$

since the cycle $\varphi_a^{-1}(\sigma_w) \subset \mathcal{F}_a(\mathcal{H}_r)$ is *effective*. Here v runs over representatives of minimal length in left coset modulo stabilizer of a. To include all permutations $v \in S_r$ one has to deal with a small perturbation $\tilde{a}$ that resolves multiple entries of a. However, since $\varphi_{\tilde{a}}^{-1}(\sigma_w) \subset \mathcal{F}_{\tilde{a}}(\mathcal{H}_r)$ is pull back of $\varphi_a^{-1}(\sigma_w) \subset \mathcal{F}_a(\mathcal{H}_r)$ via natural projection $\pi : \mathcal{F}_{\tilde{a}}(\mathcal{H}_r) \to \mathcal{F}_a(\mathcal{H}_r)$ defined in Remark 4, then decomposition of $\varphi_{\tilde{a}}^{-1}(\sigma_w)$ and $\varphi_a^{-1}(\sigma_w)$ involve the same Schubert cycles σ_v. This prove the second claim. Let's add as a warning, that the decomposition (76) actually *contains* Schubert polynomials S_v with permutations $v \notin S_r$.

The rest of the proof is purely algebraic. We'll proceed by induction on r keeping N fixed. For the first meaningful case $r = N + 1$, $\ell = 2$, as we know, only the row diagram  appears in the decomposition.

Suppose now the induction hypothesis holds for $P_r(x)$, and consider the next polynomial,

$$\begin{aligned} P_{r+1}(x) &= (x_1 + x_2 + \cdots + x_{N-1} + x_{r+1})P_r(x) \\ &= (x_1 + x_2 + \cdots + x_{N-1} + x_{r+1}) \sum_{\ell(v)=\ell} c_v S_v(x). \end{aligned} \tag{77}$$

We can find its Schubert components using a version of Monk's formula,

$$(\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 \cdots) S_v(x) = \sum_{\ell(vt_{ij})=\ell(v)+1} (\alpha_i - \alpha_j) S_{vt_{ij}},$$

where $t_{ij} = (i, j)$, $i < j < \infty$ is a transposition, see [24, p. 86]. For a typical term of (77) this gives

$$(x_1 + x_2 + \cdots + x_{N-1} + x_{r+1}) S_v \\ = \sum_{1 \le i < N \le j \ne r+1} S_{vt_{ij}} - \sum_{N \le j \ne r+1} \operatorname{sgn}(r+1-j) S_{vt_{j,r+1}}, \tag{78}$$

where the sums include only those transpositions t for which $\ell(vt) = \ell(v) + 1$. We are interested in the terms $u_\gamma = vt \in S_{r+1}$ that are shuffles coming from a Young diagram $\gamma \subset p \times (\ell+1)$ of size $\ell + 1$. Let's single out the row diagram for which Proposition 5 gives the coefficient c_γ. The remaining shuffles u_γ do not move the last index $r+1$, and therefore permutation $v = u_\gamma t_{i,j}$ has a bigger length than u_γ for $j \ge r+1$. Hence a non-row Schur component S_γ in (78) comes from the sum

$$\sum_{1 \le i < N \le j \le r} S_{vt_{ij}}$$

for $v = u_\gamma t_{ij}$, $\ell(v) = \ell(u_\gamma) - 1 = |\gamma| - 1$. Then $v \in S_r$, and $S_v(x)$ enters into decomposition (76) only for a shuffle $v = v_\tau$. In this case the relation $v_\tau = u_\gamma t_{ij}$ just means that τ is obtained from γ by removing a cell. As a result, we arrive at the recurrence relation

$$c_\gamma = \sum_{\gamma/\tau = \text{cell}} c_\tau, \tag{79}$$

that holds for all *non-row* diagrams γ. This implies that $c_\gamma > 0$ if one can obtain an even row from γ by removing cells one at a time from a non-row diagram. This can be done for any diagram different from a column or an odd row. The inequality (75) now follows from Theorem 2. □

Example 5. For a four fermion system $\wedge^4 \mathcal{H}_r$ the theorem gives inequality

$$\lambda_i + \lambda_j + \lambda_k \le 2,$$

that holds for odd rank $r \ge 7$ and pairwise distinct indices satisfying equation $i + j + k = r + 3$. For even r one has to exclude the row inequality $\lambda_1 + \lambda_2 + \lambda_r \le 2$.

For two-row diagrams Eq. (79) amounts to the Pascal recurrence relation discussed in Remark 7. In general, it allows to get an explicit formula for the coefficient c_γ that is surprisingly similar to the one given in the proof of Theorem 8, where we borrow the notations.

Corollary 4.

$$c_\gamma = \sum_{k \ge 0} (-1)^k t(\gamma/[k]) = \sum_{i > 0} t(\gamma/[2i, 1]), \tag{80}$$

where the second equality holds for diagrams γ different from rows and columns.

Proof. Applying Eq. (79) recurrently in conjunction with Proposition 5 we find out that c_γ is equal to the number of ways to obtain an even row from γ by removing cells one at a time from a non-row diagram. If γ is not a row or a column, then the last step in the process will be $[2i, 1] \mapsto [2i]$. Encoding the process by the standard tableaux, we arrived at the second formula. The first one follows from the identity $t(\gamma/[2i,1]) = t(\gamma/[2i]) - t(\gamma/[2i+1])$, cf. the proof of Theorem 8, and holds for all diagrams. □

5. Connection with Representation Theory

The solution of the ν-representability problem suggested by Theorem 2 is not feasible, except for very small systems. For example, for four fermions $\wedge^4\mathcal{H}_8$ we confront an immense symmetric group of degree $\binom{8}{4} = 70$. Besides, listing of the extremal edges for systems of this size is all but impossible. A representation theoretical interpretation of the ν-representability discussed below often allows to mollify or circumvent these difficulties.

Let's consider a composition of the Schur functors $\mathcal{H} \mapsto \mathcal{H}^\nu$ called a *plethysm*

$$[\mathcal{H}^\nu]^\mu = \sum_{|\lambda|=|\nu|\cdot|\mu|} m_\lambda^\mu \mathcal{H}^\lambda. \tag{81}$$

It splits into $\mathrm{U}(\mathcal{H})$ irreducible components $\mathcal{H}^\lambda$ of multiplicity m_λ^μ. It is instructive to treat the diagrams λ and μ as *spectra*. We are interested in their asymptotic behavior for $m_\lambda^\mu \neq 0$ and $|\mu| \to \infty$. Therefore we normalize them to a fixed size $\widetilde{\mu} = \mu/|\mu|$, $\widetilde{\lambda} = \lambda/|\mu|$, so that $\mathrm{Tr}\,\widetilde{\mu} = 1$ and $\mathrm{Tr}\,\widetilde{\lambda} = N = |\nu|$.

Theorem 9. *Every time $m_\lambda^\mu \neq 0$ the couple $(\widetilde{\lambda}, \widetilde{\mu})$ belongs to the moment polytope of the system $\mathcal{H}^\nu$, i.e. there exists its mixed state ρ^ν of spectrum $\widetilde{\mu}$, with occupation numbers $\widetilde{\lambda}$. Moreover every point of the moment polytope is a convex combination of such spectra $(\widetilde{\lambda}, \widetilde{\mu})$ of a bounded size $|\mu| \leq M < \infty$.*

The theorem is a special case of Mumford's description of the moment polytope, see his Appendix in [28]. It also holds in more general Berenstein-Sjamaar settings [1].

5.1. Practical algorithm. For a fixed M the convex hull of the spectra $(\widetilde{\lambda}, \widetilde{\mu})$ from Theorem 9 gives an inner approximation to the moment polytope, while any set of inequalities of Theorem 2 amounts to its outer approximation. This suggests the following approach to the mixed ν-representability problem, which combines both theorems.

1. Find all irreducible components $\mathcal{H}^\lambda \subset [\mathcal{H}^\nu]^\mu$ for $|\mu| \leq M$.
2. Calculate the convex hull of the corresponding spectra $(\widetilde{\lambda}, \widetilde{\mu})$ that gives an inner approximation $\mathcal{P}_M^{\mathrm{in}} \subset \mathcal{P}$ for the moment polytope $\mathcal{P}$.
3. Identify the facets of $\mathcal{P}_M^{\mathrm{in}}$ that are given by the inequalities of Theorem 2. They cut out an outer approximation $\mathcal{P}_M^{\mathrm{out}} \supset \mathcal{P}$.
4. Increase M and continue until $\mathcal{P}_M^{\mathrm{in}} = \mathcal{P}_M^{\mathrm{out}}$.

The algorithm became practical by generosity of the authors of `LiE` package [4], who made it publicly available. It allows to handle plethysms efficiently. We also benefit from

`Convex` package by Franz [13], who apply a similar approach to the quantum marginal problem for three qutrits [12,17].

One can incorporate in the algorithm additional constraints on the spectrum of the mixed state ρ^ν. In many problems this is just a restriction on the rank rk $\rho^\nu \leq p$, that bounds the number of rows of μ. For example, a pure state $\rho^\nu = |\psi\rangle\langle\psi|$ has rank one, the corresponding diagram $\mu = [m]$ reduces to a row, and the plethysm amounts to the symmetric power $S^m(\mathcal{H}^\nu)$. More generally, for spin-orbital occupation numbers of a system of electrons of total spin J, we have to deal with mixed states of rank $2J+1$, see Corollary 1 to Theorem 2, and respectively with the diagrams μ of at most that height.

5.2. Particle-hole duality. Here is another application of Theorem 9. Recall, that we arrived at the ν-representability problem from the spin-orbital decompositions (17) of Sect. 3. In this setting the Young diagram ν comes together with a rectangular frame $r \times s \supset \nu$, where r and s are dimensions of the orbital and spin spaces respectively. Let ν^* be the *complementary diagram* to ν in the frame $r \times s$, that is $\nu_i^* = s - \nu_{r+1-i}$. One can think about the representation $\mathcal{H}_r^{\nu^*}$ as describing the *holes* of the system $\mathcal{H}_r^\nu$. These are dual systems with a natural pairing $\mathcal{H}_r^\nu \otimes \mathcal{H}_r^{\nu^*} \to \mathcal{H}_r^{r\times s} = \det(\mathcal{H}_r)^{\otimes s}$, that can be extended to a pairing of the plethysms $[\mathcal{H}_r^\nu]^\mu \otimes [\mathcal{H}_r^{\nu^*}]^\mu \to \det(\mathcal{H}_r)^{\otimes sm}$, where $m = |\mu|$. The latter duality means that if $\mathcal{H}_r^\lambda$ is a component of $[\mathcal{H}_r^\nu]^\mu$, then $\mathcal{H}_r^{\lambda^*}$ is a component of $[\mathcal{H}_r^{\nu^*}]^\mu$ of the same multiplicity. Here λ^* is the complementary diagram to $\lambda \subset r \times sm$. In view of Theorem 9 this implies

Corollary 5. *The moment polytope of the hole system $\mathcal{H}_r^{\nu^*}$ is obtained from the moment polytope of $\mathcal{H}_r^\nu$ by the transformation $(\lambda, \mu) \mapsto (\lambda^*, \mu)$, where $\lambda_i^* = s - \lambda_{r+1-i}$.*

6. Analysis of Some Small Systems

Here we take the challenge to explore *all* the constraints on the occupation numbers. This is clearly a mission impossible. It moves us from a garden of the carefully selected species we dealt with in the preceding sections, into the midst of a wild jungle with no order or end in sight.

To succeed in this environment we try the algorithm of Sect. 5.1 first. However, due to computer limitation, it can be accomplished only for very small systems. For the pure N-representability problem these are the systems for which Borland and Dennis made their prophesy 35 yeas ago [3]. To move further we use any tool available, from a clever guess to numerical optimization. The final outcome of this endeavour are all the constraints for the systems of rank not exceeding 10. For $r \leq 8$ we provide a rigorous proof below. We also have a proof for the system $\wedge^3\mathcal{H}_9$ based on other ideas, not discussed here. For the remaining cases the constraints are complete only *beyond a reasonable doubt*. To resolve the doubt one has to verify independently that the vertices of the constructed polytope are legitimate occupation numbers. We did this using a variety of methods for most of the vertices, but some still evaded all efforts. For the latter we resort to numerical optimization to check that they indeed can be approached very closely within the moment polytope. The biggest system we treated $\wedge^5\mathcal{H}_{10}$ is bounded by 161 inequalities.

We are ready to bet a bottle of decent wine for every additional essential constraint found.

Table 1. N-representability inequalities for system $\wedge^3\mathcal{H}_6$

Inequalities	$v \in S_6$	$w \in S_{20}$	$c_w^v(a)$
$\lambda_1 + \lambda_6 \le 1$	(2 6 5 4 3)		1
$\lambda_2 + \lambda_5 \le 1$	(1 2 5 4 3)	(1 2 3 4 5)	1
$\lambda_3 + \lambda_4 \le 1$	(1 3)(2 4)		1
$\lambda_4 \le \lambda_5 + \lambda_6$	(1 4 3 2)	(1 2 3 4)	1

Table 2. N-representability inequalities for system $\wedge^3\mathcal{H}_7$

Inequalities	$v \in S_7$	$w \in S_{35}$	$c_w^v(a)$
$\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \le 2$	(1 2 3 4 5)		1
$\lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \le 2$	(2 3 4 6 5)	(1 2 3 4 5)	1
$\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \le 2$	(3 4 7 6 5)		1
$\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \le 2$	(3 5)(4 6)		1

6.1. Spin and orbital occupation numbers. Let's start with a simple example of constraints on spin μ and orbital λ occupation numbers for a system of three electrons of the total spin $J = 1/2$. By Corollary 1 to Theorem 2 the problem is equivalent to mixed ν-representability for $\nu = \begin{smallmatrix}\square&\square\\ \square&\end{smallmatrix}$ and Spec $\rho^\nu = (\mu_1, \mu_2)$. A calculation based on the algorithm of Sect. 5.1 shows that the constraints amount to 5 inequalities

$$\lambda_1 - \lambda_2 \le 1 + \mu_2, \quad \lambda_2 - \lambda_3 \le 1 + \mu_2, \quad \lambda_1 - \lambda_3 \le 2 - \mu_2,$$
$$\lambda_1 - \lambda_2 - \lambda_3 \le 1, \quad 2\lambda_1 - \lambda_2 + \lambda_4 \le 4 - \mu_2,$$

that apparently are independent of the rank. We test them for $r = 4, 5$. Recall that λ and μ are arranged in non-increasing order and are normalized to the traces 3 and 1 respectively.

6.2. Pure N-representability. The known solution for two fermions, together with the particle-hole duality of Sect. 5.2, bound the pure $N-$representability problem to the range $3 \le N \le r/2$. For rank $r \le 8$ this leaves us with systems $\wedge^3\mathcal{H}_6$, $\wedge^3\mathcal{H}_7$, $\wedge^3\mathcal{H}_8$, and $\wedge^4\mathcal{H}_8$.

For three of them $\wedge^3\mathcal{H}_6$, $\wedge^3\mathcal{H}_7$ and $\wedge^4\mathcal{H}_8$ the algorithm of Sect. 5.1 runs flawlessly and terminates at $M = 4, 8, 10$, respectively. The independent constraints grouped by the test spectra a, together with the coefficients $c_w^v(a)$, and cycle decomposition of the permutations v, w are given in Tables 1–3.

The remaining system $\wedge^3\mathcal{H}_8$ is much harder to resolve.

6.2.1. System $\wedge^3\mathcal{H}_8$ We managed to decompose plethysm $S^m(\wedge^3\mathcal{H}_8)$ up to degree $m = 24$, but still have had a discrepancy between the inner and the outer approximations to the moment polytope. Actually all facets of $\mathcal{P}_{24}^{\text{in}}$, except for one, fit Theorem 2. For the remaining facet

$$\lambda_1 + \lambda_5 + \lambda_6 \ge 1$$

we use a numerical minimization of the linear form $L(\lambda) = \lambda_1 + \lambda_5 + \lambda_6$ over all particle density matrices. It turns out that the form attains its minimum, equal to $\frac{27}{28}$, at the vertex

$$\frac{1}{28}(15, 15, 15, 15, 6, 6, 6, 6). \tag{82}$$

Table 3. N-representability inequalities for system $\wedge^4\mathcal{H}_8$

Inequalities	$v \in S_8$	$w \in S_{70}$	$c_w^v(a)$
$\lambda_1 \leq 1$	(1)	(1)	1
$\lambda_5 - \lambda_6 - \lambda_7 - \lambda_8 \leq 0$	(1 5 4 3 2)		1
$\lambda_1 - \lambda_2 - \lambda_7 - \lambda_8 \leq 0$	(2 3 4 5 6)		1
$\lambda_1 - \lambda_3 - \lambda_6 - \lambda_8 \leq 0$	(3 4 5 7 6)		1
$\lambda_1 - \lambda_4 - \lambda_6 - \lambda_7 \leq 0$	(4 5 8 7 6)	(1 2 3 4 5)	1
$\lambda_1 - \lambda_4 - \lambda_5 - \lambda_8 \leq 0$	(4 6)(5 7)		1
$\lambda_3 - \lambda_4 - \lambda_7 - \lambda_8 \leq 0$	(1 3 2)(4 5 6)		1
$\lambda_2 - \lambda_4 - \lambda_6 - \lambda_8 \leq 0$	(1 2)(4 5 7 6)		1
$\lambda_2 + \lambda_3 + \lambda_5 - \lambda_8 \leq 2$	(1 2 3 5 4)		1
$\lambda_1 + \lambda_3 + \lambda_6 - \lambda_8 \leq 2$	(2 3 6 5 4)		1
$\lambda_1 + \lambda_2 + \lambda_7 - \lambda_8 \leq 2$	(3 7 6 5 4)		1
$\lambda_1 + \lambda_2 + \lambda_3 - \lambda_4 \leq 2$	(4 5 6 7 8)	(1 2 3 4 5)	1
$\lambda_1 + \lambda_4 + \lambda_5 - \lambda_8 \leq 2$	(2 4)(3 5)		1
$\lambda_1 + \lambda_2 + \lambda_5 - \lambda_6 \leq 2$	(3 5 4)(6 7 8)		1
$\lambda_1 + \lambda_3 + \lambda_5 - \lambda_7 \leq 2$	(2 3 5 4)(7 8)		1

Table 4. N-representability inequalities for system $\wedge^3\mathcal{H}_8$

Inequalities	$v \in S_8$	$w \in S_{56}$	$c_w^v(a)$
$\lambda_2 + \lambda_3 + \lambda_4 + \lambda_5 \leq 2$	(1 2 3 4 5)		1
$\lambda_1 + \lambda_2 + \lambda_4 + \lambda_7 \leq 2$	(3 4 7 6 5)	(1 2 3 4 5)	1
$\lambda_1 + \lambda_3 + \lambda_4 + \lambda_6 \leq 2$	(2 3 4 6 5)		1
$\lambda_1 + \lambda_2 + \lambda_5 + \lambda_6 \leq 2$	(3 5)(4 6)		1
$\lambda_1 + \lambda_2 - \lambda_3 \leq 1$	(3 4 5 6 7 8)		1
$\lambda_2 + \lambda_5 - \lambda_7 \leq 1$	(1 2 5 4 3)(7 8)		1
$\lambda_1 + \lambda_6 - \lambda_7 \leq 1$	(2 6 5 4 3)(7 8)	(1 2 3 4 5 6)	1
$\lambda_2 + \lambda_4 - \lambda_6 \leq 1$	(1 2 4 3)(6 7 8)		1
$\lambda_1 + \lambda_4 - \lambda_5 \leq 1$	(2 4 3)(5 6 7 8)		1
$\lambda_3 + \lambda_4 - \lambda_7 \leq 1$	(1 3)(2 4)(7 8)		1
$\lambda_1 + \lambda_8 \leq 1$	(2 8 7 6 5 4 3)	(1 2 3 4 5 6 7)	1
$\lambda_2 - \lambda_3 - \lambda_6 - \lambda_7 \leq 0$	(1 2)(3 4 5 8 7 6)		1
$\lambda_4 - \lambda_5 - \lambda_6 - \lambda_7 \leq 0$	(1 4 3 2)(5 8 7 6)	(1 2 3 4 5 6 7)	1
$\lambda_1 - \lambda_3 - \lambda_5 - \lambda_7 \leq 0$	(3 4 6)(5 8 7)		1
$\lambda_2 + \lambda_3 + 2\lambda_4 - \lambda_5 - \lambda_7 + \lambda_8 \leq 2$	(1 4 8 7 5)		1
$\lambda_1 + \lambda_3 + 2\lambda_4 - \lambda_5 - \lambda_6 + \lambda_8 \leq 2$	(1 4 8 6 7 5 2)	(1 2 3 ... 10 11)	1
$\lambda_1 + 2\lambda_2 - \lambda_3 + \lambda_4 - \lambda_5 + \lambda_8 \leq 2$	(1 2)(3 4 8 5 6 7)		1
$\lambda_1 + 2\lambda_2 - \lambda_3 + \lambda_5 - \lambda_6 + \lambda_8 \leq 2$	(1 2)(3 5 4 8 6 7)		1
$\lambda_1 + \lambda_2 - 2\lambda_3 - \lambda_4 - \lambda_5 \leq 0$	(3 6 4 7 5 8)	(1 2 3 ... 11 12)	1
$\lambda_1 - \lambda_2 - \lambda_3 + \lambda_6 - 2\lambda_7 \leq 0$	(2 6)(3 4 5 8 7)		1
$\lambda_1 - \lambda_3 - \lambda_4 - \lambda_5 + \lambda_8 \leq 0$	(2 8 5 7 4 6 3)	(1 2 3 ... 12 13)	1
$\lambda_1 - \lambda_2 - \lambda_3 - \lambda_7 + \lambda_8 \leq 0$	(2 8 7 3 4 5 6)		1
$2\lambda_1 - \lambda_2 + \lambda_4 - 2\lambda_5 - \lambda_6 + \lambda_8 \leq 1$	(2 4 3 8 5 7 6)		1
$\lambda_3 + 2\lambda_4 - 2\lambda_5 - \lambda_6 - \lambda_7 + \lambda_8 \leq 1$	(1 4)(2 3 8 5)		1
$2\lambda_1 - \lambda_2 - \lambda_4 + \lambda_6 - 2\lambda_7 + \lambda_8 \leq 1$	(2 6)(3 8 7 4)	(1 2 3 ... 12 13)	1
$2\lambda_1 + \lambda_2 - 2\lambda_3 - \lambda_4 - \lambda_6 + \lambda_8 \leq 1$	(3 8)(4 5 7 6)		1
$\lambda_1 + 2\lambda_2 - 2\lambda_3 - \lambda_5 - \lambda_6 + \lambda_8 \leq 1$	(1 2)(3 8)(5 7 6)		1
$2\lambda_1 - 2\lambda_2 - \lambda_3 - \lambda_4 + \lambda_6 - 3\lambda_7 + \lambda_8 \leq 0$	(2 6 4 5 3 8 7)		1
$-\lambda_1 + \lambda_3 + 2\lambda_4 - 3\lambda_5 - 2\lambda_6 - \lambda_7 + \lambda_8 \leq 0$	(1 4 2 3 8 5)(6 7)	(1 2 3 ... 14 15)	1
$2\lambda_1 + \lambda_2 - 3\lambda_3 - 2\lambda_4 - \lambda_5 - \lambda_6 + \lambda_8 \leq 0$	(3 8)(4 7)		1
$\lambda_1 + 2\lambda_2 - 3\lambda_3 - \lambda_4 - 2\lambda_5 - \lambda_6 + \lambda_8 \leq 0$	(1 2)(3 8)(4 7 5)		1

Adding this vertex gives a polytope $\mathcal{P}$ where all facets are covered by Theorem 2. Thus $\mathcal{P}$ is the genuine moment polytope for $\wedge^3\mathcal{H}_8$ given by 31 independent inequalities listed in Table 4.

Table 5. Vertices of the moment polytope of $\wedge^4\mathcal{H}_8$ and the corresponding extremal states

Extremal states	Vertices
[1234]	(1 : 1 : 1 : 1 : 0 : 0 : 0 : 0)
[1234] + [1256] + [3456]	(1 : 1 : 1 : 1 : 1 : 1 : 0 : 0)
[1234] + [1256]	(2 : 2 : 1 : 1 : 1 : 1 : 0 : 0)
[1234] + [1256] + [1357] + [1467] + [2367] + [2457] + [3456]	(1 : 1 : 1 : 1 : 1 : 1 : 1 : 0)
[1234] + [1256] + [1357] + [1467]	(2 : 1 : 1 : 1 : 1 : 1 : 1 : 0)
$\sqrt{2}$[1234] + [1256] + [1357] + [2367]	(2 : 2 : 2 : 1 : 1 : 1 : 1 : 0)
$\sqrt{2}$[1234] + [1256] + [1357] + [2457] + [3456]	(2 : 2 : 2 : 2 : 2 : 1 : 1 : 0)
$\sqrt{3}$[1234] + $\sqrt{2}$[1256] + [1357] + [2457]	(3 : 3 : 2 : 2 : 2 : 1 : 1 : 0)
$\sqrt{2}$[1234] + $\sqrt{2}$[1256] + [1357] + [1467] + [2367] + [2457]	(3 : 3 : 2 : 2 : 2 : 2 : 2 : 0)
$\sqrt{2}$[1234] + [1256] + [1357]	(4 : 3 : 3 : 2 : 2 : 1 : 1 : 0)
[1234] + [5678]	(1 : 1 : 1 : 1 : 1 : 1 : 1 : 1)
$\sqrt{2}$[1234] + [1256] + [1278] + [1357] + [1368]	(3 : 2 : 2 : 1 : 1 : 1 : 1 : 1)
[1234] + [1256] + [1278]	(3 : 3 : 1 : 1 : 1 : 1 : 1 : 1)
$\sqrt{3}$[1234] + [1256] + [1357] + [1458] + [2358] + [2457] + [3456]	(3 : 3 : 3 : 3 : 3 : 1 : 1 : 1)
$\sqrt{2}$[1234] + $\sqrt{2}$[1256] + [1357] + [1368] + [1458] + [1467]	(4 : 2 : 2 : 2 : 2 : 2 : 1 : 1)
2[1234] + $\sqrt{2}$[1256] + [1357] + [1458] + [2358] + [2457]	(4 : 4 : 3 : 3 : 3 : 1 : 1 : 1)
2[1234] + $\sqrt{2}$[1256] + [1357] + [1368] + [2358] + [2367]	(4 : 4 : 4 : 2 : 2 : 2 : 1 : 1)
$\sqrt{2}$[1234] + [1256] + [1357] + [1458]	(5 : 3 : 3 : 3 : 3 : 1 : 1 : 1)
$\sqrt{3}$[1234] + [1256] + [1357] + [2358]	(5 : 5 : 5 : 3 : 3 : 1 : 1 : 1)
[1234] + [1256] + [1278] + [1357] + [1368] + [1458] + [1467]	(7 : 3 : 3 : 3 : 3 : 3 : 3 : 3)
$\sqrt{3}$[1234] + $\sqrt{2}$[1256] + [1357] + [1368]	(7 : 5 : 5 : 3 : 3 : 3 : 1 : 1)
$\sqrt{3}$[1234] + [1256] + [1278] + [1357] + [1368] + [2358] + [2367]	(7 : 7 : 7 : 3 : 3 : 3 : 3 : 3)

We are actually unhappy with employing of numerical optimization, that can produce no rigorous result. Nevertheless, it provides a helpful hint about missed vertices. After some guesses and trials we found the state

$$\psi = 2[123] + \sqrt{10}[145] + \sqrt{5}[347] + \sqrt{2}[\mathbf{356}] + \sqrt{2}[258] + 2[368] + [178],$$

whose occupation numbers give the vertex (82). This provides a rigorous proof of the completeness the above constraints. Here $[ijk] = e_i \wedge e_j \wedge e_k$ is the Slater determinant or, in our general notations, weight vector e_T corresponding to the semi-standard tableau T transpose to $[ijk]$. Six triplets $[ijk]$ in the support of ψ, excluding one [**356**] typeset in boldface, form a disconnected set. They are remnants of our failed attempt to produce the missed vertex by the Dadok-Kac construction in Sect. 3.2.3. Extra tableau [**356**] in the support increases the number of adjustable parameters, but makes the problem nonlinear.

For those people who don't trust a computer assisted proof we give an extremal state for every vertex of the moment polytope for the systems $\wedge^3\mathcal{H}_7$, $\wedge^3\mathcal{H}_8$, and $\wedge^4\mathcal{H}_8$ listed in Tables 5-6. They are sufficient for a computer independent proof, provided that one takes for granted the values of the coefficients $c_w^v(a)$ in Tables 2–4.

6.2.2. Systems of rank 9 and 10 The results here are less definite. Only for the smallest system $\wedge^3\mathcal{H}_9$ do we have a rigorous justification of completeness for the system of 52 independent inequalities. For the next one, $\wedge^4\mathcal{H}_9$, we found 60 constraints, that give a polytope with 103 vertices. For all of them, except for two:

$$[16, 16, 16, 6, 6, 6, 6, 6, 6]/21, \qquad [20, 14, 14, 14, 14, 4, 4, 4, 4]/23,$$

Table 6. Vertices of the moment polytope of $\wedge^3\mathcal{H}_8$ and the corresponding extremal states. The first ten lines give the same data for $\wedge^3\mathcal{H}_7$

Extremal states	Vertices
[123]	(1:1:1:0:0:0:0:0)
[123]+[145]	(2:1:1:1:1:0:0:0)
[123]+[145]+[246]+[356]	(1:1:1:1:1:1:0:0)
$\sqrt{2}$[123]+[145]+[246]	(3:3:2:2:1:1:0:0)
[123]+[145]+[167]+[246]+[257]+[347]+[356]	(1:1:1:1:1:1:1:0)
$\sqrt{2}$[123]+[167]+[246]+[257]+[145]	(2:2:1:1:1:1:1:0)
$\sqrt{2}$[123]+$\sqrt{2}$[145]+[246]+[257]+[347]+[356]	(2:2:2:2:2:1:1:0)
[123]+[145]+[167]	(3:1:1:1:1:1:1:0)
$\sqrt{2}$[123]+[145]+[246]+[347]	(3:3:3:3:1:1:1:0)
$\sqrt{3}$[123]+$\sqrt{2}$[145]+[246]+[257]	(5:5:3:3:3:1:1:0)
[178]+[368]+[258]+[567]+[347]+[246]+[145]+[123]	(1:1:1:1:1:1:1:1)
$\sqrt{2}$[178]+[368]+[567]+[246]+$\sqrt{2}$[145]+$\sqrt{2}$[123]	(2:1:1:1:1:1:1:1)
$\sqrt{2}$[178]+[258]+[567]+$\sqrt{2}$[246]+[145]+$\sqrt{3}$[123]	(2:2:1:1:1:1:1:1)
$\sqrt{3}$[123]+$\sqrt{3}$[145]+[246]+$\sqrt{2}$[347]+[356]+$\sqrt{2}$[258]	(3:3:3:3:3:1:1:1)
$\sqrt{3}$[178]+$\sqrt{2}$[567]+[347]+[246]+2[145]+$\sqrt{5}$[123]	(4:2:2:2:2:2:1:1)
[178]+[246]+[145]+$\sqrt{2}$[123]	(4:3:2:2:1:1:1:1)
[178]+[258]+[246]+[145]+$\sqrt{2}$[123]	(4:4:2:2:2:2:1:1)
[258]+[567]+[145]+$\sqrt{3}$[123]	(4:4:3:3:1:1:1:1)
$\sqrt{2}$[145]+[246]+[347]+[**356**]+$\sqrt{2}$[368]	(4:4:4:4:2:1:1:1]
$\sqrt{2}$[178]+[246]+[145]+$\sqrt{2}$[123]	(5:3:2:2:2:2:1:1)
[368]+[347]+$\sqrt{2}$[145]+$\sqrt{3}$[123]	(5:5:3:3:2:1:1:1)
2[123]+$\sqrt{10}$[145]+$\sqrt{5}$[347]+$\sqrt{2}$[**356**]+$\sqrt{2}$[258]+2[368]+[178]	(5:5:5:5:2:2:2:2)
[178]+[567]+$\sqrt{2}$[145]+$\sqrt{3}$[123]	(6:3:3:3:2:2:1:1)
2[123]+$\sqrt{2}$[246]+$\sqrt{3}$[**356**]+$\sqrt{5}$[567]+2[258]	(6:5:5:5:2:2:1:1)
$\sqrt{2}$[178]+[258]+$\sqrt{2}$[246]+[145]+$\sqrt{3}$[123]	(6:6:3:3:3:2:2:2)
2$\sqrt{2}$[145]+$\sqrt{2}$[246]+$\sqrt{2}$[347]+$\sqrt{3}$[**356**]+$\sqrt{3}$[368]	(6:6:4:4:4:1:1:1)
2$\sqrt{3}$[123]+$\sqrt{6}$[145]+$\sqrt{2}$[**356**]+2[567]+$\sqrt{3}$[258]+$\sqrt{3}$[178]	(7:5:5:5:2:2:2:2)
$\sqrt{2}$[145]+2[246]+[347]+[**356**]+$\sqrt{2}$[368]	(7:7:4:4:4:2:1:1)
$\sqrt{3}$[246]+$\sqrt{2}$[347]+$\sqrt{6}$[258]+2[368]+2$\sqrt{2}$[178]+[**124**]	(9:5:5:5:3:3:3:3)
$\sqrt{3}$[258]+[567]+$\sqrt{2}$[347]+$\sqrt{2}$[246]+2[123]	(9:6:4:4:4:3:3:3)
3[145]+$\sqrt{6}$[246]+3[347]+2[**356**]+$\sqrt{3}$[258]+$\sqrt{14}$[368]	(9:8:8:8:3:3:3:3)
$\sqrt{2}$[178]+[258]+$\sqrt{3}$[246]+$\sqrt{2}$[145]+$\sqrt{5}$[123]	(9:9:5:5:3:3:3:2)
2[123]+$\sqrt{2}$[246]+$\sqrt{2}$[**356**]+$\sqrt{3}$[567]+$\sqrt{3}$[258]+$\sqrt{2}$[368]	(9:9:9:9:4:4:2:2)
2$\sqrt{2}$[145]+$\sqrt{6}$[246]+$\sqrt{6}$[347]+$\sqrt{5}$[**356**]+$\sqrt{2}$[258]+3[368]	(10:10:10:10:4:4:3:3)
$\sqrt{5}$[178]+[347]+$\sqrt{2}$[246]+$\sqrt{2}$[145]+2[123]	(11:6:6:5:5:5:2:2)
$\sqrt{3}$[178]+[258]+2[246]+$\sqrt{2}$[145]+$\sqrt{6}$[123]	(11:11:6:6:4:4:3:3)
$\sqrt{3}$[178]+$\sqrt{2}$[567]+[246]+2[145]+$\sqrt{5}$[123]	(12:6:6:5:5:5:3:3)
[123]+$\sqrt{3}$[145]+2[347]+2[**356**]+$\sqrt{3}$[258]+$\sqrt{3}$[368]	(12:12:7:7:4:4:4:4)

we have proved rigorously that they belong to the moment polytope. The remaining two vertices were checked only numerically. It turns out that the same two vertices would provide the completeness of 125 constraints for $\wedge^4\mathcal{H}_{10}$. The occupation numbers of the remaining systems $\wedge^3\mathcal{H}_{10}$ and $\wedge^5\mathcal{H}_{10}$ are bounded by 93 and 161 inequalities, but many vertices are still waiting a confirmation by non-numerical methods.

The facets and vertices of the moment polytopes for all systems of rank $\leq$ 10 are available as electronic supplementary material in the online version of this article doi:10.1007/s00220-008-0552-z.

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Communicated by M.B. Ruskai