



The face lattice of the set of reduced density matrices and its coatoms

Stephan Weis¹ · João Gouveia²

Received: 21 February 2022 / Revised: 1 January 2023 / Accepted: 19 February 2023 /
Published online: 9 March 2023
© The Author(s), under exclusive licence to Springer Nature Singapore Pte Ltd. 2023

Abstract

The lattice of faces of the convex set of reduced density matrices is essential for the construction of the information projection to a hierarchical model. The lattice of faces is also important in quantum state tomography. Yet, the description and computation of these faces is elusive in the simplest examples. Here, we study the face lattice of the set of two-body reduced density matrices: We show that the three-qubit lattice has no elements of rank seven and that it has a family of coatoms of rank five. This contrasts with the three-bit lattice, where every coatom has rank six. We discovered the coatoms of rank five using a novel experimental method, which employs convex duality, semidefinite programming, and algebra. We also discuss nonexposed points for three and six qubits. Using frustration-free Hamiltonians, we provide a new characterization of probability distributions that factor.

Keywords Information projection · Reduced density matrices · Face lattice · Exposed face · Joint numerical range · Spectrahedron · Semidefinite programming · Local Hamiltonian · Frustration-free

Mathematics Subject Classification 81P45 · 94A15 · 90C22 · 52A20

Communicated by Nihat Ay.

✉ Stephan Weis
maths@weis-stephan.de
João Gouveia
jgouveia@mat.uc.pt

¹ Wald-Gymnasium Berlin, Berlin, Germany

² Department of Mathematics, University of Coimbra, Coimbra, Portugal

1 Introduction

Information geometry is concerned with statistical manifolds in a differential geometrical framework [4]. One important aspect is the projection of a probability distribution to a statistical manifold, a special case of which is the reverse information projection [16], which we call information projection in the sequel.

In the quantum setting, there is the Gibbs family of trace-normalized states,

$$\mathcal{E} = \left\{ \frac{\exp(A)}{\text{Tr}(\exp(A))} : A \in \mathcal{U} \right\},$$

defined by the exponential map, given a vector space \mathcal{U} of hermitian matrices. The information projection of a density matrix ρ is the unique point in \mathcal{E} having the same expected values as ρ with respect to all elements in \mathcal{U} . The information projection has the same fibers as the orthogonal projection of the set of density matrices onto \mathcal{U} with respect to the Hilbert-Schmidt inner product. We call the image of the set of density matrices under the orthogonal projection joint numerical range [11], see Sect. 3.4 for details. As a compact and convex set, the joint numerical range contains its own boundary, whereas the Gibbs family \mathcal{E} has no points in the fibers over this boundary. We resolved this problem by constructing a boundary to \mathcal{E} , the pieces of which are defined in terms of the faces of the joint numerical range [48].

This paper is about many-body systems. An economical way to work with the set of density matrices of exponentially large dimension is to collect the relevant information in the reduced density matrices. For example, the k -body reduced density matrices capture all information a k -local Hamiltonian, which ignores subsystems of more than k units, can observe [14, 54]. If \mathcal{U} is the space of k -local Hamiltonians, then the Gibbs family \mathcal{E} is the hierarchical model of k -body interactions [49] and the information projection has the same fibers as the linear map that assigns the reduced density matrices to a density matrix.

Density matrices can represent probability distributions in the commutative setting of diagonal matrices [21]. Here, the information projection of an empirical distribution to a Gibbs family \mathcal{E} is the maximum-likelihood estimate. It is well-known that the boundary of \mathcal{E} is required in order to have the information projection and the maximum-likelihood estimate defined with probability one [8, Sect. 9.3], [16]. The space of local Hamiltonians is known as a hierarchical model subspace [27] and the reduced density matrices are the marginals of a distribution [7, Section 2.9]. Again, with the goal to define the information projection with probability one, algebraic [23] and approximate [43] approaches have been developed for the computation of the faces of the convex set of marginals.

As an application, the information projection to a hierarchical model can be employed to compute the entropy distance from a hierarchical model. Quantifying the complexity of the many-body system, the entropy distance is important in the neural sciences [3, 7] and in condensed matter theory [34, 49, 54, 55]. Understanding the faces of the set of reduced density matrices is even more important than understanding

the faces of the set of marginals, in the sense that the maximum-entropy inference,¹ and hence the information projection, is discontinuous in the quantum setting [47]. Continuous approximations are possible in commutative settings, such as probability distributions [8, Sect. 9.3], or quantum stabilizer states [55].

Despite decades of research in quantum chemistry [18, 38] and more recent research in state tomography [13–15, 25, 28, 54], the face lattice of the convex set of reduced density matrices is widely unexplored. An example is the set of two-body reduced density matrices of three qubits. We only have accurate knowledge of its extreme points [15, 28]. A description of the set of (AB, BC) reduced density matrices of a three-qubit system ABC is still an open problem, see [52] and [54, Section 4.4.2]. Even the extreme points can be challenging for small systems. For instance, while the set of two-body reduced density matrices of three qubits has no nonexposed points, the set of two-body reduced density matrices of six qubits has nonexposed points [25], as we will discuss in Sect. 4.6. Here, we distinguish an exposed face, the set of minimizers of a linear functional, from a nonexposed face that cannot be written as a set of minimizers.

In this paper, we explore the exposed faces of the set of reduced density matrices with a focus on the coatoms (maximal faces). Coatoms are important for several reasons. They are dual to the extreme points of the dual convex set, a spectrahedron. All exposed faces are intersections of coatoms. These are special properties of the set of reduced density matrices, see Sections 4 and 6 in [50]. Numerically, the sampling procedure described below typically yields extreme points of the dual spectrahedron and leads to coatoms through duality.

We propose an experimental method to analyze coatoms in three steps, see Remark 2. First, we search for extreme points of the spectrahedron, which we achieve efficiently with the help of semidefinite programming [33] (the computational complexity has a meaning in information geometry [24]). Secondly, we guess algebraic expressions for the samples. Thirdly, we confirm or reject that the expressions are extreme points, using linear algebra and lattice theory. Notably, a lattice isomorphisms from the exposed faces of the set of reduced density matrices to the ground projectors of the local Hamiltonians associates the notion of a matrix rank to each coatom.

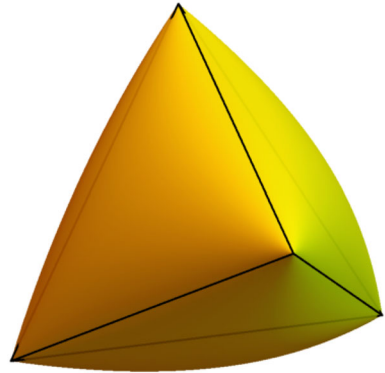
The experimental method works well for the two-body reduced density matrices of three qubits. We present a family of coatoms of rank five in the lattice of ground projectors in Sect. 4.5, whereas all coatoms have rank six in the setting of probability distributions. We owe the low-rank coatoms to the high-rank extreme points on the curved boundary portions of the dual spectrahedron. An instructive example is the spectrahedron

$$\left\{ (x, y, z) \in \mathbb{R}^3 \mid \begin{pmatrix} 1 & x & y \\ x & 1 & z \\ y & z & 1 \end{pmatrix} \succeq 0 \right\},$$

which contains the one-skeleton of a tetrahedron and which is bounded by the Cayley cubic, see Fig. 1. The four vertices of the underlying tetrahedron correspond to rank one matrices, while the rest of the yellow surface corresponds to rank two matrices.

¹ Finding the maximum-entropy state is computationally hard [17], even if the face is known.

Fig. 1 Spectrahedron bounded by the Cayley cubic



The relative interiors of the six edges of the tetrahedron constitute the set of boundary points that are not extreme.

Some of our results only address probability distributions. We describe the faces of the set of two-body marginals of three bits in Sect. 4.4. In Sect. 4.2 look at hierarchical models of probability distributions. It is well known that their elements factor. For a distribution of full support this means the distribution is the exponential of a local Hamiltonian (by the Hammersley-Clifford theorem [19, 27]). The equivalence was extended from maximal to nonmaximal support, employing algebraic varieties and a combinatorial condition on the support projectors [19]. We add to the topic of nonmaximal support in Sect. 4.2 using frustration-free Hamiltonians. This is refined aspect to the lattice of faces of the set of marginals, as the ground projectors of only some local Hamiltonians support probability distributions that factor. It would be interesting to clarify a similar meaning of frustration-free Hamiltonians [22, 32, 54] in the context of hierarchical models of quantum states.

The article is structured as follows. Section 2 introduces matrix algebras. Section 3 explains the experimental method in the general setting of the joint numerical range. Section 4 addresses reduced density matrices and marginals.

Remark 1 (Complexity) Two computational problems may be responsible for the difficulty to grasp the faces of the set of reduced density matrices. The first problem is estimating the ground state energy of a local Hamiltonian, the second is the marginal problem of deciding whether a collection of states is the collection of reduced density matrices of a state. Both problems are QMA-complete, meaning they cannot be solved efficiently on a quantum computer [26, 29]. The marginal problem can be solved by a hierarchy of semidefinite programs [53]. This problem is trivial for non-overlapping subsystems, but it becomes QMA-complete again for indistinguishable particles, fermions or bosons [30, 44], where a spectral polytope describes the solution [5, 31, 39, 40].

2 Matrix *-algebras

This section introduces the algebras we employ throughout the paper.

2.1 Lattices, state spaces, projectors

A *lattice* [10] is a partially ordered set in which any pair of elements has an infimum and a supremum. A lattice is *complete* if every subset has an infimum and a supremum. Let \mathcal{L} be a lattice with least element 0 and greatest element 1. An *atom* of \mathcal{L} is a minimal element of $\mathcal{L} \setminus \{0\}$. A *coatom* of \mathcal{L} is a maximal element of $\mathcal{L} \setminus \{1\}$. The lattice \mathcal{L} is *atomistic* if each of its element is the supremum of a set of atoms (such a lattice is called atomic in [10]). The lattice \mathcal{L} is *coatomistic* if each of its element is the infimum of a set of coatoms.

Let M_d denote the $*$ -algebra of complex $d \times d$ matrices, and I_d the $d \times d$ identity matrix. We write the matrix product of $A, B \in M_d$ in the form $A.B$ to distinguish it from the tensor product $AB = A \otimes B$ in Sect. 4.1. We will work with a $*$ -algebra $\mathcal{A} \subseteq M_d$ over the reals as this give us the possibility to decrease the dimension (see Sect. 2.4). This also includes the $*$ -algebras over the complex field. The *Hilbert-Schmidt inner product* on \mathcal{A} is defined by $\langle A, B \rangle = \text{Tr}(A^*. B)$ for all $A, B \in \mathcal{A}$. The real vector space of hermitian matrices

$$\mathcal{H}(\mathcal{A}) = \{A \in \mathcal{A} : A^* = A\}$$

is a Euclidean space with the restricted Hilbert-Schmidt inner product. The set $\mathcal{H}(\mathcal{A})$ is partially ordered by the *Loewner order* $A \preceq B$, or equivalently $B \succeq A$, which is valid if $B - A$ is positive semidefinite for all $A, B \in \mathcal{H}(\mathcal{A})$. We denote the set of positive semidefinite matrices by

$$\mathcal{A}^+ = \{A \in \mathcal{A} : A \succeq 0\}.$$

The *state space* [2] of the algebra \mathcal{A} is the set

$$\mathcal{D}(\mathcal{A}) = \{\rho \in \mathcal{A}^+ : \text{Tr}(\rho) = 1\}.$$

The set \mathcal{A}^+ is a closed, convex cone and $\mathcal{D}(\mathcal{A})$ is a compact, convex set. The elements of $\mathcal{D}(\mathcal{A})$ are called *density matrices* or *quantum states* [9]. The extreme points of $\mathcal{D}(\mathcal{A})$ are called the *pure states* of \mathcal{A} . Endowed with the restricted Loewner order, the set of *projectors* in \mathcal{A} ,

$$\mathcal{P}(\mathcal{A}) = \{P \in \mathcal{A} : P = P^* = P^2\},$$

is a complete lattice [2].

Rank one projectors are important, as they are the atoms of $\mathcal{P}(M_d)$. Every rank one projector $P \in \mathcal{P}(M_d)$ is a pure state and we write it as $P = |\psi\rangle\langle\psi|$ in Dirac’s notation, where $|\psi\rangle \in \mathbb{C}^d$ is any unit vector in the image of P . If every atom of $\mathcal{P}(\mathcal{A})$ has rank one, then the converse holds: Every pure state of \mathcal{A} is a rank one projector.

From now on, we assume the $*$ -algebra \mathcal{A} contains the $d \times d$ identity matrix I_d . In contrast, the multiplicative identity of the $*$ -algebra

$$P.\mathcal{A}.P = \{P.A.P : A \in \mathcal{A}\}$$

is P for all projectors $P \in \mathcal{P}(\mathcal{A})$. The assumption of $I_d \in \mathcal{A}$ guarantees that every eigenvalue of a matrix $A \in \mathcal{A}$ is a spectral value of A in the algebra \mathcal{A} , which is important in our definition of a ground projector in Sect. 3.3.

2.2 Diagonal matrices

Given a finite set X , the space \mathbb{C}^X of functions $X \rightarrow \mathbb{C}$ is a $*$ -algebra. Let $\delta_x \in \mathbb{C}^X$ be defined by $\delta_x(y) = 0$ if $x \neq y$ and $\delta_x(y) = 1$ if $x = y$, for all $x, y \in X$. The *support* of a function $f \in \mathbb{C}^X$ is the set of points $\{x \in X \mid f(x) \neq 0\}$. We identify the set of functions $C(d) \rightarrow \mathbb{C}$ on the *configuration space* $C(d) = \{0, \dots, d - 1\}$ with the set of $d \times d$ diagonal matrices, in such a way that $f \in \mathbb{C}^{C(d)}$ corresponds to the diagonal matrix $\text{diag}(f(0), f(1), \dots, f(d - 1))$. In the notation of Sect. 2.1, the space $\mathcal{H}(\mathbb{C}^{C(d)})$ of hermitian matrices is the set of real functions $C(d) \rightarrow \mathbb{R}$, the state space $\mathcal{D}(\mathbb{C}^{C(d)})$ is the simplex of probability distributions on $C(d)$, and the set $\mathcal{P}(\mathbb{C}^{C(d)})$ of projectors is the set of $\{0, 1\}$ -valued functions on $C(d)$. There is a lattice isomorphism

$$\mathcal{P}(\mathbb{C}^{C(d)}) \rightarrow 2^{C(d)}, \quad P \mapsto \text{supp}(P), \tag{1}$$

from the set of projectors to the power set of the configuration space $C(d)$, which maps the rank one projector δ_x to x for all $x \in C(d)$.

2.3 The qubit-algebra

The *qubit* is the information unit of quantum theory. The algebra associated with the qubit is the complex $*$ -algebra of 2×2 matrices M_2 , spanned by the identity matrix

$$I = I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and the *Pauli matrices*

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These matrices also span the real space $\mathcal{H}(M_2)$ of hermitian matrices. Any traceless hermitian matrix can be written in the form

$$\hat{n} \cdot \vec{\sigma} = n_x X + n_y Y + n_z Z$$

where $\hat{n} = (n_x, n_y, n_z) \in \mathbb{R}^3$ is the *Bloch vector* and $\vec{\sigma} = (X, Y, Z)$ the *Pauli vector*. The matrix $\hat{n} \cdot \vec{\sigma}$ has the eigenvalues $\pm |\hat{n}|$ and the spectral decomposition

$$\hat{n} \cdot \vec{\sigma} = |\hat{n}|(I + \frac{\hat{n}}{|\hat{n}|} \cdot \vec{\sigma})/2 - |\hat{n}|(I - \frac{\hat{n}}{|\hat{n}|} \cdot \vec{\sigma})/2, \quad \hat{n} \neq 0.$$

The state space of M_2 is the *Bloch ball*

$$\mathcal{D}(M_2) = \left\{ (I + \hat{n} \cdot \vec{\sigma})/2 : \hat{n} \in \mathbb{R}^3, |\hat{n}| \leq 1 \right\}.$$

The set of pure states is the *Bloch sphere* $\{(I + \hat{n} \cdot \vec{\sigma})/2 : \hat{n} \in \mathbb{R}^3, |\hat{n}| = 1\}$.

2.4 The disk-algebra

The real $*$ -algebra $M_2(\mathbb{R}) = \text{span}_{\mathbb{R}}\{I, X, Z, iY\}$ is interesting as it is noncommutative and has a smaller dimension than M_2 . The space of hermitian matrices is

$$\mathcal{H}(M_2(\mathbb{R})) = \text{span}_{\mathbb{R}}\{I, X, Z\}.$$

The state space is the disk $\mathcal{D}(M_2(\mathbb{R})) = \{\rho \in \mathcal{D}(M_2) : \langle \rho, Y \rangle = 0\}$, a cross section of the Bloch ball.

2.5 The bit-algebra

The information unit of digital computers is the *bit*, which has the configuration space $C(2) = \{0, 1\}$. Thinking of the elements of $\mathbb{C}^{C(2)}$ as 2-by-2 diagonal matrices as in Sect. 2.2, we write $\mathbb{C}^{C(2)}$ as the span of the identity matrix I and the Pauli matrix Z introduced in Sect. 2.3. As per the lattice isomorphism (1), the rank one projectors

$$\frac{1}{2}(I + (-1)^x Z), \quad x = 0, 1,$$

of $\mathbb{C}^{C(2)}$ are in a one-to-one correspondence with the configurations 0 and 1.

3 Experimental approach to the coatoms of the lattice of exposed faces of the joint numerical range

This section focusses on the joint numerical range \mathcal{W} , the convex set which is the projection of the state space $\mathcal{D}(\mathcal{A})$ of the $*$ -algebra \mathcal{A} onto a vector space of hermitian matrices. The main result is an experimental method, described in Remark 2 in Sect. 3.6, that allows us to calculate coatoms of the lattice of exposed faces of \mathcal{W} . The experimental method is based on convex geometry and lattice isomorphisms (summarized in Fig. 2). The gist of the lattice isomorphism is Thm. 3, which leads to the random search (step one) of the experimental method.

We begin by discussing exposed faces and normal cones in Sect. 3.1, and convex duality in Sect. 3.2. The purpose of Sect. 3.3 is to write exposed faces and normal cones of the state space in terms of ground projectors. Sect. 3.4 introduces the joint numerical range \mathcal{W} and describes the lattice of exposed faces of \mathcal{W} in terms of the lattice of ground projectors of the underlying space of hermitian matrices. Based on the normal cones of \mathcal{W} , Sect. 3.5 develops computational approaches to the lattice

of ground projections, which lead to the verification (step three) of the experimental method. The dual spectrahedron to \mathcal{W} defined in Sect. 3.6 completes the bouquet of convex sets, lattices, and isomorphisms needed in the experimental method.

We refer to [37, 41] regarding convex geometry, and to [6] regarding the convex geometry of quantum states.

3.1 Exposed faces and normal cones

Let $(\mathbb{E}, \langle \cdot, \cdot \rangle)$ be a Euclidean space and $C \subseteq \mathbb{E}$ a convex subset. An *exposed face* of C is a subset of C , which is either empty or equal to the set of points at which a linear function attains its minimum on C . We denote the set of exposed faces of C by $\mathcal{F}(C)$. If C is compact then the minimum $\mu_{C,u} = \min_{x \in C} \langle x, u \rangle$ exists for all $u \in \mathbb{E}$ and we define the map

$$F_C : \mathbb{E} \rightarrow \mathcal{F}(C), \quad u \mapsto \{x \in C : \langle x, u \rangle = \mu_{C,u}\}.$$

We call $F_C(u)$ the exposed face of C *exposed* by the vector u . A point $x \in C$ is an *exposed point* if $\{x\}$ is an exposed face. Partially ordered by inclusion, the set $\mathcal{F}(C)$ is a complete lattice, and the infimum is the intersection.

The *normal cone* to C at a point $x \in C$ is the closed convex cone

$$N_C(x) = \{u \in \mathbb{E} \mid \langle y - x, u \rangle \geq 0 \ \forall y \in C\}.$$

The *normal cone* to C at a nonempty convex subset $G \subseteq C$ is defined as the intersection $N_C(G) = \bigcap_{x \in G} N_C(x)$. We put $N_C(\emptyset) = \mathbb{E}$. Partially ordered by inclusion, the set $\mathcal{N}(C)$ of normal cones to C is a complete lattice, and the infimum is the intersection.

In a slight abuse of the symbol N_C , we define the map

$$N_C : \mathcal{F}(C) \rightarrow \mathcal{N}(C), \quad F \mapsto N_C(F). \quad (2)$$

If C is not a singleton, then this map is an antitone lattice isomorphism. The statements of this section are proved in [46].

3.2 Convex duality

Let $(\mathbb{E}, \langle \cdot, \cdot \rangle)$ be a Euclidean space and denote the orthogonal projection onto a subspace $U \subseteq \mathbb{E}$ by $\pi_U : \mathbb{E} \rightarrow \mathbb{E}$. The *dual convex cone* to a subset $C \subseteq \mathbb{E}$ is the closed convex cone

$$C^\vee = \{u \in \mathbb{E} \mid \langle u, x \rangle \geq 0 \ \forall x \in C\}.$$

If C is a closed convex cone, then $C = (C^\vee)^\vee$ holds. If $C = C^\vee$, then C is called a *self-dual convex cone*. The *dual convex set* to any subset $C \subseteq \mathbb{E}$ is

$$C^\circ = \{u \in \mathbb{E} \mid 1 + \langle u, x \rangle \geq 0 \ \forall x \in C\}.$$

The set C° is a closed convex set containing the origin. If C is a compact, convex set containing the origin as an interior point, then the dual convex set C° is compact and contains the origin as an interior point, too [37, 41].

Section 3.6 uses the following one-to-one correspondence between normal cones of C and exposed faces of C° . If C is a compact, convex set containing the origin as an interior point and if $\dim(\mathbb{E}) \geq 1$, then the map

$$\chi_C : \mathcal{N}(C) \rightarrow \mathcal{F}(C^\circ), \quad N \mapsto \begin{cases} N \cap \partial C^\circ & \text{if } N \neq \mathbb{E}, \\ C^\circ & \text{if } N = \mathbb{E}, \end{cases} \tag{3}$$

is an isotone lattice isomorphism, where ∂C° is the boundary of C° . The composition of the maps (2) and (3) is the antitone lattice isomorphism $\mathcal{F}(C) \rightarrow \mathcal{F}(C^\circ)$ that maps an exposed face to its *conjugate face* [41]. The inverse isomorphism to (3) is

$$\chi_C^{-1} : \mathcal{F}(C^\circ) \rightarrow \mathcal{N}(C), \quad F \mapsto \text{pos}(F), \tag{4}$$

where $\text{pos}(F) = \{\lambda x : \lambda \geq 0, x \in F\}$ is the positive hull of any nonempty exposed face F of C° , and $\text{pos}(\emptyset) = \{0\}$, see for example [46, Section 8]. Lemma 7.2 of [46] shows that the cone $\chi_C^{-1}(F)$ is the normal cone to C at the exposed face $F_C(u)$ of C which is exposed by any nonzero vector u in the relative interior of $\chi_C^{-1}(F)$, for all exposed faces $F \neq C^\circ$ of C° .

The following construction is fundamental in Sect. 3.6. Let $C \subseteq \mathbb{E}$ be a closed convex cone with interior point $\epsilon \neq 0$. Then

$$B_{C,\epsilon} = \{u \in C^\vee : \langle u, \epsilon \rangle = 1\}$$

is a compact convex set, which is a *base* of C^\vee . Let $U \subseteq \mathbb{E}$ be a linear subspace incident with ϵ , let

$$V_{U,\epsilon} = \{u \in U : \langle u, \epsilon \rangle = 0\}$$

be the orthogonal complement to ϵ in U , and

$$S_{C,U,\epsilon} = \{x \in V_{U,\epsilon} : \epsilon + x \in C\}$$

an affine section of the cone C .

Lemma 1 *Let $C \subseteq \mathbb{E}$ be a closed convex cone and let $\epsilon \neq 0$ be an interior point of C . Let $U \subseteq \mathbb{E}$ be a linear subspace incident with ϵ . Then $S_{C,U,\epsilon}$ is the dual convex set to $\pi_{V_{U,\epsilon}}(B_{C,\epsilon})$ with respect to the Euclidean space $V_{U,\epsilon}$.*

Proof Let $x \in V_{U,\epsilon}$ and let $B = B_{C,\epsilon}$. Then

$$\begin{aligned} x \in S_{C,U,\epsilon} &\iff \epsilon + x \in C \iff \forall u \in C^\vee : \langle u, \epsilon + x \rangle \geq 0 \\ &\iff \forall u \in B : \langle u, \epsilon + x \rangle \geq 0 \iff \forall u \in B : 1 + \langle u, x \rangle \geq 0 \\ &\iff \forall u \in \pi_{V_{U,\epsilon}}(B) : 1 + \langle u, x \rangle \geq 0. \end{aligned}$$

This proves the claim. \square

3.3 Geometry of the state space

The exposed faces and the normal cones of the state space $\mathcal{D}(\mathcal{A})$ are represented in terms of projectors.

Let $P_0 : \mathcal{H}(\mathcal{A}) \rightarrow \mathcal{P}(\mathcal{A})$ denote the map from the set of hermitian matrices to the set of projectors, where $P_0(A)$ is the spectral projector of A corresponding to the smallest eigenvalue of A . We call $P_0(A)$ the *ground projector* of A by its name in physics if A represents an energy observable.

The exposed face of the state space $\mathcal{D}(\mathcal{A})$ exposed by $A \in \mathcal{H}(\mathcal{A})$ is

$$F_{\mathcal{D}(\mathcal{A})}(A) = \mathcal{D}(P_0(A) \cdot A \cdot P_0(A)).$$

Note that

$$F_{\mathcal{D}(\mathcal{A})}(A) = \{\rho \in \mathcal{D}(\mathcal{A}) \mid S(\rho) \leq P_0(A)\},$$

where $S(\rho)$ is the *support projector* of ρ , the sum of the spectral projectors corresponding to the nonzero eigenvalues. Moreover, the map

$$\phi_{\mathcal{A}} : \mathcal{P}(\mathcal{A}) \rightarrow \mathcal{F}(\mathcal{D}(\mathcal{A})), \quad P \mapsto \mathcal{D}(P \cdot A \cdot P) \quad (5)$$

is an isotone lattice isomorphism from the lattice of projectors $\mathcal{P}(\mathcal{A})$ to the lattice of exposed faces of $\mathcal{D}(\mathcal{A})$, see for example [2] or [45, Section 2.3]. As

$$F_{\mathcal{D}(\mathcal{A})}(A) = (\phi_{\mathcal{A}} \circ P_0)(A), \quad A \in \mathcal{H}(\mathcal{A}), \quad (6)$$

the map $F_{\mathcal{D}(\mathcal{A})} : \mathcal{H}(\mathcal{A}) \rightarrow \mathcal{F}(\mathcal{D}(\mathcal{A}))$ factors through $\mathcal{P}(\mathcal{A})$.

The concatenation of the maps (5) and (2) is the antitone lattice isomorphism

$$\nu_{\mathcal{A}} : \mathcal{P}(\mathcal{A}) \rightarrow \mathcal{N}(\mathcal{D}(\mathcal{A})), \quad P \mapsto (N_{\mathcal{D}(\mathcal{A})} \circ \phi_{\mathcal{A}})(P), \quad (7)$$

where

$$\nu_{\mathcal{A}}(P) = \{A \in \mathcal{H}(\mathcal{A}) \mid P \leq P_0(A)\}$$

is the normal cone to $\mathcal{D}(\mathcal{A})$ at the exposed face $\phi_{\mathcal{A}}(P)$, see [51, Section 3]. Here, the Euclidean space to define normal cones in Eqn. (2) is $\mathbb{E} = \mathcal{H}(\mathcal{A})$. We ignore the case $\mathcal{A} \cong \mathbb{C}$ where $\mathcal{D}(\mathcal{A}) = \{I_d/d\}$ and (7) is not injective.

3.4 The joint numerical range and its exposed faces

In the sequel, let $\mathcal{U} \subseteq \mathcal{H}(\mathcal{A})$ be a vector space of hermitian matrices, and let $\pi_{\mathcal{U}} : \mathcal{H}(\mathcal{A}) \rightarrow \mathcal{H}(\mathcal{A})$ denote the orthogonal projection onto \mathcal{U} .

If F_1, \dots, F_k is a spanning set of \mathcal{U} , then the map

$$\text{Av} : \mathcal{H}(\mathcal{A}) \rightarrow \mathbb{R}^k, \quad A \mapsto \langle A, F_i \rangle_{i=1}^k,$$

factors through \mathcal{U} as per $\text{Av} = \text{Av} \circ \pi_{\mathcal{U}}$. The map $\mathcal{U} \xrightarrow{\text{Av}} \text{Av}(\mathcal{U})$ is a linear isomorphism, see [45, Remark 1.1], which restricts to the bijection

$$\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A})) \xrightarrow{\text{Av}} \text{Av}(\mathcal{D}(\mathcal{A})).$$

The set $\text{Av}(\mathcal{D}(\mathcal{A}))$ is known as the *joint numerical range* [11] of F_1, \dots, F_k . Here we call the set $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$ *joint numerical range* of \mathcal{U} . In physics, $\text{Av}(\rho)$ is the vector of expected values or averages of the observables F_1, \dots, F_k if the state of the system is represented by the density matrix $\rho \in \mathcal{D}(\mathcal{A})$.

Equation (6) shows that the function which maps a hermitian matrix A to the exposed face of $\mathcal{D}(\mathcal{A})$ exposed by A factors through the lattice of ground projectors. If $A \in \mathcal{U}$ then the map factors also through the lattice of exposed faces of the joint numerical range,

$$F_{\mathcal{D}(\mathcal{A})}(A) = (\phi_{\mathcal{A}} \circ P_0)(A) = (\pi_{\mathcal{U}}|_{\mathcal{D}(\mathcal{A})}^{-1} \circ \pi_{\mathcal{U}} \circ \phi_{\mathcal{A}} \circ P_0)(A), \quad A \in \mathcal{U}. \quad (8)$$

Note that the orthogonal projection $\pi_{\mathcal{U}} : \mathcal{H}(\mathcal{A}) \rightarrow \mathcal{H}(\mathcal{A})$ operates as a set-valued map here. The operator $\pi_{\mathcal{U}}|_{\mathcal{D}(\mathcal{A})}^{-1}$ maps a subset of the subspace \mathcal{U} to its pre-image inside the state space $\mathcal{D}(\mathcal{A})$. As detailed in Section 3.1 of [45], by endowing the set of ground projectors

$$\mathcal{P}_0(\mathcal{U}) = \{P_0(A) : A \in \mathcal{U}\} \cup \{\emptyset\}$$

with the Loewner order and the set of exposed faces $F_{\mathcal{D}(\mathcal{A})}(\mathcal{U}) \cup \{\emptyset\}$ with the partial order of inclusion, one obtains the lattice isomorphisms

$$\mathcal{P}_0(\mathcal{U}) \xrightarrow{\phi_{\mathcal{A}}} \phi_{\mathcal{A}}(\mathcal{P}_0(\mathcal{U})) = F_{\mathcal{D}(\mathcal{A})}(\mathcal{U}) \cup \{\emptyset\} \begin{matrix} \xrightarrow{\pi_{\mathcal{U}}} \\ \xleftarrow{\pi_{\mathcal{U}}|_{\mathcal{D}(\mathcal{A})}^{-1}} \end{matrix} \mathcal{F}(\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))). \quad (9)$$

The lattices $\mathcal{P}_0(\mathcal{U})$, $\phi_{\mathcal{A}}(\mathcal{P}_0(\mathcal{U}))$, and $\mathcal{F}(\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A})))$ are complete, coatomistic lattices [50, Corollary 6.5]. The infimum in the lattices $\phi_{\mathcal{A}}(\mathcal{P}_0(\mathcal{U}))$ and $\mathcal{F}(\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A})))$ is the intersection. The infimum in $\mathcal{P}_0(\mathcal{U})$ is the same as the infimum in the lattice $\mathcal{P}(\mathcal{A})$ of all projectors, restricted to subsets of $\mathcal{P}_0(\mathcal{U})$, of course [51, Section 4].

3.5 Normal cones of the joint numerical range

We discuss the antitone isomorphism between the ground projectors and the normal cones of the joint numerical range. The atoms (rays) of the lattice of normal cones characterize the coatoms of the lattice of ground projectors.

If $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$ is not a singleton, then the lattice isomorphisms (9) and (2) concatenate to the antitone lattice isomorphism

$$\mathcal{P}_0(\mathcal{U}) \rightarrow \mathcal{N}(\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))), \quad P \mapsto v_{\mathcal{A}}(P) \cap \mathcal{U}. \tag{10}$$

Here, the Euclidean space to define normal cones in Eqn. (2) is $\mathbb{E} = \mathcal{U}$. Also, $v_{\mathcal{A}}(P)$ is a normal cone to the state space, see Eqn. (7), and

$$v_{\mathcal{A}}(P) \cap \mathcal{U} = \{A \in \mathcal{U} \mid P \preceq P_0(A)\}$$

is the normal cone to the joint numerical range $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$ at the convex subset $\pi_{\mathcal{U}} \circ \phi_{\mathcal{A}}(P)$ for all $P \in \mathcal{P}(\mathcal{A})$. See [51, Section 4] for more details.

From now on we assume that the space of hermitian matrices $\mathcal{U} \subseteq \mathcal{H}(\mathcal{A})$ contains the $d \times d$ identity matrix I_d . A somewhat simpler object than the normal cone $v_{\mathcal{A}}(P) \cap \mathcal{U}$ is the cone

$$\begin{aligned} \mathcal{K}(P) &= P'.\mathcal{A}^+.P' \cap \mathcal{U} \\ &= \{A \in \mathcal{U} \mid A \succeq 0, P \preceq \ker(A)\}, \quad P \in \mathcal{P}(\mathcal{A}). \end{aligned} \tag{11}$$

Here, $P' = I_d - P$ denotes the complementary projector to P .

The following statement is Theorem 5.1 of [51]. We use it in Sect. 4.4 to identify elements in the lattice of ground projectors.

Theorem 1 *Let $\mathcal{U} \subseteq \mathcal{H}(\mathcal{A})$ be a linear subspace containing the identity matrix $I_d \in \mathcal{U}$ and let $P \in \mathcal{P}(\mathcal{A})$. Then P lies in $\mathcal{P}_0(\mathcal{U})$ if and only if P is the greatest element of the set of all $Q \in \mathcal{P}(\mathcal{A})$ which satisfy $\mathcal{K}(Q) = \mathcal{K}(P)$.*

Thm. 1 yields a necessary condition for projectors to lie in $\mathcal{P}_0(\mathcal{U})$.

Corollary 1 *Let $\mathcal{U} \subseteq \mathcal{H}(\mathcal{A})$ be a linear subspace with $I_d \in \mathcal{U}$ and let $P \neq I_d$ be a projector in \mathcal{A} . If there exists a hermitian matrix $A \in \mathcal{H}(\mathcal{A})$ orthogonal to \mathcal{U} and a nonzero number $\lambda \neq 0$ such that $P'.A.P' = \lambda P'$, then $P \notin \mathcal{P}_0(\mathcal{U})$.*

Proof Let $A \in \mathcal{U}^\perp$ and $\lambda \neq 0$ such that $P'.A.P' = \lambda P'$ and let $U \in \mathcal{K}(P)$. Since $U = P'.U.P'$, we have

$$\lambda \operatorname{Tr}(U) = \lambda \langle P', U \rangle = \langle P'.A.P', U \rangle = \langle A, U \rangle = 0.$$

Since $\lambda \neq 0$ we get $\operatorname{Tr}(U) = 0$. As $U \succeq 0$ this implies $U = 0$. The claim follows from Thm. 1 as $\mathcal{K}(I_d) = \{0\}$. □

Thm. 2 is proved as Theorem 6.1 of [51]. The second statement of Thm. 2 is clear, as the cone of positive semidefinite matrices \mathcal{A}^+ contains no lines. We use this result (and Lemma 2 below) in the experimental method (third step) described in Remark 2.

Theorem 2 *Let $\mathcal{U} \subseteq \mathcal{H}(\mathcal{A})$ be a linear subspace containing the identity matrix $I_d \in \mathcal{U}$ and let $P \in \mathcal{P}_0(\mathcal{U})$. Then P is a coatom of $\mathcal{P}_0(\mathcal{U})$ if and only if $\mathcal{K}(P)$ is a ray. This happens if and only if $\dim \mathcal{K}(P) = 1$.*

Finding the dimension of the cone $\mathcal{K}(P)$ is a problem of linear algebra.

Lemma 2 *Let $\mathcal{U} \subseteq \mathcal{H}(\mathcal{A})$ be a linear subspace with $I_d \in \mathcal{U}$ and let $P \in \mathcal{P}_0(\mathcal{U})$. Then the real span of the cone $\mathcal{K}(P)$ is $\mathcal{H}(P'.\mathcal{A}.P') \cap \mathcal{U}$.*

Proof The cone $\mathcal{K}(0) = \mathcal{A}^+ \cap \mathcal{U}$ has the span \mathcal{U} as required, as $I_d \in \mathcal{U}$. Let $P \neq 0$. As $P \in \mathcal{P}_0(\mathcal{U})$ and as $I_d \in \mathcal{U}$, there is a (positive semidefinite) matrix $U \in \mathcal{U}$ such that $P = P_0(U)$ and $U.P = 0$. Hence, U is invertible in the algebra $P'.\mathcal{A}.P'$. Thus, U is an interior point of the cone of positive semidefinite matrices $P'.\mathcal{A}^+.P'$ with respect to the topology of $\mathcal{H}(P'.\mathcal{A}.P')$, see Prop. 2.7 of [45]. This proves the claim. \square

3.6 Finding coatoms via semidefinite programming

We show that the coatoms of the lattice of ground projectors $\mathcal{P}_0(\mathcal{U})$ are in a one-to-one correspondence with the extreme points of a spectrahedron. This yields a numerical algorithm to find candidates for coatoms, and an algebraic method to verify the candidates are indeed coatoms.

Besides the hypothesis that $I_d \in \mathcal{U}$, we assume $\dim(\mathcal{U}) \geq 2$ from now on. We introduce the space

$$\mathcal{V} = \{A \in \mathcal{U} : \langle A, I_d \rangle = 0\} = \{A \in \mathcal{U} : \text{Tr}(A) = 0\}.$$

The joint numerical ranges $\pi_{\mathcal{V}}(\mathcal{D}(\mathcal{A})) = \pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A})) - I_d/d$ are translates of each other, and the lattices of ground projectors $\mathcal{P}_0(\mathcal{V}) = \mathcal{P}_0(\mathcal{U})$ coincide. The affine section

$$\mathcal{S}(\mathcal{U}) = \{A \in \mathcal{V} : I_d + A \in \mathcal{A}^+\}$$

of the cone of positive semidefinite matrices is a *spectrahedron* [36]

It is well known that the cone of positive semidefinite matrices $(M_d)^+$ is a self-dual convex cone within the Euclidean space of hermitian matrices $\mathcal{H}(M_d)$. The analogue is true for every real $*$ -algebra $\mathcal{A} \subseteq M_d$, see Corollary 2.8 of [45]. Therefore, Lemma 1 shows

$$\mathcal{S}(\mathcal{U}) = \mathcal{W}^\circ \tag{12}$$

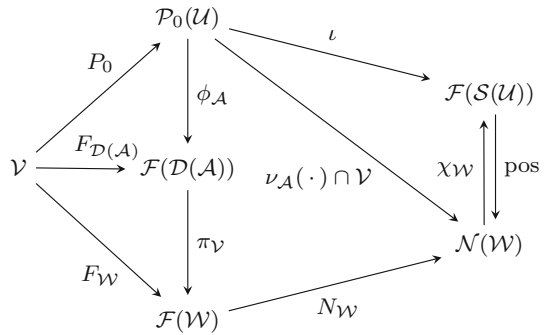
where the whole space \mathbb{E} assumed in defining \mathcal{W}° is \mathcal{V} , and where

$$\mathcal{W} = \pi_{\mathcal{V}}(\mathcal{D}(\mathcal{A}))$$

denotes the joint numerical range. That is to say, the spectrahedron $\mathcal{S}(\mathcal{U})$ is the dual convex set to \mathcal{W} .

Combining two lattice isomorphisms, we identify $\mathcal{P}_0(\mathcal{U})$ and the set of exposed faces of $\mathcal{S}(\mathcal{U})$. Equation (10) provides an antitone lattice isomorphism $\mathcal{P}_0(\mathcal{U}) \rightarrow \mathcal{N}(\mathcal{W})$ to the lattice of normal cones of \mathcal{W} , as \mathcal{W} is not a singleton under the chosen

Fig. 2 Commutative diagram with isomorphisms between the lattices $\mathcal{P}_0(\mathcal{U})$, $\mathcal{F}(\mathcal{W})$, $\mathcal{N}(\mathcal{W})$, and $\mathcal{F}(\mathcal{S}(\mathcal{U}))$



assumptions. As \mathcal{W} is compact, Equation (3) provides the isomorphism $\mathcal{N}(\mathcal{W}) \rightarrow \mathcal{F}(\mathcal{S}(\mathcal{U}))$. The function composition of (10) and (3) is the antitone lattice isomorphism

$$\iota : \mathcal{P}_0(\mathcal{U}) \rightarrow \mathcal{F}(\mathcal{S}(\mathcal{U})), \quad P \mapsto \begin{cases} \nu_{\mathcal{A}}(P) \cap \partial \mathcal{S}(\mathcal{U}) & \text{if } P \neq 0, \\ \mathcal{S}(\mathcal{U}) & \text{if } P = 0, \end{cases} \quad (13)$$

where $\nu_{\mathcal{A}}(P) \cap \mathcal{V}$ is a normal cone to \mathcal{W} , as introduced in Equation (10).

We invert the isomorphism (13). Note that all faces of the spectrahedron $\mathcal{S}(\mathcal{U})$ are exposed faces [36]. In particular, all extreme points are exposed points.

Theorem 3 *Let $\mathcal{U} \subseteq \mathcal{H}(\mathcal{A})$ be a subspace with $\dim(\mathcal{U}) \geq 2$ and $I_d \in \mathcal{U}$. Let $(P, F) \neq (0, \mathcal{S}(\mathcal{U}))$ be a point in the graph of the isomorphism ι . Then $P = P_0(A)$ holds for any nonzero matrix A in the relative interior of the positive hull $\text{pos}(F)$. The map ι restricts to the bijection*

$$\left\{ \text{coatoms of } \mathcal{P}_0(\mathcal{U}) \right\} \rightarrow \left\{ \{A\} \mid A \text{ is an exposed point of } \mathcal{S}(\mathcal{U}) \right\}. \quad (14)$$

Let $(P, \{A\})$ be a point in the graph of the map (14). Then A is the unique matrix in \mathcal{V} with ground projector $P = P_0(A)$ for which $I_d + A$ is positive semidefinite of nonmaximal rank. If $P \in \mathcal{U}$ then $A = \frac{\text{Tr}(P)}{\text{Tr}(P')}P' - P$.

Proof The commutative diagram in Fig. 2 provides an overview of the maps introduced in Sect. 3, which are relevant to this proof. By applying the positive hull operator to the equation $\iota(P) = F$, we obtain

$$\nu_{\mathcal{A}}(P) \cap \mathcal{V} = \text{pos}(F).$$

Let A be a nonzero point in the relative interior of $\text{pos}(F)$. As discussed below of Equation (4), the convex cone $\text{pos}(F)$ is the normal cone to \mathcal{W} at the exposed face $F_{\mathcal{W}}(A)$, that is to say

$$v_{\mathcal{A}}(P) \cap \mathcal{V} = N_{\mathcal{W}} \circ F_{\mathcal{W}}(A).$$

The commutative diagram then shows $P = P_0(A)$.

The isomorphism ι restricts to the bijection (14), since every atom of the lattice of exposed faces of $\mathcal{S}(\mathcal{U})$ is an exposed point. To prove this, it suffices to show that every nonempty exposed face F of $\mathcal{S}(\mathcal{U})$ contains an exposed point of $\mathcal{S}(\mathcal{U})$. Since F is compact, it has an extreme point A by Minkowski’s theorem [41]. As F is a face of $\mathcal{S}(\mathcal{U})$, the point A is an extreme point of $\mathcal{S}(\mathcal{U})$, and hence an exposed point of $\mathcal{S}(\mathcal{U})$.

Let P be a coatom of $\mathcal{P}_0(\mathcal{U})$ and let A be an exposed point of $\mathcal{S}(\mathcal{U})$ such that $\{A\} = \iota(P)$. Since A is in the relative interior of the ray $\text{pos}(\{A\})$, we get $P = P_0(A)$ as above. As P is a coatom of $\mathcal{P}_0(\mathcal{U})$, the relation $P \preceq P_0(B)$ implies $P = P_0(B)$ for all nonzero traceless matrices $B \in \mathcal{U}$. Hence, the ray

$$v_{\mathcal{A}}(P) \cap \mathcal{V} = \text{pos}(\{A\})$$

consists of all matrices $B \in \mathcal{V}$ such that $P = P_0(B)$, and of zero, as per the definition of $v_{\mathcal{A}}(P)$ in Equation (7). The ray intersects the boundary $\partial\mathcal{S}(\mathcal{U})$ only in A . This completes the characterization of A , because boundary points B of the spectrahedron $\mathcal{S}(\mathcal{U})$ are characterized by $I_d + B$ being positive semidefinite of nonmaximal rank. If $P \in \mathcal{U}$, then the matrix $\frac{\text{Tr}(P)}{\text{Tr}(P')}P' - P$ fulfills the characterizing conditions of A . \square

Theorem 3 underpins the initial idea to the experimental method in Remark 2 and to this article, which is to sample extreme points from the dual spectrahedron, in order to find coatoms of the lattice of exposed faces of the joint numerical range. Sect. 4.5 shows how this works in an example of reduced density matrices.

Remark 2 (Experimental Method) The search for coatoms of the lattice of exposed faces of the joint numerical range \mathcal{W} works in three steps.

The first step is a numerical random search. The coatoms of the lattice $\mathcal{F}(\mathcal{W})$ of exposed faces of the joint numerical range $\mathcal{W} = \pi_{\mathcal{V}}(\mathcal{D}(\mathcal{A}))$ are amenable to a numerical exploration, since the map from the exposed faces of \mathcal{W} to their conjugate faces defines an antitone isomorphism $\mathcal{F}(\mathcal{W}) \rightarrow \mathcal{F}(\mathcal{S}(\mathcal{U}))$ to the lattice of exposed faces of the spectrahedron $\mathcal{S}(\mathcal{U})$. This map induces a one-to-one correspondence between the coatoms of $\mathcal{F}(\mathcal{W})$ and the atoms of $\mathcal{F}(\mathcal{S}(\mathcal{U}))$, which are the extreme points of $\mathcal{S}(\mathcal{U})$. Numerically, one can draw linear functionals from the dual space \mathcal{V}^* of \mathcal{V} at random, and minimize them on $\mathcal{S}(\mathcal{U})$. The minimum of a generic linear functional is attained at a single extreme point of $\mathcal{S}(\mathcal{U})$. This means that this random search will allow us to sample extreme points, or at least numerical approximations of such. The minimization can be done efficiently, using semidefinite programming [33].

To illustrate some subtleties of the underlying process let us revisit the Cayley cubic example of Fig. 1. In that case there are two types of extreme points, the four rank one vertices and the surface of rank two extreme points. While there are only four rank one extreme points, their normal cones have a high volume, hence it is quite likely that while searching in a random direction we end up sampling those points. In Fig. 3 one can see the possible search directions in \mathbb{R}^3 , color coded by which type of extreme point they lead to. The directions that lead to rank one matrices form four

Fig. 3 Search directions in the Cayley cubic



equal spherical caps pairwise tangent. One can easily calculate that a random search would therefore lead to a rank one matrix around 84.5% of the times, and a rank two matrix otherwise. The exceptional directions that would lead to linear forms that are minimized in higher dimensional faces are the six tangency points of the caps.

This gives us some hint of possible issues if one wants to find representatives for all classes of extreme points. In high dimensions, if the union of the normal cones of the extreme points in some class is of very low volume, it might be hard to sample by a uniformly generated random search direction. This problem should not be as acute in moderate dimensions, and does not stop us from attempting to find new interesting classes of extreme points.

The second step of the experimental method is the guesswork to find possible algebraic expressions for the numerical extreme points from step one.

The third step is the algebraic verification that the algebraic expressions from step two are indeed extreme points. The lattice $\mathcal{F}(\mathcal{W})$ is isomorphic to the lattice $\mathcal{P}_0(\mathcal{U})$ of ground projectors by Eqn. (9). This brings about a one-to-one correspondence between the coatoms of $\mathcal{F}(\mathcal{W})$ and the coatoms of $\mathcal{P}_0(\mathcal{U})$. Let $A \in \mathcal{V}$ be an arbitrary matrix, for example an output of the random search described above. Then the ground projector $P = P_0(A)$ lies in the lattice $\mathcal{P}_0(\mathcal{U})$. Thm. 2 and Lemma 2 above prove that P is a coatom of $\mathcal{P}_0(\mathcal{U})$ if and only if the real vector space

$$\mathcal{H}(P'.A.P') \cap \mathcal{U} \quad (15)$$

is a line (here, $P' = I_d - P$). Verifying that the vector space in equation (15) has dimension one allows us to confirm that $P = P_0(A)$ is a coatom.

4 Reduced density matrices

We discuss examples of two-body reduced density matrices. The highlight is the application of the experimental method of Remark 2 to the reduced density matrices of three qubits.

The basic notation of a many-body system is settled in Sect. 4.1. The Sects. 4.3 and 4.5 examine two-body reduced density matrices of three qubits. Sec. 4.3 shows that no two-local Hamiltonian has a ground projector of rank seven. Sect. 4.5 applies the experimental method of Remark 2 to the convex set of two-body reduced density matrices of three qubits. We examine the commutative case of three bits in Sect. 4.4. Sect. 4.6 comments on nonexposed points of the set of two-body reduced density matrices of three and six qubits in the context of quantum state tomography.

Section 4.2 goes beyond the case of two-body interaction. It addresses probability distributions that factor.

4.1 Reduced density matrices and local Hamiltonians

We specify an interaction pattern on a many-body system of $N \in \mathbb{N}$ units by choosing a family \mathfrak{g} of subsets of $\Omega = \{1, 2, \dots, N\}$. Let (d_1, d_2, \dots, d_N) be a sequence of natural numbers and $\mathfrak{a} = (\mathcal{A}_1, \mathcal{A}_2, \dots, \mathcal{A}_N)$ a sequence of $*$ -algebras, where \mathcal{A}_i is included in M_{d_i} and contains the $d_i \times d_i$ identity matrix I_{d_i} for all $i \in \Omega$.

The $*$ -algebra of the subsystem with units in a subset $\nu \subseteq \Omega$ is the tensor product $\mathcal{A}_\nu := \bigotimes_{i \in \nu} \mathcal{A}_i$. We omit the tensor product symbol \otimes when no confusion arises. That is to say, we write AB in place of $A \otimes B$ for two matrices A, B . We denote the multiplicative identity of \mathcal{A}_ν by I_ν , and write $\bar{\nu} = \Omega \setminus \nu$. The *partial trace* $\text{Tr}_{\bar{\nu}} : \mathcal{A}_\Omega \rightarrow \mathcal{A}_\nu$ over the subsystem $\bar{\nu}$ is the adjoint to the embedding $\mathcal{A}_\nu \rightarrow \mathcal{A}_\Omega$, $A \mapsto AI_{\bar{\nu}}$. The matrix $\text{Tr}_{\bar{\nu}}(\rho)$ is a state in $\mathcal{D}(\mathcal{A}_\nu)$, called the *reduced density matrix* in physics [18, 54], for every state $\rho \in \mathcal{D}(\mathcal{A}_\Omega)$. Let

$$\text{red}_{(\mathfrak{g}, \mathfrak{a})} : \mathcal{H}(\mathcal{A}_\Omega) \rightarrow \times_{\nu \in \mathfrak{g}} \mathcal{H}(\mathcal{A}_\nu), \quad A \mapsto (\text{Tr}_{\bar{\nu}}(A))_{\nu \in \mathfrak{g}} \tag{16}$$

denote the map which assigns reduced density matrices with respect to the pair $(\mathfrak{g}, \mathfrak{a})$. A \mathfrak{g} -local Hamiltonian [15] (also, quasi-local Hamiltonian [25]) is an element of the real vector space of hermitian matrices

$$\mathcal{U}(\mathfrak{g}, \mathfrak{a}) = \left\{ \sum_{\nu \in \mathfrak{g}} A_\nu I_{\bar{\nu}} : A_\nu \in \mathcal{H}(\mathcal{A}_\nu), \nu \in \mathfrak{g} \right\}. \tag{17}$$

We write

$$\mathcal{P}_0(\mathfrak{g}, \mathfrak{a}) = \mathcal{P}_0(\mathcal{U}(\mathfrak{g}, \mathfrak{a})) \cup \{0\}$$

to denote the lattice of ground projectors of $\mathcal{U}(\mathfrak{g}, \mathfrak{a})$.

In statistics [27], the space $\mathcal{U}(\mathfrak{g}, \mathfrak{a})$ is known as a *hierarchical model subspace*. Strictly speaking, one has to distinguish between the quantum mechanical concept of a Hamiltonian, or more generally of an observable, and its mathematical representation in terms of a hermitian matrix or a self-adjoint operator [9]. As it is common in theoretical physics [54], we refer with a local Hamiltonian to a matrix. Similarly, we apply to following notions of an interaction and of a frustration-free Hamiltonian to matrices.

Without changing the space $\mathcal{U}(\mathfrak{g}, \mathfrak{a})$, one can reduce \mathfrak{g} to the antichain of its maximal elements (partially ordered by inclusion) and one can augment \mathfrak{g} by adding all subsets of its elements as new elements. In the reduced form, \mathfrak{g} is known as the *generating class* of $\mathcal{U}(\mathfrak{g}, \mathfrak{a})$ in statistics [19, 27]. If \mathfrak{g} has the augmented form we call \mathfrak{g} a *hypergraph*.

It is useful to decompose local Hamiltonians into interaction terms. A matrix $A \in \mathcal{H}(\mathcal{A}_\Omega)$ is a ν -factor interaction, $\nu \subseteq \Omega$, if $A \in \mathcal{U}(\{\nu\}, \mathfrak{a})$ and A is perpendicular to $\mathcal{U}(\{\mu\}, \mathfrak{a})$ for all $\mu \subset \nu$. In statistics, ν -factor interactions are called $|\nu|$ -factor interactions [27, Section B.2]. If \mathfrak{g} is a hypergraph, then $\mathcal{U}(\mathfrak{g}, \mathfrak{a})$ is the direct sum

$$\mathcal{U}(\mathfrak{g}, \mathfrak{a}) = \bigoplus_{\nu \in \mathfrak{g}} \{A \in \mathcal{H}(\mathcal{A}_\Omega) \text{ is a } \nu\text{-factor interaction}\}. \tag{18}$$

We construct a basis for each summand in the direct sum (18). Let \mathcal{B}_i be an orthogonal basis of $\mathcal{H}(\mathcal{A}_i)$, $i \in \Omega$. Then the matrices $B_1 B_2 \dots B_N$, where $B_i \in \mathcal{B}_i$, $i \in \Omega$, are an orthogonal basis of $\mathcal{H}(\mathcal{A}_\Omega)$. If \mathcal{B}_i contains the identity matrix I_{d_i} for each $i \in \Omega$, then the set

$$\{B_1 B_2 \dots B_N \mid B_i \in \mathcal{B}_i \text{ and } B_i = I_{d_i} \text{ if and only if } i \in \bar{\nu} \text{ for all } i \in \Omega\}$$

is an orthogonal basis for the space of ν -factor interactions, the dimension of which is therefore $\prod_{i \in \nu} (\dim \mathcal{H}(\mathcal{A}_i) - 1)$.

As per $\text{red}_{(\mathfrak{g}, \mathfrak{a})} = \text{red}_{(\mathfrak{g}, \mathfrak{a})} \circ \pi_{\mathcal{U}(\mathfrak{g}, \mathfrak{a})}$, the map $\text{red}_{(\mathfrak{g}, \mathfrak{a})}$ factors through the space $\mathcal{U}(\mathfrak{g}, \mathfrak{a})$. The map restricts to the linear isomorphism

$$\mathcal{U}(\mathfrak{g}, \mathfrak{a}) \xrightarrow{\text{red}_{(\mathfrak{g}, \mathfrak{a})}} \text{red}_{(\mathfrak{g}, \mathfrak{a})}(\mathcal{H}(\mathcal{A}_\Omega)),$$

as its injectivity follows from equation (18). The map restricts to the bijection

$$\pi_{\mathcal{U}(\mathfrak{g}, \mathfrak{a})}(\mathcal{D}(\mathcal{A}_\Omega)) \xrightarrow{\text{red}_{(\mathfrak{g}, \mathfrak{a})}} \text{red}_{(\mathfrak{g}, \mathfrak{a})}(\mathcal{D}(\mathcal{A}_\Omega)), \tag{19}$$

between the joint numerical range and the set of reduced density matrices. The dimension of the set of reduced density matrices is therefore $\dim(\mathcal{U}(\mathfrak{g}, \mathfrak{a})) - 1$.

Theorem 4 *The lattice of exposed faces $\mathcal{F}(\text{red}_{(\mathfrak{g}, \mathfrak{a})}(\mathcal{D}(\mathcal{A}_\Omega)))$ of the convex set of reduced density matrices $\text{red}_{(\mathfrak{g}, \mathfrak{a})}(\mathcal{D}(\mathcal{A}_\Omega))$ is isomorphic to the lattice of exposed faces $\mathcal{F}(\pi_{\mathcal{U}(\mathfrak{g}, \mathfrak{a})}(\mathcal{D}(\mathcal{A}_\Omega)))$ of the joint numerical range $\pi_{\mathcal{U}(\mathfrak{g}, \mathfrak{a})}(\mathcal{D}(\mathcal{A}_\Omega))$. Both lattices are isomorphic to the lattice of ground projectors $\mathcal{P}_0(\mathfrak{g}, \mathfrak{a})$ of the space of local Hamiltonians $\mathcal{U}(\mathfrak{g}, \mathfrak{a})$.*

Proof The affine isomorphism in Equation (19) induces a lattice isomorphism between the lattices of exposed faces in the first statement. The lattice isomorphism (9) completes the proof. \square

Thm. 4 allows us to employ the experimental method of Remark 2 to search for coatoms in the lattice of exposed faces of the set of reduced density matrices.

In the sequel, we focus mainly on three-body systems, where $\Omega = \{1, 2, 3\}$. Up to permutations, there are only two generating classes with overlapping subsets, the

edge sets $\{\{1, 2\}, \{2, 3\}\}$ and $\{\{1, 2\}, \{2, 3\}, \{3, 1\}\}$ of the *path graph* P_3 and the *cycle graph* C_3 , respectively. We denote their hypergraphs by

$$p_3 = \{\emptyset, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{2, 3\}\}$$

and

$$c_3 = \{\emptyset, \{1\}, \{2\}, \{3\}, \{1, 2\}, \{2, 3\}, \{3, 1\}\},$$

respectively. By Equation (18), we have

$$\dim \mathcal{U}(c_3, \mathfrak{a}) = \prod_{i=1}^3 \dim \mathcal{H}(\mathcal{A}_i) - \prod_{i=1}^3 (\dim \mathcal{H}(\mathcal{A}_i) - 1)$$

and

$$\dim \mathcal{U}(p_3, \mathfrak{a}) = \dim \mathcal{U}(c_3, \mathfrak{a}) - (\dim \mathcal{H}(\mathcal{A}_1) - 1)(\dim \mathcal{H}(\mathcal{A}_3) - 1).$$

This gives $\dim \mathcal{U}(c_3, \mathfrak{a}) = 37$ and $\dim \mathcal{U}(p_3, \mathfrak{a}) = 28$ for three qubits.

We denote the set of all subsets of cardinality k of Ω by $\binom{N}{k}$. An $\binom{N}{k}$ -local Hamiltonian is called a *k-local Hamiltonian* [54] and $\text{red}_{\binom{N}{k}, \mathfrak{a}}(\mathcal{D}(\mathcal{A}_\Omega))$ is the set of *k-body reduced density matrices*. We will focus on the interaction pattern $\binom{3}{2} = c_3$ of three-body systems.

Remark 3 A special class of local Hamiltonians appears in information theory and statistical mechanics frequently. A matrix $A \in \mathcal{H}(\mathcal{A}_\Omega)$ is a *frustration-free Hamiltonian* [22, 32, 54] with respect to the pair $(\mathfrak{g}, \mathfrak{a})$ if there are $A_\nu \in \mathcal{H}(\mathcal{A}_\nu)$, $\nu \in \mathfrak{g}$, such that

$$A = \sum_{\nu \in \mathfrak{g}} A_\nu I_{\bar{\nu}},$$

and such that the ground projectors satisfy $P_0(A) \preceq P_0(A_\nu I_{\bar{\nu}})$ with respect to the Loewner order for all $\nu \in \mathfrak{g}$. Hence, the set of ground projectors of all frustration-free Hamiltonians, together with the zero projector, is the set

$$\mathcal{P}_0^{\text{ff}}(\mathfrak{g}, \mathfrak{a}) = \left\{ \bigwedge_{\nu \in \mathfrak{g}} P_\nu I_{\bar{\nu}} : P_\nu \in \mathcal{P}(\mathcal{A}_\nu), \nu \in \mathfrak{g} \right\}. \tag{20}$$

As per the associativity of the infimum, the infimum of any subset of $\mathcal{P}_0^{\text{ff}}(\mathfrak{g}, \mathfrak{a})$ in the Loewner order on $\mathcal{P}(\mathcal{A}_\Omega)$ lies in $\mathcal{P}_0^{\text{ff}}(\mathfrak{g}, \mathfrak{a})$. Hence, $\mathcal{P}_0^{\text{ff}}(\mathfrak{g}, \mathfrak{a})$ is a complete lattice [10, Section I.4]. Furthermore, the lattice $\mathcal{P}_0^{\text{ff}}(\mathfrak{g}, \mathfrak{a})$ is coatomistic. The set of coatoms of $\mathcal{P}_0^{\text{ff}}(\mathfrak{g}, \mathfrak{a})$ is

$$\bigcup_{\nu \in \mathfrak{g}} \{P_\nu I_{\bar{\nu}} : P_\nu \text{ is a coatom of } \mathcal{P}(\mathcal{A}_\nu)\} \tag{21}$$

if \mathfrak{g} is a generating class.

4.2 Probability distributions that factor

This section adds a refined aspect to the lattice of faces of the set of marginals, as the ground projectors of only some local Hamiltonians support probability distributions that factor. The projectors have to satisfy a certain condition [19]. We show that the condition is that the projector is the ground projector of a frustration-free Hamiltonian.

Let $\mathcal{A}_i = \mathbb{C}^{C(d_i)}$ be the $*$ -algebra of complex functions on the configuration space $C(d_i) = \{0, 1, \dots, d_i - 1\}$, $i \in \Omega$, introduced in Sect. 2.2. The algebra \mathcal{A}_ν of the subsystem $\nu \subseteq \Omega$ is the set $\mathcal{A}_\nu = \mathbb{C}^{C_\nu}$ of complex functions on the configuration space

$$C_\nu = \prod_{i \in \nu} C_i.$$

If $x = (x_i)_{i \in \Omega}$ is an element of C_Ω and $\nu \subseteq \Omega$, then x_ν denotes the truncation of x to ν , that is to say, $x_\nu = ((x_\nu)_i)_{i \in \nu}$ is the element of C_ν which satisfies $(x_\nu)_i = x_i$ for all $i \in \nu$. Let \mathfrak{g} be a family of subsets of Ω and let

$$C_{\mathfrak{g}} = \{(\nu, y) \mid y \in C_\nu, \nu \in \mathfrak{g}\}$$

denote the disjoint union of the configuration spaces C_ν , $\nu \in \mathfrak{g}$. The matrix $M = (m_{(\nu,y),x})$ of the map (16) has the coefficients

$$\begin{aligned} m_{(\nu,y),x} &= \text{red}_{(\mathfrak{g},\mathfrak{a})}(\delta_x)(\nu, y) \\ &= \text{Tr}_{\bar{\nu}}(\delta_x)(y) = \delta_{x_\nu}(y), \quad (\nu, y) \in C_{\mathfrak{g}}, x \in C_\Omega, \end{aligned} \tag{22}$$

with respect to the bases $(\delta_x)_{x \in C_\Omega}$ of \mathbb{R}^{C_Ω} and $(\delta_{(\nu,y)})_{(\nu,y) \in C_{\mathfrak{g}}}$ of $\prod_{\nu \in \mathfrak{g}} \mathbb{R}^{C_\nu}$. The set of marginals is the convex hull of the columns of the matrix M , which is called the marginal polytope [43].

By definition, a probability distribution $P \in \mathcal{D}(\mathcal{A}_\Omega)$ factors with respect to \mathfrak{g} if there exist a function $\psi_\nu : C_\nu \rightarrow \mathbb{R}$ for each $\nu \in \mathfrak{g}$ such that

$$P(x) = \prod_{\nu \in \mathfrak{g}} \psi_\nu(x_\nu), \quad x \in C_\Omega.$$

It is well known [19] that a probability distribution $P \in \mathcal{D}(\mathcal{A}_\Omega)$ factors with respect to \mathfrak{g} if and only if $P = P_\theta$ for some $\theta \in [-\infty, \infty)^{C_{\mathfrak{g}}}$, where

$$P_\theta(x) = \frac{1}{Z(\theta)} e^{(\theta, T(x))}, \quad x \in C_\Omega. \tag{23}$$

Here, $T(x) = (m_{(\nu,y),x})_{(\nu,y) \in C_{\mathfrak{g}}}$ is the column with index $x \in C_\Omega$ of the matrix M defined above in Equation (22). The bracket $\langle \cdot, \cdot \rangle$ is the inner product on $\mathbb{R}^{C_{\mathfrak{g}}}$ restricted to nonnegative values in the second argument and extended to minus infinity in the first, by defining $(-\infty) \cdot 0 = 0$ and $(-\infty) \cdot t = -\infty$ for all $t > 0$. The number $Z(\theta)$ is a normalization constant. As $e^{-\infty} = 0$, the Equation (23) defines a probability distribution if and only if $(\theta, T(x)) > -\infty$ holds for at least one $x \in C_\Omega$. Parametric

models of the form (23) are called *hierarchical models* in the literature [7, 27], they are special cases of *exponential families* or *log-linear models* [19].

Probability distributions that factor have been characterized in terms of support sets and commutative algebra. A subset $F \subseteq C_\Omega$ is *M-feasible* if

$$\text{supp } T(x) \not\subseteq \bigcup_{y \in F} \text{supp } T(y), \quad \text{for all } x \in C_\Omega \setminus F.$$

Here, $\text{supp } T(x)$ is the subset of points $(v, y) \in C_{\mathfrak{g}}$ for which the coefficients of $T(x)$ are nonzero (and hence equal to one). This means that (v, y) belongs to $\text{supp } T(x)$ if and only if $x_v = y$. The *nonnegative toric variety* X_M is the set of all vectors $\xi = (\xi_x)_{x \in C_\Omega}$ in $[0, \infty)^{C_\Omega}$ which satisfy

$$\prod_{x \in C_\Omega} \xi_x^{u_x} = \prod_{x \in C_\Omega} \xi_x^{v_x}$$

whenever $u = (u_x)_{x \in C_\Omega}, v = (v_x)_{x \in C_\Omega} \in \mathbb{Z}^{C_\Omega}$ are vectors of nonnegative integers such that $u - v$ is in the kernel of M .

Theorem 5 (Geiger et al. [19]) *Let $\mathcal{A}_i = \mathbb{C}^{C(d_i)}$ for all $i \in \Omega$ and let $P \in \mathcal{D}(\mathcal{A}_\Omega)$ be a probability distribution. Then P factors with respect to \mathfrak{g} if and only if the support of P is M -feasible and P lies in the nonnegative toric variety X_M .*

We describe the support condition of Theorem 5 in terms of ground projectors. We use the map (1) to identify projectors in \mathcal{A}_v and subsets of $C_v, v \subseteq \Omega$. The complementary projector to $P \subseteq C_v$ is $P' = C_v \setminus P = I_v - P$.

Lemma 3 *Let $\mathcal{A}_i = \mathbb{C}^{C(d_i)}$ for all $i \in \Omega$ and let $P \in \mathcal{P}(\mathcal{A}_\Omega)$ be a projector. The following assertions are equivalent.*

1. P is M -feasible,
2. $P = \bigcap_{x \in P'} \bigcap_{v \in \mathfrak{g}_x} \{x_v\}' I_{\bar{v}}$, where $\mathfrak{g}_x = \{v \in \mathfrak{g} \mid x_v \neq y_v \text{ for all } y \in P\}$,
3. there exists a frustration-free \mathfrak{g} -local Hamiltonian $A \in \mathcal{U}(\mathfrak{g}, \mathfrak{a})$ such that $P = P_0(A)$ is the ground projector of A .

Proof Let P be M -feasible. Then for all $x \in P'$ there exists $v \in \mathfrak{g}$ such that $x_v \neq y_v$ holds for all $y \in P$. This shows that the set \mathfrak{g}_x above is nonempty for all $x \in P'$. Without any assumptions on the projector P , the inclusion “ \subseteq ” of the assertion 2) holds. Since each of the sets $\mathfrak{g}_x, x \in P'$, is nonempty, the right-hand side of the equation 2) cannot contain any points of P' . This proves 1) \Rightarrow 2). The implication 2) \Rightarrow 3) was discussed in Equation (20).

Let $P = \bigcap_{v \in \mathfrak{g}} P_v I_{\bar{v}}$, where $P_v \in \mathcal{P}(\mathcal{A}_v)$ for all $v \in \mathfrak{g}$, and let $x \in P'$. Then there exists $v \in \mathfrak{g}$ such that $x \notin P_v I_{\bar{v}}$, that is to say, $x_v \notin P_v$. Since $y_v \in P_v$ holds for all $y \in P$, this proves that P is M -feasible, hence 3) \Rightarrow 1). □

Corollary 2 *Let $\mathcal{A}_i = \mathbb{C}^{C(d_i)}, i \in \Omega$, and let $P \in \mathcal{P}(\mathcal{A}_\Omega)$ be a nonzero projector. Then P is the ground projector of a frustration-free \mathfrak{g} -local Hamiltonian if and only if there are functions $A_v \in \mathbb{R}^{C_v}, v \in \mathfrak{g}$, such that $P = \prod_{v \in \mathfrak{g}} A_v I_{\bar{v}}$. If this is the case, then there are projectors $P_v \in \mathcal{P}(\mathcal{A}_v), v \in \mathfrak{g}$, such that $P = \prod_{v \in \mathfrak{g}} P_v I_{\bar{v}}$.*

Proof If the projector P factors, then the uniform probability distribution $\frac{P}{|P|}$ on the set P factors. Theorem 5 then shows that P is M -feasible and Lemma 3 concludes that P is the ground projector of a frustration-free Hamiltonian. Conversely, if P is the ground projector of a frustration-free Hamiltonian, then Equation (20) shows $P = \bigcap_{\nu \in \mathfrak{g}} P_\nu I_{\bar{\nu}}$, where $P_\nu \in \mathcal{P}(\mathcal{A}_\nu)$, $\nu \in \mathfrak{g}$. This proves the claim, as $\bigcap_{\nu \in \mathfrak{g}} P_\nu I_{\bar{\nu}} = \prod_{\nu \in \mathfrak{g}} P_\nu I_{\bar{\nu}}$. \square

4.3 A first glimpse at three qubits

We consider a system of $N \in \mathbb{N}$ qubits. The algebras

$$\mathfrak{a}_{N,\text{qu}} = \underbrace{(M_2, M_2, \dots, M_2)}_{N \text{ copies}}$$

of the units are all equal to the algebra M_2 of a single qubit (Sect. 2.3). The algebra

$$\mathcal{A}_\Omega = M_2^{\otimes N} = M_{2^N}$$

of the full system is the N -fold tensor product of M_2 . The space of hermitian matrices $\mathcal{H}(\mathcal{A}_\Omega)$ has the orthogonal basis

$$\{A_1 A_2 \dots A_N : A_i \in \{I, X, Y, Z\}, i \in \Omega = \{1, 2, \dots, N\}\}.$$

We begin with an observation regarding the space $\mathcal{U}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}})$ of two-local three-qubit Hamiltonians.

Lemma 4 *The space $\mathcal{U}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}})$ contains no matrix of rank one. In other words, the lattice of ground projectors $\mathcal{P}_0(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}})$ contains no projector of rank seven.*

Proof Let $P = |\psi\rangle\langle\psi|$ be the projector onto the line spanned by a unit vector $\psi \in (\mathbb{C}^{C(2)})^{\otimes 3}$. It is known [1] that, up to a local unitary transformation, there are $\kappa_0, \kappa_1, \dots, \kappa_4 \geq 0$ and $\theta \in [0, \pi)$ such that

$$\psi = \kappa_0 e^{i\theta} |000\rangle + \kappa_1 |001\rangle + \kappa_2 |010\rangle + \kappa_3 |100\rangle + \kappa_4 |111\rangle.$$

Let us assume that P lies in $\mathcal{U}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}})$. Then the inner products of P with all three-factor interactions vanish. In particular

$$0 = \langle P, ZZZ \rangle = \kappa_0^2 - \kappa_1^2 - \dots - \kappa_4^2,$$

which is only possible if $\kappa_0 = 1/\sqrt{2}$, as ψ is a unit vector. Hence,

$$\begin{aligned} \langle P, ZZ X \rangle &= \sqrt{2} \kappa_1 \cos(\theta), & \langle P, Z X Z \rangle &= \sqrt{2} \kappa_2 \cos(\theta), \\ \langle P, X Z Z \rangle &= \sqrt{2} \kappa_3 \cos(\theta), & \langle P, X X X \rangle &= \sqrt{2} \kappa_4 \cos(\theta), \end{aligned}$$

which shows $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_4 = 0$ if $\theta \neq \frac{\pi}{2}$ modulo π . Also,

$$\begin{aligned} \langle P, ZZY \rangle &= -\sqrt{2} \kappa_1 \sin(\theta), & \langle P, ZYZ \rangle &= -\sqrt{2} \kappa_2 \sin(\theta), \\ \langle P, YZZ \rangle &= -\sqrt{2} \kappa_3 \sin(\theta), & \langle P, YYY \rangle &= \sqrt{2} \kappa_4 \sin(\theta), \end{aligned}$$

shows $\kappa_1 = \kappa_2 = \kappa_3 = \kappa_4 = 0$ if $\theta = \frac{\pi}{2}$ modulo π . In any case,

$$1/2 = \kappa_0^2 + \kappa_1^2 + \kappa_2^2 + \kappa_3^2 + \kappa_4^2 = \langle \psi | \psi \rangle = 1$$

is a contradiction. □

4.4 All about three bits

We consider a system of $N \in \mathbb{N}$ bits, which is a special case of the setup discussed in Sect. 4.2. The configuration space of a bit is $C(2) = \{0, 1\}$. The algebras

$$\mathfrak{a}_{N,\text{cl}} = \underbrace{(\mathbb{C}^{C(2)}, \mathbb{C}^{C(2)}, \dots, \mathbb{C}^{C(2)})}_{N \text{ copies}}$$

of the units are all equal to the algebra $\mathbb{C}^{C(2)}$ of 2-by-2 diagonal matrices, associated with a single bit (Sect. 2.5). The algebra

$$\mathcal{A}_\Omega = (\mathbb{C}^{C(2)})^{\otimes N} = \mathbb{C}^{C_\Omega}$$

of the full system is the N -fold tensor product of $\mathbb{C}^{C(2)}$, which is the set of complex functions on C_Ω . The set

$$\{A_1 A_2 \dots A_N : A_i \in \{I, Z\}, i \in \Omega\}$$

is an orthogonal basis of the space of hermitian matrices $\mathcal{H}(\mathcal{A}_\Omega) = \mathbb{R}^{C_\Omega}$. We identify two representations of rank one projectors in \mathcal{A}_Ω , using the isomorphism of Equation (1),

$$x_1 x_2 \dots x_N = \frac{1}{2^N} (I + (-1)^{x_1} Z) (I + (-1)^{x_2} Z) \dots (I + (-1)^{x_N} Z), \tag{24}$$

for all N -digit binary numbers $x = x_1 x_2 \dots x_N \in C_\Omega$. On the left-hand side of Equation (24) there is an element of the configuration space C_Ω , and on the right-hand side there is a diagonal $2^N \times 2^N$ matrix. The number x marks the position of the diagonal entry 1 of this matrix, which has all other entries equal to 0. The position increases from $x = 00 \dots 0$ at the top left to $x = 11 \dots 1$ at the bottom right of the diagonal.

We focus on $N = 3$ where $\Omega = \{1, 2, 3\}$. In Lemma 5 we simplify the characterization of the coatoms of the lattice of ground projectors of the space $\mathcal{U}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{cl}})$ of two-local three-bit Hamiltonians [51]. We also describe the ground projectors of

frustration-free Hamiltonians, in Lemma 6, and of Hamiltonians interacting along a path without a cycle, in Lemma 7.

Note that the space $\mathcal{U}(c_3, a_{3,cl})$ is the orthogonal complement to $f = ZZZ$ in $\mathcal{H}(\mathcal{A}_\Omega)$. We have

$$f(x_1x_2x_3) = (-1)^{x_1+x_2+x_3}, \quad x_1, x_2, x_3 \in C(2),$$

$$f = \text{diag}(+1, -1, -1, +1, -1, +1, +1, -1).$$

We identify the vertex set of the complete bi-partite graph $K_{4,4}$ with C_Ω , the bi-partition being defined by the two fibers of f . In other words, $\{x, y\} \subseteq C_\Omega$ is an edge of $K_{4,4}$ if and only if the digit sums of x and y differ modulo two.

The projectors in \mathcal{A}_Ω are in a one-to-one correspondence with the subsets of C_Ω by means of the isomorphism (1). The complementary projector to $P \subseteq C_\Omega$ is $P' = C_\Omega \setminus P = III - P$.

Lemma 5 *Let $P \subseteq C(2)^{\times 3}$ be a subset. The projector P is a coatom of $\mathcal{P}_0(c_3, a_{3,cl})$ if and only if P' is an edge of the graph $K_{4,4}$. The projector P lies in $\mathcal{P}_0(c_3, a_{3,cl})$ if and only if P' is a union of edges of $K_{4,4}$ (possibly empty).*

Proof We abbreviate $\mathcal{U} = \mathcal{U}(c_3, a_{3,cl})$ and $\mathcal{P}_0 = \mathcal{P}_0(c_3, a_{3,cl})$. The lattice \mathcal{P}_0 has no elements of rank seven by Lemma 4.

If $P \in \mathcal{P}_0$ has rank at most five, then P is not a coatom. Indeed, as f is perpendicular to \mathcal{U} , Cor. 1 shows that f is nonconstant on P' . Hence, there are mutually distinct points $x, y, z \in P'$ such that $f(x) \neq f(y) = f(z)$. Then the space $\mathcal{H}(P' \cdot \mathcal{A}_\Omega \cdot P') \cap \mathcal{U}$ has dimension at least two, as it contains the linearly independent rank two projectors $\{x, y\}$ and $\{x, z\}$. According to Equation (15), this proves that P is not a coatom of \mathcal{P}_0 .

The preceding part of the proof shows that a projector $P \subseteq C(2)^{\times 3}$ is a coatom of \mathcal{P}_0 if and only if $P \in \mathcal{P}_0$ and $|P| = 6$. Let $P' = \{x, y\}$ with $x \neq y$ and consider the cone $\mathcal{K}(P) = P' \cdot \mathcal{A}_\Omega^+ \cdot P' \cap \mathcal{U}$ defined in Equation (11). If $f(x) \neq f(y)$ then $\mathcal{K}(P)$ is the ray spanned by $\{x, y\}$. If $f(x) = f(y)$ then $\mathcal{K}(P) = \{0\}$. Thus, Thm. 1 completes the assertion on coatoms.

The second assertion is true since the infimum in \mathcal{P}_0 is the intersection and since \mathcal{P}_0 is coatomistic by Thm. 2. □

We describe the coatoms of $\mathcal{P}_0(c_3, a_{3,cl})$ in terms of matrices and extreme points.

Remark 4 (Edges, Matrices, and Extreme Points) Lemma 5 above characterizes the coatoms of $\mathcal{P}_0(c_3, a_{3,cl})$ as those projectors $P \subseteq C(2)^{\times 3}$ for which the complementary projectors P' are edges of the complete bi-partite graph $K_{4,4}$. Table 1 and Table 2 list the sixteen edges of $K_{4,4}$ in the matrix notation of Equation (24). By Theorem 3, the matrix $4P' - III$ is an extreme point of the spectrahedron $\mathcal{S}(\mathcal{U}(c_3, a_{3,cl}))$ for all sixteen coatoms P of $\mathcal{P}_0(c_3, a_{3,cl})$, because they are two-local Hamiltonians. All extreme points of the spectrahedron $\mathcal{S}(\mathcal{U}(c_3, a_{3,cl}))$ are obtained in this way.

Lemma 6 *Let $P \subseteq C(2)^{\times 3}$ be a subset. The projector P is a coatom of the lattice $\mathcal{P}_0^{\text{ff}}(c_3, a_{3,cl})$ if and only if P' is an edge of the graph $K_{4,4}$ which connects two vertices*

Table 1 Edges of $K_{4,4}$ that connect vertices differing in exactly one digit

$\{000, 001\} = \text{diag}(1, 1, 0, 0, 0, 0, 0, 0) = \frac{1}{4}(I + Z)I$
$\{010, 011\} = \text{diag}(0, 0, 1, 1, 0, 0, 0, 0) = \frac{1}{4}(I + Z)(I - Z)I$
$\{100, 101\} = \text{diag}(0, 0, 0, 0, 1, 1, 0, 0) = \frac{1}{4}(I - Z)I(I + Z)$
$\{110, 111\} = \text{diag}(0, 0, 0, 0, 0, 0, 1, 1) = \frac{1}{4}(I - Z)(I - Z)I$
$\{000, 010\} = \text{diag}(1, 0, 1, 0, 0, 0, 0, 0) = \frac{1}{4}(I + Z)I(I + Z)$
$\{001, 011\} = \text{diag}(0, 1, 0, 1, 0, 0, 0, 0) = \frac{1}{4}(I + Z)I(I - Z)$
$\{100, 110\} = \text{diag}(0, 0, 0, 0, 1, 0, 1, 0) = \frac{1}{4}(I - Z)I(I + Z)$
$\{101, 111\} = \text{diag}(0, 0, 0, 0, 0, 1, 0, 1) = \frac{1}{4}(I - Z)I(I - Z)$
$\{000, 100\} = \text{diag}(1, 0, 0, 0, 1, 0, 0, 0) = \frac{1}{4}I(I + Z)(I + Z)$
$\{001, 101\} = \text{diag}(0, 1, 0, 0, 0, 1, 0, 0) = \frac{1}{4}I(I + Z)(I - Z)$
$\{010, 110\} = \text{diag}(0, 0, 1, 0, 0, 0, 1, 0) = \frac{1}{4}I(I - Z)(I + Z)$
$\{011, 111\} = \text{diag}(0, 0, 0, 1, 0, 0, 0, 1) = \frac{1}{4}I(I - Z)(I - Z)$

Table 2 Edges of $K_{4,4}$ that connect vertices differing in all three digits

$\{000, 111\} = \text{diag}(1, 0, 0, 0, 0, 0, 0, 1) = \frac{1}{4}(III + IZZ + ZIZ + ZZI)$
$\{001, 110\} = \text{diag}(0, 1, 0, 0, 0, 0, 1, 0) = \frac{1}{4}(III - IZZ - ZIZ + ZZI)$
$\{010, 101\} = \text{diag}(0, 0, 1, 0, 0, 1, 0, 0) = \frac{1}{4}(III - IZZ + ZIZ - ZZI)$
$\{100, 011\} = \text{diag}(0, 0, 0, 1, 1, 0, 0, 0) = \frac{1}{4}(III + IZZ - ZIZ - ZZI)$

that differ in exactly one digit. The projector P lies in $\mathcal{P}_0^{\text{ff}}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{cl}})$ if and only if P' is a union of the described edges.

Proof Let $\mathcal{P}_0^{\text{ff}} = \mathcal{P}_0^{\text{ff}}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{cl}})$. By Equation (21), the set of coatoms of $\mathcal{P}_0^{\text{ff}}$ is

$$\bigcup_{i=1}^3 \{PI_{\{i\}} : P \text{ is a coatom of } \mathcal{P}(\mathcal{A}_{\Omega \setminus \{i\}})\}.$$

The complementary projector to the coatom $PI_{\{i\}}$ can be written as

$$(PI_{\{i\}})' = I_{\Omega} - PI_{\{i\}} = QI_{\{i\}},$$

where $Q = I_{\Omega \setminus \{i\}} - P$ is an atom of the lattice $\mathcal{P}(\mathcal{A}_{\Omega \setminus \{i\}})$. Since $\mathcal{A}_{\Omega \setminus \{i\}}$ is isomorphic to the two-bit algebra $\mathbb{C}^{C(2)} \otimes \mathbb{C}^{C(2)}$, the projector Q is a rank one projector, which we write as a two-digit binary number $Q = xy$ for some $x, y \in C(2)$. This shows that the two elements in the subset

$$(PI_{\{i\}})' = QI_{\{i\}} \subseteq C(2)^{\times 3}$$

differ exactly in the i -th digit. Conversely, $(I_{\Omega \setminus \{i\}} \setminus \{xy\})I_{\{i\}}$ is a coatom of $\mathcal{P}_0^{\text{ff}}$, again by Equation (21), for all $i \in \Omega$ and $x, y \in C(2)$. The second statement is true as the

infimum in $\mathcal{P}_0^{\text{ff}}$ is the intersection and since $\mathcal{P}_0^{\text{ff}}$ is coatomistic, see the discussion in Sect. 4.1. □

We turn to the interaction pattern \mathfrak{p}_3 with generating class $\{\{1, 2\}, \{2, 3\}\}$, the edge set of the path graph P_3 . The space $\mathcal{U}(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}})$ is the orthogonal complement of the span of $f = ZZZ$ and $g = ZIZ$ in $\mathcal{H}(\mathcal{A}_\Omega) = \mathbb{R}^{C^\Omega}$. We have

$$g(x_1x_2x_3) = (-1)^{x_1+x_3}, \quad x_1, x_2, x_3 \in \{0, 1\},$$

$$g = \text{diag}(+1, -1, +1, -1, -1, +1, -1, +1).$$

Lemma 7 *Let $P \subseteq C(2)^{\times 3}$ be a subset. The projector P is a coatom of the lattice $\mathcal{P}_0(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}})$ if and only if P' is an edge of the graph $K_{4,4}$ which connects two vertices that differ exactly in the first digit or exactly in the third. The projector P lies in $\mathcal{P}_0(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}})$ if and only if P' is a union of the described edges. Every nonzero element of $\mathcal{P}_0(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}})$ is the ground projector of a frustration-free \mathfrak{p}_3 -local three-bit Hamiltonian.*

Proof We abbreviate $\mathcal{U} = \mathcal{U}(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}})$ and $\mathcal{P}_0 = \mathcal{P}_0(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}})$. The lattice \mathcal{P}_0 has no elements of rank seven by Lemma 4.

If $P \in \mathcal{P}_0$ has rank at most five, then P is not a coatom. Indeed, since f and g are perpendicular to \mathcal{U} , Cor. 1 shows that both f and g are nonconstant on P' . As $|P'| \geq 3$, there are three mutually distinct points $x, y, z \in P'$, such that both f and g are nonconstant on $\{x, y, z\}$. First, let both f and g be nonconstant on a subset of size two of $\{x, y, z\}$. Then P is not a coatom of \mathcal{P}_0 by a similar reasoning as in Lemma 5 above. Otherwise, by multiplying f and g with ± 1 and permuting the labels of the points x, y, z , we can assume without loss of generality that

$$+1 = f(x) \neq f(y) = f(z) = -1,$$

$$+1 = g(x) = g(y) \neq g(z) = -1.$$

Second, if $P' = \{x, y, z\}$ then the cones $\mathcal{K}(P)$ and $\mathcal{K}(\{x, z\}')$, defined in Equation (11), are equal to the ray spanned by $\{x, z\}$. Thm. 1 then shows $P \notin \mathcal{P}_0$. Third, let $\eta \in P' \setminus \{x, y, z\}$. If $f(\eta) = f(a)$ and $g(\eta) = g(a)$ for a point $a \in \{x, y, z\}$, then $P \notin \mathcal{P}_0$ again by a similar reasoning as in Lemma 5. Finally, if $f(\eta) = +1$ and $g(\eta) = -1$ then the space $\mathcal{H}(P', \mathcal{A}_\Omega, P') \cap \mathcal{U}$ contains the linearly independent rank two projectors $\{x, z\}$ and $\{y, \eta\}$, hence P is not a coatom by Equation (15).

Let $P \subseteq C(2)^{\times 3}$. The preceding part of the proof shows that P is a coatom of \mathcal{P}_0 if and only if $P \in \mathcal{P}_0$ and $|P| = 6$. Let $P' = \{x, y\}$ for $x \neq y$. As cone $\mathcal{K}(p)$ is a ray if and only if $f(x) \neq f(y)$ and $g(x) \neq g(y)$, Thm. 2 confirms the assertion on coatoms.

The second assertion, regarding general elements of \mathcal{P}_0 , is true since the infimum in \mathcal{P}_0 is the intersection and because \mathcal{P}_0 is coatomistic (see the last paragraph of Sect. 3.4).

The third assertion follows from the fact that every coatom P of \mathcal{P}_0 is the ground projector of its complementary projector P' , and that P' is a frustration-free \mathfrak{p}_3 -local three-bit Hamiltonian, see the rows 1–4 or 9–12 of Table 1. □

Lemma 7, Lemma 6, and Lemma 5 describe the lattices of ground projectors

$$\mathcal{P}_0^{\text{ff}}(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}}) = \mathcal{P}_0(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}}) \subset \mathcal{P}_0^{\text{ff}}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{cl}}) \subset \mathcal{P}_0(\mathfrak{c}_3, \mathfrak{a}_{3,\text{cl}}).$$

The coatoms in each lattice are projectors of rank six, which are complements to certain edges of the graph $K_{4,4}$. The eight edges in Table 1, rows 1–4 and 9–12, belong to the coatoms in the lattices $\mathcal{P}_0^{\text{ff}}(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}}) = \mathcal{P}_0(\mathfrak{p}_3, \mathfrak{a}_{3,\text{cl}})$. All twelve edges in Table 1 pertain to the lattice of ground projectors of the frustration-free two-local Hamiltonians. The sixteen edges of Table 1 and Table 2 together belong to the lattice of ground projectors of all two-local Hamiltonians. All other lattice elements are intersections of coatoms in each of the lattices.

4.5 A family of coatoms of rank five

We present a family of coatoms of rank five in the lattice $\mathcal{P}_0(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}})$ of ground projectors of the space $\mathcal{U}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}})$ of two-local three-qubit Hamiltonians. This is in contrast with the lattice $\mathcal{P}_0(\mathfrak{c}_3, \mathfrak{a}_{3,\text{cl}})$ in the commutative setting, where Lemma 5 rules out the existence of coatoms of rank five. We found the family of coatoms with the help of the semidefinite programming strategy that samples extreme points from the dual spectrahedron proposed in Sect. 3.6. Whereas this is a two-parameter family, it covers a higher-dimensional family of extreme points in the spectrahedron of dimension up to eleven. In fact [12], the generic dimension of the orbit of a mixed (or pure) N -qubit state under local unitary transformations is $3N$ if $N \geq 2$. The question as to whether our family provides two nonlocal parameters can be rigorously studied using invariant theory, see [20, 35, 42] and the references therein.

4.5.1 The numerical procedure

Recall that we are trying to find extreme points of the spectrahedron $\mathcal{S}(\mathcal{U}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}}))$. By what was seen in Sect. 4.1, this spectrahedron is given by

$$\mathcal{S}(\mathcal{U}(\mathfrak{c}_3, \mathfrak{a}_{3,\text{qu}})) = \left\{ x \in \mathbb{R}^{36} : I_8 + \sum_{i=1}^{36} x_i A_i \geq 0 \right\},$$

where the A_i range over all the matrices of the form $B_1 B_2 B_3$ where $B_j \in \{I, X, Y, Z\}$, for $j = 1, 2, 3$, at least one of them is I , but not all three are I .

This is then a 36-dimensional object defined by an 8×8 positive semidefinite condition, an object that is quite amenable to semidefinite programming. Using MOSEK 9.2.10, we optimized in randomly generated directions in \mathbb{R}^{36} and recorded the ranks of the corresponding matrices. After 65000 we recorded the following rank distribution

Rank	2	3	4
Frequency	83.62%	9.57%	6.81%

Note that the ranks indicated are numerical, obtained by cutting off eigenvalues of sufficiently small magnitude, and do not provide exact certificates of the existence of

such extreme points. This, however, strongly suggests that in addition to the rank 6 coatoms in $\mathcal{U}(c_3, a_{3,cl})$, there exist rank 4 and 5 coatoms in $\mathcal{U}(c_3, a_{3,qu})$.

By carefully looking at the samples we were obtaining with rank 3, and after some ad hoc algebraic manipulations we were able to identify some of them that seem to come from the two-parameter family

$$\begin{aligned}
 M(a, t) &= \begin{pmatrix} a^2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 4 \cos(t)^2 & -\sqrt{\eta} \sin(2t) & 0 & 0 & 0 & 0 \\ 0 & 0 & -\sqrt{\eta} \sin(2t) & \eta \sin(t)^2 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4 \sin(t)^2 & \sqrt{\eta} \sin(2t) & 0 & 0 \\ 0 & 0 & 0 & 0 & \sqrt{\eta} \sin(2t) & \eta \cos(t)^2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \\
 &= III + \frac{a^2}{4} [IIZ + \sin(t)^2 IZI + \cos(t)^2 ZII] \\
 &\quad + \frac{\sqrt{\eta}}{2} \sin(2t) (IZ - ZI) X \\
 &\quad + \frac{a^2}{8} (IZ + ZI) Z - \frac{1}{8} (8 - a^2) \cos(2t) (IZ - ZI) Z - \frac{\eta}{4} ZZI,
 \end{aligned}$$

where $\eta = 4 - a^2$, $0 \leq a \leq 2$, and $t \in [0, \pi)$.

This suggests that the matrices in this family correspond to a family of extreme points of $\mathcal{S}(\mathcal{U}(c_3, a_{3,qu}))$ whose normal cones collectively have some non-negligible positive volume. The last task remaining is to, from this heuristically derived family, derive an exact certificate that it is indeed a family of extreme points. In what follows, we illustrate that procedure.

4.5.2 Algebraic certificates

We show that the ground projector $P = P_0(M(a, t))$ defined in the prior section is a coatom of the lattice $\mathcal{P}_0(c_3, a_{3,qu})$ except for special parameters.

By Equation (15) in Remark 2, it suffices to show that the intersection of the space $\mathcal{H}(P'.\mathcal{A}_\Omega.P')$ of hermitian matrices in the algebra $P'.\mathcal{A}_\Omega.P'$ with the space $\mathcal{U}(c_3, a_{3,qu})$ of two-local three-qubit Hamiltonians is the line spanned by $M(a, t)$. If P is a coatom, then we also learn from Theorem 3 that the hermitian matrix $M(a, t) - III$ is an extreme point of the spectrahedron $\mathcal{S}(\mathcal{U}(c_3, a_{3,qu}))$. Here, $P' = III - P$, and $\mathcal{A}_\Omega = \mathcal{A}_{\{1,2,3\}} = M_2^{\otimes 3}$ is the algebra associated with three qubits.

Let us recover the matrix $M(a, t)$ from P in the sense that $\mathcal{H}(P'.\mathcal{A}_\Omega.P') \cap \mathcal{U}(c_3, a_{3,qu})$ is the line spanned by $M(a, t)$, under the condition that $a \notin \{0, 2\}$ and $t \notin \{0, \frac{\pi}{2}\}$. The matrix $M(a, t)$ is positive semidefinite of rank three, and its kernel is spanned by the vectors

$$\begin{aligned}
 &|001\rangle, \quad |110\rangle, \quad |111\rangle, \\
 &|\psi_1\rangle = \sqrt{\eta} \sin(2t)|010\rangle + 4 \cos(t)^2|011\rangle, \\
 &|\psi_2\rangle = \sqrt{\eta} \sin(2t)|100\rangle - 4 \sin(t)^2|101\rangle.
 \end{aligned}$$

Let $A \in \mathcal{U}(c_3, a_{3,qu})$ be an arbitrary two-local Hamiltonian. We can write $A = \sum_{i=1}^{37} z_i A_i$ for some $z \in \mathbb{R}^{37}$, where the A_i range over all the matrices of the form $B_1 B_2 B_3$ where $B_j \in \{I, X, Y, Z\}$, for $j = 1, 2, 3$ and at least one of them is I . Assuming that A lies in the algebra $P' \cdot \mathcal{A}_\Omega \cdot P'$, we can set the real and imaginary parts of the vectors $A|001\rangle$, $A|110\rangle$, and $A|111\rangle$ to zero, as the vectors $|001\rangle$, $|110\rangle$, $|111\rangle$ lie in the kernel of every matrix from $P' \cdot \mathcal{A}_\Omega \cdot P'$. This allows us to get rid of 29 of the z_i 's with the help of Wolfram Mathematica 9. One eliminates by hand seven of the remaining eight parameters by requiring that the real and imaginary parts of the vectors $A|\psi_1\rangle$ and $A|\psi_2\rangle$ are zero. This is the only place where the variables a and t play a role, as far as $a \notin \{0, 2\}$ and $t \notin \{0, \frac{\pi}{2}\}$ guarantees that the seven variables can be eliminated.

Out of curiosity, we discuss the special parameter values. As the matrix $M(0, t)$ has rank two, Theorem 3 and Lemma 4 show that the point $M(0, t) - III$ is an extreme point of the spectrahedron $\mathcal{S}(\mathcal{U}(c_3, a_{3,qu}))$. The corresponding coatom of the lattice $\mathcal{P}_0(c_3, a_{3,qu})$ is the matrix $III - \frac{1}{4}M(0, t)$, as the positive eigenvalues of $M(0, t)$ are equal for all $t \in [0, \pi)$. The matrix $M(2, t)$ belongs to the commutative algebra $(\mathbb{C}^{C(2)})^{\otimes 3}$ and has rank three unless $t = 0$ or $t = \frac{\pi}{2}$, in which case it has rank two. By Lemma 5, the ground projector $P_0(M(2, t))$ is not a coatom of $\mathcal{U}(c_3, a_{3,cl})$ if $M(2, t)$ has rank three. It follows that the point $M(2, t) - III$ is an extreme point of the spectrahedron $\mathcal{S}(\mathcal{U}(c_3, a_{3,qu}))$ if and only if $t \in \{0, \frac{\pi}{2}\}$. The matrix $M(a, 0)$ belongs to the commutative algebra $(\mathbb{C}^{C(2)})^{\otimes 3}$ and has rank three unless $a = 0$ or $a = 2$, in which case it has rank two. It follows that $M(a, 0) - III$ is an extreme point of the spectrahedron $\mathcal{S}(\mathcal{U}(c_3, a_{3,qu}))$ if and only if $a \in \{0, 2\}$. The same happens at $t = \frac{\pi}{2}$, where the point $M(a, \frac{\pi}{2}) - III$ is an extreme point of the spectrahedron $\mathcal{S}(\mathcal{U}(c_3, a_{3,qu}))$ if and only if $a \in \{0, 2\}$.

4.6 Tomography and nonexposed faces

Karuvade et al. [25] discovered a six-qubit state that is uniquely determined by its two-body reduced density matrices, but which is not the unique ground state of any two-local Hamiltonian. We discuss the convex geometric consequences of this result. Related observations have been made earlier [15, 38].

A basic problem of quantum state tomography is to find conditions under which a state can be recovered from certain data, for example from its image under the projection $\pi_{\mathcal{U}}$ onto a space of hermitian matrices \mathcal{U} . We say a state $\rho \in \mathcal{D}(\mathcal{A})$ is *uniquely determined* by $\pi_{\mathcal{U}}$ if $\rho = \sigma$ whenever $\pi_{\mathcal{U}}(\rho) = \pi_{\mathcal{U}}(\sigma)$ for all states $\sigma \in \mathcal{D}(\mathcal{A})$. We say a subset of $\mathcal{D}(\mathcal{A})$ is *uniquely determined* by $\pi_{\mathcal{U}}$ if all its elements are.

Another problem of tomography is concerned with ground states. A state $\rho \in \mathcal{D}(\mathcal{A})$ is a *ground state* of a hermitian matrix $A \in \mathcal{H}(\mathcal{A})$ if ρ is supported by the ground projector $P_0(A)$, that is to say, if ρ lies in $\phi_{\mathcal{A}}(P_0(A))$, as defined in Equation (5). A state ρ is the *unique ground state* of A if we have $\{\rho\} = \phi_{\mathcal{A}}(P_0(A))$. In this case $\rho = P_0(A) / \text{Tr}(P_0(A))$ holds.

The above notions of tomography have counterparts in terms of faces of the joint numerical range $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$. A *face* of a convex set C in a Euclidean space is a convex

subset F of C such that whenever $(1 - \lambda)x + \lambda y$ lies in F for some $\lambda \in (0, 1)$ and $x, y \in C$, then x and y are also in F . It is well known that every exposed face of C is a face of C . A face that is not an exposed face is called a *nonexposed* face. If $x \in C$ and $\{x\}$ is a face or nonexposed face, then x is called an *extreme point* or *nonexposed point*, respectively.

A subset F of $\mathcal{D}(\mathcal{A})$ is *lift-invariant* under $\pi_{\mathcal{U}}$ if $F = \pi_{\mathcal{U}}|_{\mathcal{D}(\mathcal{A})}^{-1}(\pi_{\mathcal{U}}(F))$. Note that every subset of $\mathcal{D}(\mathcal{A})$ which is uniquely determined by $\pi_{\mathcal{U}}$ is lift-invariant under $\pi_{\mathcal{U}}$.

Lemma 8 *A subset $F \subseteq \mathcal{D}(\mathcal{A})$ is the preimage $\pi_{\mathcal{U}}|_{\mathcal{D}(\mathcal{A})}^{-1}(G)$ of a face G of $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$ if and only if F is a face of $\mathcal{D}(\mathcal{A})$ which is lift-invariant under $\pi_{\mathcal{U}}$. If F is a face of $\mathcal{D}(\mathcal{A})$ lift-invariant under $\pi_{\mathcal{U}}$, then $\pi_{\mathcal{U}}(F)$ is an exposed face of $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$ if and only if $F = \phi_{\mathcal{A}}(P_0(A))$ holds for some $A \in \mathcal{U}$.*

Proof The first statement is proved in Prop. 5.7 in [46] for faces F . This and the fact that preimages of faces are faces prove the statement for general subsets F . The second statement follows from Equation (8). □

We remark that the inverse isomorphism $\phi_{\mathcal{A}}^{-1}$, introduced in Equation (5), can be applied to the preimage $F = \pi_{\mathcal{U}}|_{\mathcal{D}(\mathcal{A})}^{-1}(G)$ of every face G of $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$, not only to the exposed faces. In the context of \mathfrak{g} -local Hamiltonians (17), the image $P(\mathbb{C}^d) \subseteq \mathbb{C}^d$ of the projector $P = \phi_{\mathcal{A}}^{-1}(F)$ associated with F has been called a *\mathfrak{g} -correlated space* [15].

Corollary 3 *For any state $\rho \in \mathcal{D}(\mathcal{A})$, the singleton $\{\rho\}$ is the preimage of an extreme point of $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$ if and only if ρ is a pure state of \mathcal{A} which is uniquely determined by $\pi_{\mathcal{U}}$. If ρ is a pure state of \mathcal{A} uniquely determined by $\pi_{\mathcal{U}}$, then $\pi_{\mathcal{U}}(\rho)$ is an exposed point of $\pi_{\mathcal{U}}(\mathcal{D}(\mathcal{A}))$ if and only if ρ is the unique ground state of a matrix $A \in \mathcal{U}$.*

Proof The claim follows from Lemma 8 as every lift-invariant singleton is uniquely determined by $\pi_{\mathcal{U}}$. □

It was an open problem [14, 15] whether the set of reduced density matrices can have nonexposed faces. Here, we discuss prior work [15, 25] regarding two-body reduced density matrices of N qubits. Using the notation of the Sects. 4.1 and 4.3, we employ the algebra $\mathcal{A}_i = M_2$ for each unit $i \in \Omega = \{1, 2, \dots, N\}$. We denote the linear map (16), which maps a density matrix to its reduced density matrices, by

$$\text{red}_N = \text{red}_{\left(\binom{N}{2}, \alpha_{N,\text{qu}}\right)}$$

and the space of two-local N -qubit Hamiltonians (17) by

$$\mathcal{U}_N = \mathcal{U}\left(\binom{N}{2}, \alpha_{N,\text{qu}}\right).$$

Equation (19) shows that the map red_N factors through \mathcal{U}_N and that

$$\pi_{\mathcal{U}_N}(\mathcal{D}(\mathcal{A}_{\Omega})) \xrightarrow{\text{red}_N} \text{red}_N(\mathcal{D}(\mathcal{A}_{\Omega})) \tag{25}$$

is a bijection from the joint numerical range onto the set of two-body reduced density matrices of N qubits. The set $\text{red}_6(\mathcal{D}(\mathcal{A}_{\Omega}))$ has a nonexposed point.

Remark 5 (Six Qubits) Using dissipative quantum control theory, Karuvade et al. [25, Section IV.B] discovered a pure six-qubit state $\rho \in \mathcal{D}(\mathcal{A}_\Omega)$ that is uniquely determined by its two-body reduced density matrices, but which is not the unique ground state of any matrix in \mathcal{U}_6 , the space of two-local six-qubit Hamiltonians. Equation (25) shows that ρ is uniquely determined by the projection $\pi_{\mathcal{U}_6}$. Hence the point $\pi_{\mathcal{U}_6}(\rho)$ is a nonexposed point of the joint numerical range $\pi_{\mathcal{U}_6}(\mathcal{D}(\mathcal{A}_\Omega))$ by Corollary 3, and the point $\text{red}_6(\rho)$ is a nonexposed point of the set $\text{red}_6(\mathcal{D}(\mathcal{A}_\Omega))$ of two-body reduced density matrices of six qubits, again by Equation (25).

Lemma 9 (Three Qubits) *The set $\text{red}_3(\mathcal{D}(\mathcal{A}_\Omega))$ of two-body reduced density matrices of three qubits has no nonexposed points.*

Proof Let x be an extreme point of the convex set $\text{red}_3(\mathcal{D}(\mathcal{A}_\Omega))$. Then $x = \text{red}_3(\rho)$ is the image of an extreme point (pure state) ρ of the state space $\mathcal{D}(\mathcal{A})$. First, let ρ be of the GHZ type [9]

$$|\text{GHZ}\rangle = \alpha|000\rangle + \beta|111\rangle$$

for some $\alpha, \beta \in \mathbb{C}$ satisfying $|\alpha|^2 + |\beta|^2 = 1$. That is to say,

$$\rho = U_1 U_2 U_3 \cdot |\text{GHZ}\rangle\langle\text{GHZ}| \cdot U_1^* U_2^* U_3^*$$

for some unitaries $U_1, U_2, U_3 \in U(2)$. Applying a unitary similarity, we can take $U_i = I, i = 1, 2, 3$, without loss of generality. Then the two-body reduced density matrices are $\text{red}_3(\rho) = y(|\beta|^2)$, where

$$y(\lambda) = (\sigma, \sigma, \sigma) \quad \text{and} \quad \sigma = (1 - \lambda)|00\rangle\langle 00| + \lambda|11\rangle\langle 11|, \quad 0 \leq \lambda \leq 1.$$

Since the segment $\{y(\lambda) \mid 0 \leq \lambda \leq 1\}$ lies in $\text{red}_3(\mathcal{D}(\mathcal{A}_\Omega))$ and since the point $x = y(|\beta|^2)$ is an extreme point, we have $\sigma = |ii\rangle\langle ii|$ and $\rho = |iii\rangle\langle iii|$ either for $i = 0$ or $i = 1$. This shows that ρ is the unique ground state of the two-local Hamiltonian

$$(I_{\{1,2\}} - \sigma)I_{\{3\}} + I_{\{1\}}(I_{\{2,3\}} - \sigma).$$

Second, if the pure state ρ is not of the GHZ type, then ρ is the unique ground state of a two-local Hamiltonian, too [15, Section V.A].

In both cases, the state ρ is the unique ground state of a two-local Hamiltonian. Equation (9) then shows that $\pi_{\mathcal{U}_3}(\rho)$ is an exposed point of the joint numerical range $\pi_{\mathcal{U}_3}(\mathcal{D}(\mathcal{A}_\Omega))$. Equation (25) proves that $\text{red}_3(\rho)$ is an exposed point of the set of reduced density matrices $\text{red}_3(\mathcal{D}(\mathcal{A}_\Omega))$. □

Remark 5 and Lemma 9 prompt the question of whether the convex sets $\text{red}_4(\mathcal{D}(\mathcal{A}_\Omega))$ and $\text{red}_5(\mathcal{D}(\mathcal{A}_\Omega))$ have nonexposed points. It would also be interesting to establish whether the convex set $\text{red}_3(\mathcal{D}(\mathcal{A}_\Omega))$ has nonexposed faces of higher dimensions 1, 2, . . . , 34.

Acknowledgements We thank Tomasz Maciążek and Adam Sawicki for bringing the papers [31, 53] and [40], respectively, to our attention. We thank the anonymous referees for their valuable feedback.

Data Availability There is no data associated with this paper.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

References

1. Acín, A., Andrianov, A., Jané, E., Tarrach, R.: Three-qubit pure-state canonical forms. *J. Phys. A* **34**(35), 6725–6739 (2001)
2. Alfsen, E.M., Shultz, F.W.: *State Spaces of Operator Algebras: Basic Theory, Orientations, and C*-Products*. Birkhäuser, Boston (2001)
3. Amari, S.-I.: Information geometry on hierarchy of probability distributions. *IEEE Trans. Inf. Theory* **47**(5), 1701–1711 (2001)
4. Amari, S., Nagaoka, H.: *Methods of Information Geometry*. AMS, Providence (2000)
5. Altunbulak, M., Klyachko, A.: The Pauli principle revisited. *Commun. Math. Phys.* **282**(2), 287–322 (2008)
6. Aubrun, G., Szarek, S.J.: *Alice and Bob Meet Banach: The Interface of Asymptotic Geometric Analysis and Quantum Information Theory*. AMS, Providence (2017)
7. Ay, N., Jost, J., Lê, H.V., Schwachhöfer, L.: *Information Geometry*. Springer, New York (2017)
8. Barndorff-Nielsen, O.: *Information and Exponential Families*. John Wiley and Sons, Chichester (2014)
9. Bengtsson, I., Życzkowski, K.: *Geometry of Quantum States: An Introduction to Quantum Entanglement*, 2nd edn. Cambridge University Press, Cambridge (2017)
10. Birkhoff, G.: *Lattice Theory*, 3rd edn. AMS, Providence (1973)
11. Bonsall, F.F., Duncan, J.: *Numerical Ranges of Operators on Normed Spaces and of Elements of Normed Algebras*. Cambridge University Press, London (1971)
12. Carteret, H.A., Linden, N., Popescu, S., Sudbery, A.: Multiparticle entanglement. *Found. Phys.* **29**(4), 527–552 (1999)
13. Chen, J., Dawkins, H., Ji, Z., Johnston, N., Kribs, D., Shultz, F., Zeng, B.: Uniqueness of quantum states compatible with given measurement results. *Phys. Rev. A* **88**(1), 012109 (2013)
14. Chen, J., Ji, Z., Ruskai, M.B., Zeng, B., Zhou, D.-L.: Comment on some results of Erdahl and the convex structure of reduced density matrices. *J. Math. Phys.* **53**(7), 072203 (2012)
15. Chen, J., Ji, Z., Zeng, B., Zhou, D.L.: From ground states to local Hamiltonians. *Phys. Rev. A* **86**(2), 022339 (2012)
16. Csiszár, I., Matúš, F.: Information projections revisited. *IEEE Trans. Inf. Theory* **49**(6), 1474–1490 (2003)
17. Di Giorgio, S., Mateus, P.: On the complexity of finding the maximum entropy compatible quantum state. *Mathematics* **9**(2), 193 (2021)
18. Erdahl, R.M.: The convex structure of the set of N-representable reduced 2-matrices. *J. Math. Phys.* **13**(10), 1608–1621 (1972)
19. Geiger, D., Meek, C., Sturmfels, B.: On the toric algebra of graphical models. *Ann. Stat.* **34**(3), 1463–1492 (2006)
20. Grassl, M., Rötteler, M., Beth, T.: Computing local invariants of quantum-bit systems. *Phys. Rev. A* **58**(3), 1833–1839 (1998)
21. Ingarden, R.S.: Quantum information theory. *Rep. Math. Phys.* **10**(1), 43–72 (1976)
22. Ji, Z., Wei, Z., Zeng, B.: Complete characterization of the ground-space structure of two-body frustration-free Hamiltonians for qubits. *Phys. Rev. A* **84**(4), 042338 (2011)
23. Kahle, T.: *On Boundaries of Statistical Models*, PhD thesis, Universität Leipzig (2010)
24. Kakiyama, S., Ohara, A., Tsuchiya, T.: Information geometry and interior-point algorithms in semidefinite programs and symmetric cone programs. *J. Optim. Theory Appl.* **157**(3), 749–780 (2013)

25. Karuvade, S., Johnson, P.D., Ticozzi, F., Viola, L.: Uniquely determined pure quantum states need not be unique ground states of quasi-local Hamiltonians. *Phys. Rev. A* **99**(6), 062104 (2019)
26. Kitaev, A., Shen, A., Vyalii, M.: *Classical and Quantum Computation*. AMS, Providence (2002)
27. Lauritzen, S.L.: *Graphical Models*. Clarendon Press, Oxford (1996)
28. Linden, N., Popescu, S., Wootters, W.: Almost every pure state of three qubits is completely determined by its two-particle reduced density matrices. *Phys. Rev. Lett.* **89**(20), 207901 (2002)
29. Liu, Y.-K.: Consistency of local density matrices is QMA-complete. In: Díaz, J., et al. (eds.) *Approximation, Randomization, and Combinatorial Optimization*. Lecture Notes in Computer Science, vol. 4110, pp. 438–449. Springer, Berlin (2006)
30. Liu, Y.-K., Christandl, M., Verstraete, F.: Quantum computational complexity of the N-representability problem: QMA complete. *Phys. Rev. Lett.* **98**(11), 110503 (2007)
31. Maciazek, T., Tsanov, V.: Quantum marginals from pure doubly excited states. *J. Phys. A* **50**(46), 465304 (2017)
32. Movassagh, R., Farhi, E., Goldstone, J., Nagaj, D., Osborne, T.J., Shor, P.W.: Unfrustrated qudit chains and their ground states. *Phys. Rev. A* **82**(1), 012318 (2010)
33. Nesterov, Y., Nemirovskij, A.: *Interior-Point Polynomial Algorithms in Convex Programming*, 3rd printing. SIAM, Philadelphia (2001)
34. Niekamp, S., Galla, T., Kleinmann, M., Gühne, O.: Computing complexity measures for quantum states based on exponential families. *J. Phys.* **46**(12), 125301 (2013)
35. Rains, E.M.: Polynomial invariants of quantum codes. *IEEE Trans. Inform. Theory* **46**(1), 54–59 (2000)
36. Ramana, M., Goldman, A.J.: Some geometric results in semidefinite programming. *J. Global Optim.* **7**(1), 33–50 (1995)
37. Rockafellar, R.T.: *Convex Analysis*. Princeton University Press, Princeton (1970)
38. Rosina, M.: Some theorems on uniqueness and reconstruction of higher-order density matrices. In: Cioslowski, J. (ed.) *Many-Electron Densities and Reduced Density Matrices*, pp. 19–32. Springer, Boston (2000)
39. Schilling, C., Gross, D., Christandl, M.: Pinning of Fermionic occupation numbers. *Phys. Rev. Lett.* **110**(4), 040404 (2013)
40. Schilling, C., Benavides-Riveros, C.L., Lopes, A., Maciazek, T., Sawicki, A.: Implications of pinned occupation numbers for natural orbital expansions: I. Generalizing the concept of active spaces. *New J. Phys.* **22**, 023001 (2020)
41. Schneider, R.: *Convex Bodies: The Brunn-Minkowski Theory, Second Expanded*. Cambridge University Press, New York (2014)
42. Sun, B.-Z., Fei, S.-M., Wang, Z.-X.: On local unitary equivalence of two and three-qubit states. *Sci. Rep.* **7**(1), 4869 (2017)
43. Wang, N., Rauh, J., Massam, H.: Approximating faces of marginal polytopes in discrete hierarchical models. *Ann. Statist.* **47**(3), 1203–1233 (2019)
44. Wei, T.-C., Mosca, M., Nayak, A.: Interacting boson problems can be QMA hard. *Phys. Rev. Lett.* **104**(4), 040501 (2010)
45. Weis, S.: Quantum convex support. *Linear Algebra Appl.* **435**(12), 3168–3188 (2011)
46. Weis, S.: A note on touching cones and faces. *J. Convex Anal.* **19**(2), 323–353 (2012)
47. Weis, S., Knauf, A.: Entropy distance: new quantum phenomena. *J. Math. Phys.* **53**(10), 102206 (2012)
48. Weis, S.: Information topologies on non-commutative state spaces. *J. Convex Anal.* **21**(2), 339–399 (2014)
49. Weis, S., Knauf, A., Ay, N., Zhao, M.-J.: Maximizing the divergence from a hierarchical model of quantum states. *Open Syst. Inf. Dyn.* **22**(1), 1550006 (2015)
50. Weis, S.: Operator systems and convex sets with many normal cones. *J. Convex Anal.* **25**(1), 41–64 (2018)
51. Weis, S.: A variational principle for ground spaces. *Rep. Math. Phys.* **82**(3), 317–336 (2018)
52. Werner, R.F.: An application of Bell’s inequalities to a quantum state extension problem. *Lett. Math. Phys.* **17**(4), 359–363 (1989)
53. Yu, X.-D., Simnacher, T., Wyderka, N., Nguyen, H.C., Gühne, O.: A complete hierarchy for the pure state marginal problem in quantum mechanics. *Nat. Commun.* **12**, 1012 (2021)
54. Zeng, B., Chen, X., Zhou, D.-L., Wen, X.-G.: *Quantum Information Meets Quantum Matter*. Springer, New York (2019)
55. Zhou, D.-L.: Efficient numerical algorithm on irreducible multiparty correlations. *Commun. Theor. Phys.* **61**(2), 187–190 (2014)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.