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by

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CONTINUITY OF THE MAXIMUM-ENTROPY INFERENCE: CONVEX GEOMETRY AND NUMERICAL RANGES APPROACH

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Abstract. We study the continuity of an abstract generalization of the maximum-entropy inference — a maximizer. It is defined as a right-inverse of a linear map restricted to a convex body which uniquely maximizes on each fiber of the linear map a continuous function on the convex body. Using convex geometry we prove, amongst others, the existence of discontinuities of the maximizer at limits of extremal points not being extremal points themselves and apply the result to quantum correlations. Further, we use numerical range methods in the case of quantum inference which refers to two observables. One result is a complete characterization of points of discontinuity for 3×3 matrices.

Key Words: Maximum-entropy inference, quantum inference, continuity, convex body, irreducible many-party correlation, quantum correlation, numerical range.

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1. Introduction

The maximum-entropy principle is a topic in physics since the 19^{th} century in the work of Boltzmann, Gibbs, von Neumann, Jaynes and many others [40, 23]. The continuity issue of the maximum-entropy inference under linear constraints in the quantum context was studied by one of the authors in [48] (jointly with A. Knauf), and then further in [44]–[46]. Discontinuity points of the maximum-entropy inference are a distinguished quantum phenomenon because they are missing in the analogous maximum-entropy inference of probability distributions which is formally included in the quantum setting by viewing probability vectors as diagonal matrices. The discontinuity points were recently discussed by Chen et al. [13] in condensed matter physics.

Convex geometry has proved powerful for the problem of discontinuity in our preceding contribution [45]. The crucial difference with the simplex of probability distributions is that a quantum state space, consisting of density matrices, has curved and flat boundary portions. Already its planar linear images have a very rich geometry. They correspond to the notion of *numerical range* in operator theory whose shapes are well understood for 2×2 (the classical elliptical range theorem) and 3×3 matrices, see the work of Kippenhahn [24] and earlier papers by the first two authors [26] (jointly with D. Keeler) and [36].

Let us briefly return to the condensed matter note which is a substantial motivation for this work. Definitions of a phase transition in statistical mechanics include symmetry breaking, such as melting crystals, and long-range correlations which may be certified by a power law correlation function, see for example Yeomans [51]. Quantum phase transitions are not necessarily associated with symmetry breaking or long-range correlations, for example see the discussion by Wen [49], Sec. 1.4. Still, correlations explain quantum phase transitions in some cases: Liu et al. [31] have recognized that a quantum phase transition in Kitaev's toric code model can be seen in the six-body correlations of the ground states of a 3×4 torus model. We demonstrate by an example that our methods are suitable to obtain analytical results about the correlation quantities used by Liu et al. which are known as *irreducible many-party correlations* and which were defined by Linden et al. and Zhou [30, 52] based on the maximum-entropy principle.

The aim of this article is to contribute to the continuity theory of the maximum-entropy inference and of the irreducible correlation using techniques from convex geometry and operator theory (numerical range). Convex geometrical methods will be developed in reference to a maximizer H which is defined as a right-inverse of a linear map f restricted to a convex body K which uniquely maximizes on each fiber of $f|_K$ a continuous function on K. We have in mind the example where H is an abstract generalization of the maximum-entropy inference (defined in Sec. 2) and the continuous function is a generalization of the von Neumann entropy.

Our analysis will be based on our continuity result [45] which we recall in Sec. 2 and which allows us to study the continuity of the maximizer without solving the respective inverse problem explicitly. This is possible by studying the *openness* of the restricted linear map $f|_K$. Continuity results follow as corollaries of openness results.

The results presented in Sec. 3 have appeared earlier in the paper [45] by the fourth author and are based on gauge functions of the domain $L := f(K)$ of the maximizer. Here we provide a new unified proof in terms of the notion of *simplicial point* which is a point-wise defined variant of a locally simplicial set in the sense of Rockafellar [35]. We prove that the maximizer is continuous at all simplicial points — in particular it is continuous in the restriction to a polytope or to a relatively open convex subset.

Further, we present two new results inspired by examples by Chen et al. [13]. In Sec. 4 we prove a *dichotomy* with regard to the partition of the domain L of the maximizer H: the continuity of H is equivalent to the continuity of its restriction to the relative boundary of L and can be decided in terms of its restriction to the relative interior of L.

In Sec. 5 we prove a necessary condition for the continuity of H in terms of the *face function* studied by Klee and Martin [25] and others. The face function maps every point of L to the unique face of L which contains the given point in its relative interior. For example, we prove under mild assumptions (which are satisfied by the maximum-entropy inference) that the maximizer is discontinuous at points $w \in L$ which are limit points of extremal points of L but not extremal points themselves. In that case we remark in Exa. 5.2 that the discontinuity at w is not removable from the restriction of H to the relative boundary of L by changing only the value at w. Discontinuities of the (unrestricted) maximizer H are never removable as we will point out in Sec. 4.

In the three last sections we specialize to the convex body K equal to a quantum state space. The aim of Sec. 6 is to demonstrate that convex geometry is an essential part of the topology of quantum correlations. We use the face function method to point out discontinuities in the *irreducible three-party correlation* of three qubits which is possible because this correlation quantity is based on the maximum-entropy principle. We check our analysis by consulting a result in the context of pure state reconstruction by Linden et al. [30].

In Secs. 7 and 8 we consider two hermitian $d \times d$ matrices, $d \in \mathbb{N}$, having the meaning of quantum observables. Then the domain L of the maximizer is planar and can be identified with the *numerical range* of a complex $d \times d$ matrix A, that is $W(A) := \{x^* A x \mid x \in \mathbb{C}S^d\}$ where $\mathbb{C}S^d$ denotes the unit-sphere in $\mathbb{C}^d$. We determine the maximum number of discontinuities in dimension $d = 4, 5$ (new methods are needed for $d \geq 6$). Further, in Sec. 8 we give a complete characterization of points of discontinuity of the maximum-entropy inference for $d = 3$. These results essentially are corollaries of the Theorem 7.3 which connects to the paper [28] by T. Leake, B. Lins and the second author, devoted to the numerical range. One of the proof ideas is that the notion of simplicial point, mentioned above, is a complement of the notion of *round boundary point* in the second author's papers [15] (jointly with D. Corey, C.R. Johnson, R. Kirk and B. Lins) and [27, 28] (jointly with T. Leake and B. Lins) on the numerical range. The second idea is concerned with *singularly generated* points which were defined in [28] as having exactly one linearly independent unit vector in the pre-image under the map $\mathbb{C}S^d \to \mathbb{C}$, $x \mapsto x^* A x$.

It is worth mentioning that similar pre-image problems of the numerical range are of a broader interest, see for example Carden [9]. In particular, pre-image problems for more than two observables appear in quantum state reconstruction, see for example Gross et al., Heinosaari et al. and Chen et al. [17, 19, 12], and in quantum chemistry, see for example Erdahl, Ocko et al. and Chen et al. [16, 33, 11].

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2. Preliminaries

In this section we introduce the central objects and concepts of this article including the notions of state space and maximum-entropy inference in quantum mechanics, starting with their abstract counterparts of convex body and maximizer, as well as the joint numerical range and the topological notion of open map.

Definition 2.1 (Maximizer)**.** Let X, Y be finite-dimensional real normed vector spaces, let $f : X \to Y$ be a continuous map and let $K \subset X$ be compact. The compact set $L := f(K) \subset Y$ parametrizes the fibers

$$f|_K^{-1}(w) = \{v \in K \mid f(v) = w\}, \qquad w \in L,$$

of $f|_K$. We assume the inverse problem of selecting a point in each fiber is solved by maximizing a continuous function $g : K \to \mathbb{R}$ which attains a unique maximum on each fiber. The *maximizer* is defined by

$$H : L \to K, \qquad w \mapsto \operatorname{argmax}\{g(v) \mid v \in f|_K^{-1}(w)\}.$$

All sets which will be introduced in the sequel are tacitly assumed to be subsets of a finite-dimensional real normed vector space. Unless otherwise stated we will always assume that f is linear and that K is a *convex body*, that is a compact and convex set.

We remark that the domain of f is X rather than K by consistency with our main example (2.1). Since K is compact, this choice is no restriction because, by the Tietze extension theorem, any continuous function $K \to Y$ can be extended to a continuous function $X \to Y$.

On $K \subset X$ and $L = f(K) \subset Y$ we use the subspace topology induced by X and of Y, respectively. A *neighborhood* of a point x in a topological space $\widetilde{X}$ is any subset of $\widetilde{X}$ containing an open set containing x. We call a map $\gamma : \widetilde{X} \to \widetilde{Y}$ between topological spaces $\widetilde{X}, \widetilde{Y}$ *open* at $x \in \widetilde{X}$ if for any neighborhood $N \subset \widetilde{X}$ of x the image $\gamma(N)$ is a neighborhood of $\gamma(x)$ in $\widetilde{Y}$. We say γ is *open on* a given subset of $\widetilde{X}$ if γ is open at each point in the subset. Finally, γ is *open* if γ is open on $\widetilde{X}$.

In Thm. 4.9 in [45] one of the authors has proved the following.

Fact 2.2 (Continuity-openness equivalence)**.** Let $K \subset X$ be an arbitrary compact subset, not necessarily convex, and let $f : X \to Y$ be an arbitrary continuous function, not necessarily linear. Then for any $w \in L$ the maximizer H is continuous at w if and only if $f|_K$ is open at $H(w)$.

From now on we make the global assumption that K is a convex body and that f is linear. We will argue in terms of the openness of $f|_K$. All results may, and some will, be translated into continuity statements of H using Fact 2.2.

Our main example of convex body K will be the state space of a matrix algebra which is studied in operator theory [1]. Let M_d, $d \in \mathbb{N}$, denote the full matrix algebra of $d \times d$-matrices with complex coefficients. The algebra M_d is a complex C*-algebra with identity $\mathbb{1}_d$. We shall also write $0 = 0_d$ for the zero in M_d. Let $\mathcal{A}$ denote a (complex) C*-subalgebra of M_d. For example, we will introduce in Fact 5.1 the C*-algebras $pM_dp = \{pap \mid a \in M_d\}$ where $p \in M_d$ is a projection, that is a hermitian idempotent $p = p^* = p^2$. See Lemma 9.1 for other relevant examples of C*-algebras.

We denote by $\mathcal{A}^{\mathrm{h}} = \{a \in \mathcal{A} \mid a^* = a\}$ the real vector space of hermitian matrices in $\mathcal{A}$, known as *observables* in physics, and we endow it with the scalar product $\langle a, b\rangle := \mathrm{tr}(ab)$, $a, b \in \mathcal{A}^{\mathrm{h}}$ which makes $\mathcal{A}^{\mathrm{h}}$ a Euclidean space. We call *state space* of $\mathcal{A}$ the convex body

$$\mathcal{M}(\mathcal{A}) := \{\rho \in \mathcal{A} \mid \rho \succeq 0, \mathrm{tr}(\rho) = 1\}.$$

Here $a \succeq 0$ means the matrix $a \in \mathcal{A}$ is positive semi-definite, that is $a^* = a$ and all eigenvalues of a are non-negative. Elements of $\mathcal{M}(\mathcal{A})$ are called *density matrices* in physics [1, 5, 32]. They are in one-to-one correspondence to the positive normalized linear functionals $\mathcal{A} \to \mathbb{C}$

called *states*, see for example [1], Sec. 4. We use the terms state and density matrix synonymously.

Now we confine definitions to the full matrix algebra M_d and we write $\mathcal{M}_d := \mathcal{M}(M_d)$. Given a number $r \in \mathbb{N}$ of fixed observables $u_i \in M_d^{\rm h}$, $i = 1, \ldots, r$, we write $\mathbf{u} = (u_1, \ldots, u_r)$ and we define the *expected value function*

$$\mathbb{E} = \mathbb{E}_{\mathbf{u}} : M_d^{\rm h} \to \mathbb{R}^r, \qquad a \mapsto (\langle u_1, a\rangle, \ldots, \langle u_r, a\rangle). \tag{2.1}$$

In our earlier papers [42, 45] we have called the set of expected values

$$L(\mathbf{u}) = L(u_1, \ldots, u_r) := \{\mathbb{E}_{\mathbf{u}}(\rho) \mid \rho \in \mathcal{M}_d\} \subset \mathbb{R}^r$$

the *convex support*. This name is motivated by probability theory [3]. The probability vectors of length d, embedded as diagonal matrices into M_d, are the states of the algebra of diagonal matrices. Random variables on $\{1, \ldots, d\}$ correspond to diagonal matrices $u_1, \ldots, u_r$ and the set of their expected value tuples, called convex support in [3], equals $L(\mathbf{u})$ by Lemma 9.1.

Given expected values $\alpha \in L(\mathbf{u})$ the maximum-entropy state $\rho^*(\alpha)$ is the unique state in the fiber $\mathbb{E}|_{\mathcal{M}_d}^{-1}(\alpha)$ which maximizes on $\mathbb{E}|_{\mathcal{M}_d}^{-1}(\alpha)$ the *von Neumann entropy*

$$S(\rho) = -\mathrm{tr}(\rho \cdot \ln \rho).$$

Functional calculus with respect to the continuous function $[0, 1] \to \mathbb{R}$, $x \mapsto x \cdot \ln(x)$ where $0 \cdot \ln 0 = 0$ can be used to define S. The mapping

$$\rho^* : L(\mathbf{u}) \to \mathcal{M}_d, \qquad \alpha \mapsto \rho^*(\alpha) \tag{2.2}$$

is called the *maximum-entropy inference*, see [23, 50, 22] for more details. In physics, the von Neumann entropy quantifies the uncertainty in a state [41]. The state $\rho^*(\alpha)$ is considered the most non-committal, most unbiased or least informative state with regard to all missing information beyond the expected values α [23].

Although ρ^* can be discontinuous it is smooth up to boundary points. We denote by $\overline{C}$ the norm closure of any set C. The *relative interior* $\mathrm{ri}(C)$ of C is the interior of C in the topology of the affine hull of C, and C is *relatively open* if $C = \mathrm{ri}(C)$ holds. The *relative boundary* of C is $\mathrm{rb}(C) := \overline{C} \setminus \mathrm{ri}(C)$. The following statement is proved in [50], Thm. 2b.

Fact 2.3 (Real analyticity)**.** The maximum-entropy inference $\rho^*(\alpha)$ is real analytic in the relative interior of $L(\mathbf{u})$.

Now we turn to the joint numerical range which will be useful to address the continuity of ρ^* for two ($r = 2$) observables. It will be convenient to denote the inner product of $x, y \in \mathbb{C}^d$ by $x^*y := \overline{x_1}y_1 +$

$\cdots + \overline{x_d} y_d$ and to denote by $xy^* : \mathbb{C}^d \to \mathbb{C}^d$ the linear map defined for $z \in \mathbb{C}^d$ by $(xy^*)(z) := (y^* z)x$. Vectors in $\mathbb{C}^n$, $n \in \mathbb{N}$, will be understood as column vectors. To save space we will write them equivalently in the column and row forms

$$\begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = (x_1, \ldots, x_n), \qquad x_1, \ldots, x_n \in \mathbb{C}.$$

Definition 2.4. The *joint numerical range* of $\mathbf{u} = (u_1, \ldots, u_r)$ is the subset of $\mathbb{R}^r$ defined by

$$W(\mathbf{u}) = W(u_1, \ldots, u_r) := \{(x^* u_1 x, \ldots, x^* u_r x) \mid x \in \mathbb{C}^d, x^* x = 1\}.$$

Let us recall that the convex hull of the joint numerical range is the convex support. We denote the convex hull of any set C by $\mathrm{conv}(C)$. For all $d, r \in \mathbb{N}$ we have

$$\mathrm{conv}(W(\mathbf{u})) = L(\mathbf{u}). \tag{2.3}$$

See [18], Thm. 1, for the identity (2.3) formulated as an affine isomorphism. For two observables ($r = 2$), if we identify $\mathbb{R}^2 \cong \mathbb{C}$, then the joint numerical range $W(u_1, u_2)$ equals the numerical range $W(u_1 + iu_2)$ which is convex by the *Toeplitz-Hausdorff theorem*. Hence (2.3) implies

$$L(u_1, u_2) = W(u_1, u_2). \tag{2.4}$$

A proof of (2.4) can be found in [6], Thm. 3. For three observables ($r = 3$) the joint numerical range $W(u_1, u_2, u_3)$ is also convex but only for matrix size $d \geq 3$, see [2, 29].

Let us discuss easy properties and example of the convex support.

Remark 2.5. The following transformations do not essentially alter $L(\mathbf{u})$, $W(\mathbf{u})$, and $\rho^*(\alpha)$.

(1) Remove any u_i which is a (real) linear combination of $u_1, \ldots, u_{i-1}, u_{i+1}, \ldots, u_r$. Conversely, add observables which are linear combinations of $u_1, \ldots, u_r$.

(2) Replace u_i with $u_i + c_i \mathbb{1}$, where $c_i \in \mathbb{R}$, for any i.

(3) Replace u_i with $T^* u_i T$ for all i, where $T \in M_d$ is a unitary.

The state space $\mathcal{M}_2$ of M_2 is a three-dimensional Euclidean ball, known as *Bloch ball* [5]. Its surface is known as the *Bloch sphere* [5, 32] or *Poincaré sphere* [1]. The openness of $\mathbb{E}|_{\mathbb{CP}^1}$ on the Bloch sphere is proved in Coro. 6 in [15]. The openness of $\mathbb{E}|_{\mathcal{M}_2}$ on the Bloch ball is shown in Example 4.15.2 in [45]:

Fact 2.6. The expected value function $\mathbb{E}|_{\mathcal{M}_2}$ is open.

The possible convex support sets $L(\mathbf{u})$ of $\mathcal{M}_2$ are the linear images of the Bloch ball and they are easily identified algebraically. By Rem. 2.5(1,2) we may assume that $r \leq 3$ and that $u_1, u_2, u_3 \in M_2^{\mathrm{h}}$ are zero-trace and mutually orthogonal. If $r = 3$, then by Rem. 2.5(3) we can take the observables equal to the *Pauli matrices*

$$\sigma_1 := \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 := \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 := \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{2.5}$$

It is well known (and easy to check) that $L(\sigma_1, \sigma_2, \sigma_3)$ is the unit ball in $\mathbb{R}^3$. Notice that the joint numerical range $W(\sigma_1, \sigma_2, \sigma_3)$ is the unit sphere in $\mathbb{R}^3$ which is not convex. If $r = 2$, then we can take $u_1 = \sigma_1$, $u_2 = \sigma_2$. Then $L(\mathbf{u})$ is the numerical range of

$$\sigma_1 + i\sigma_2 = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix}$$

which is the unit disk in $\mathbb{C}$ centered at zero. If $r = 1$, then $L(\mathbf{u})$ is a line segment (we ignore the trivial case when $L(\mathbf{u})$ is a singleton).

3. Simplicial Points

In this section we recapitulate results from [45] now with a unified proof in terms of simplicial points. The term of simplicial point has another advantage that it complements the term of round boundary point in Lemma 7.1.

The main idea is the gauge condition in Fact 3.1 from our work [45] which is somewhat similar to the idea of our Thm. 4 in [15]. Let $\widetilde{X}$ be a finite-dimensional real normed vector space and let C be a convex subset of $\widetilde{X}$. The *gauge* of C is defined by

$$\gamma_C(v) := \inf\{\lambda \geq 0 \mid v \in \lambda C\}, \quad v \in \widetilde{X}.$$

Recall that the gauge of the unit ball in $\widetilde{X}$ is the norm. More generally, γ_C is positively homogeneous of degree one and convex [35]. If $C \neq \emptyset$ then the *positive hull* of C is defined by $\mathrm{pos}(C) := \{\lambda v \mid \lambda \geq 0, v \in C\}$.

In [45], Prop. 4.11, one of the authors has proved the following.

Fact 3.1 (Gauge condition)**.** If $w \in L$ and if the gauge γ_{L-w} is bounded on the set of unit vectors in $\mathrm{pos}(L - w)$ with respect to an arbitrary norm on Y then $f|_K$ is open on $f|_K^{-1}(w)$.

The assumptions of Fact 3.1 are fulfilled for example at the apices of the skew cone (5.1). The following Prop. 3.2 does not apply there but it will suffice for the purposes of this article.

We call a point x in a convex set C a *simplicial point* if there exists a finite set of simplices $S_1, \dots, S_m \subset C$ such that the union $S_1 \cup \dots \cup S_m$ is a neighborhood of x in C. A convex set C is *locally simplicial* [35] if all its elements are simplicial points.

Proposition 3.2 (Simplicial points)**.** *If $w \in L$ is a simplicial point of L then $f|_K$ is open on $f|_K^{-1}(w)$.*

Proof: Let $S_1, \dots, S_m \subset L$, $m \in \mathbb{N}$, be a set of simplices such that the union $U := S_1 \cup \dots \cup S_m$ is a neighborhood of w in L. Since L is convex, the convex hull P of U is also a neighborhood of w in L. Therefore $\text{pos}(L - w) = \text{pos}(P - w)$ holds. Since $P - w \subset L - w$ holds we have for all vectors $u \in \text{pos}(P - w)$ the inequality

$$\gamma_{L-w}(u) \leq \gamma_{P-w}(u).$$

For unit vectors u in $\text{pos}(P - w)$ the right-hand side is bounded because $P - w$ is polyhedral convex and contains the origin, see Rem. 3.1 in [39]. Therefore Fact 3.1 implies the claim. □

We mention some examples where we will apply Prop. 3.2. The relative interior of L and polytopes included in L are locally simplicial sets [35]. So the maximizer H is continuous on the relative interior of L and globally continuous if L is a polytope. Moreover, the restriction $H|_P$ is continuous for every polytope $P \subset L$. For example, the convex support $L(\mathbf{u})$ is a polytope for commutative observables $u_1, \dots, u_r$, see Sec. 2 in [45].

As the last example we mention that relative interior points of facets are simplicial points and we leave the proof to the reader because the openness of $f|_K$ on the fibers of these points is also proved in Coro. 4.4 in the next section.

Recall that a *face* [35] of a convex set C is any convex subset $F \subset C$ which contains all segments in C which meet F with an interior point. A face which is a singleton is called an *extremal point*. A face of codimension one in C is a *facet* of C.

4. Boundary-Interior Dichotomy

We show that the continuity of the maximizer H is certified by its restriction to the relative interior $\text{ri}(L)$ of L and also by the restriction to the relative boundary $\text{rb}(L)$ of L.

We begin with the relative interior by citing from Lemma 4.8 in our paper [45]:

Fact 4.1 (Norm closure)**.** We have $H(L) \subset \overline{H(\text{ri}(L))}$.

This statement was proved earlier in the context of the maximum-entropy inference (2.2) in Thm. 2d in [50]. The continuity of the maximizer H can be decided using $H|_{\mathrm{ri}(L)}$. In fact, given $w \in L$, if

$$f|_K^{-1}(w) \cap \overline{H(\mathrm{ri}(L))}$$

is a singleton $\{v\}$ then H is continuous at w and $H(w) = v$. Otherwise H is discontinuous at w. Fact 4.1 shows also that discontinuities of H are not removable.

Turning to the relative boundary we will use the property that for every $w \in \mathrm{rb}(L)$ the convex hull of a neighborhood of w in $\mathrm{rb}(L)$ and of a point in $\mathrm{ri}(L)$ is a neighborhood of w in L. This is easy to check for a Euclidean ball L with center w. The following fact, proved in Sec. 8.1 in [7], generalizes this from the ball to arbitrary convex bodies. Recall from [35] that a mapping $\gamma : \mathbb{R}^n \to \mathbb{R}^n$, $n \in \mathbb{N}$, is *positively homogeneous of degree one* if for each $x \in \mathbb{R}^n$ we have $\gamma(\lambda x) = \lambda\gamma(x)$, $0 < \lambda < \infty$.

Fact 4.2 (Thm. of Sz. Nagy)**.** Let $C \subset \mathbb{R}^n$, $n \in \mathbb{N}$, be a convex body containing the origin in its interior. Then there exists a homeomorphism from C onto the standard Euclidean unit ball of $\mathbb{R}^n$ which is positively homogeneous of degree one.

Theorem 4.3. *Let $\widetilde{K} := f|_K^{-1}(\mathrm{rb}(L))$. For all $\widetilde{v} \in \widetilde{K}$ the map $f|_K$ is open at $\widetilde{v}$ if and only if $f|_{\widetilde{K}}$ is open at $\widetilde{v}$.*

Proof: One direction follows by taking intersections of neighborhoods. Let us prove conversely that the openness of $f|_{\widetilde{K}}$ at $\widetilde{v} \in \widetilde{K}$ implies the openness of $f|_K$ at $\widetilde{v}$.

Let $N \subset K$ be a neighborhood of $\widetilde{v}$ in K. Then $N \cap \widetilde{K}$ is a neighborhood of $\widetilde{v}$ in $\widetilde{K}$. By assumptions $f|_{\widetilde{K}}$ is open at $\widetilde{v}$ so the image $f(N \cap \widetilde{K})$ is a neighborhood of $f(\widetilde{v})$ in $\mathrm{rb}(L)$. Since X is locally convex, we can assume that N is convex so $\mathrm{conv}(v, N \cap \widetilde{K}) \subset N$ for a given point $v \in N \setminus \widetilde{K}$. The linearity of f shows

$$f(N) \supset f(\mathrm{conv}(v, N \cap \widetilde{K})) = \mathrm{conv}(f(v), f(N \cap \widetilde{K})). \tag{4.1}$$

Since $f(v)$ lies in the relative interior of L the discussion in the paragraph before Fact 4.2 proves that $\mathrm{conv}(f(v), f(N \cap \widetilde{K}))$ is a neighborhood of $f(\widetilde{v})$ in L. Then (4.1) shows that $f(N)$ is a neighborhood of $f(\widetilde{v})$ in L which completes the proof. □

Thm. 4.3 applies to any facet F of L because F is a neighborhood in $\mathrm{rb}(L)$ of the relative interior points of F.

Corollary 4.4. *Let F be a facet of L and let $w \in \mathrm{ri}(F)$. Then $f|_K$ is open on $f|_K^{-1}(w)$.*

5. The Face Function of L

We prove a necessary continuity condition of the maximizer H in terms of the lower semi-continuity of the face function of L. The lower semi-continuity of the face function implies that a limit of extremal points is an extremal point [34].

An example where a limit of extremal points is not an extremal point is given by the convex hull of

$$\{(s,t,0) \in \mathbb{R}^3 \mid (s-1)^2 + t^2 = 1\} \cup \{(0,0,\pm 1)\}. \tag{5.1}$$

Here the set of extremal points $\{(s,t,0) \in \mathbb{R}^3 \mid (s-1)^2+t^2 = 1, s \neq 0\}$ contains $(0,0,0)$ which is an interior point of the segment connecting $(0,0,-1)$ and $(0,0,1)$.

To provide an example with the state space $\mathcal{M}_3$ we need algebraic representations of faces. A subset F of a convex set C is an *exposed face* of C if $F = \emptyset$ or if F equals the set of maximizers in C of a linear functional. One can show that every exposed face of C is a face of C. An exposed extremal point is called *exposed point*.

Fact 5.1 (Faces of state spaces)**.**

(1) The non-empty faces of the state space $\mathcal{M}_d$ are of the form $\mathcal{M}(pM_dp)$ where $p \in M_d$ is a non-zero projection, see for example [42], Sec. 2.3.

(2) Consider the exposed face $F = \mathrm{argmax}\{\alpha^*\lambda \mid \alpha \in L(\mathbf{u})\}$ of $L(\mathbf{u})$ where $\lambda = (\lambda_1,\ldots,\lambda_r) \in \mathbb{R}^r$. Then $\mathbb{E}|_{\mathcal{M}_d}^{-1}(F) = \mathcal{M}(pM_dp)$ where p is the spectral projection of the matrix $\mathbf{u}(\lambda) = \lambda_1 u_1 + \cdots + \lambda_r u_r$ corresponding to the maximal eigenvalue of $\mathbf{u}(\lambda)$. This follows from $\langle \rho, \mathbf{u}(\lambda)\rangle = \mathbb{E}(\rho)^*\lambda$, $\rho \in \mathcal{M}_d$, $\lambda \in \mathbb{R}^r$, and from [42], Thm. 2.9.

(3) Extremal points of the state space $\mathcal{M}_d$ are called *pure states*. A state is a pure state if and only if it is of the form xx^* for some unit vector $x \in \mathbb{C}^d$, see for example [1], Sec. 4.

We now discuss a three-dimensional linear image of $\mathcal{M}_3$ which has appeared as Exa. 4 in [13]. This linear image has a sequence of extremal points which converge to a point which is not an extremal point. A three-dimensional cross-section of $\mathcal{M}_3$ with this property is discussed in Rem 5.9 in [45].

Example 5.2. We consider the convex support $L(u_1, u_2, u_3)$ of

$$u_1 := \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad u_2 := \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & -1 \end{bmatrix}, \quad u_3 := \begin{bmatrix} 1 & 0 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & -1 \end{bmatrix}.$$

A limit of extremal points. Let $\epsilon \in \mathbb{R}$ and $\xi(\epsilon) := \sqrt{(1-\epsilon)^2 + 2\epsilon^2}$. The eigenvalues of $u_1 - \epsilon u_2$ are $\{1-\epsilon, \pm\xi(\epsilon)\}$. If $\epsilon \neq 0$ then the maximal eigenvalue $\xi(\epsilon)$ is non-degenerate and $v(\epsilon) := (1, 1, \epsilon \cdot x(\epsilon))$ is a corresponding eigenvector, where $x(\epsilon) := (\xi(\epsilon) + \epsilon - 1)/\epsilon^2$. By Fact 5.1(2) the pure state $\rho(\epsilon) := c(\epsilon) \cdot v(\epsilon)v(\epsilon)^*$, where $c(\epsilon) > 0$ is for normalization, defines the exposed point

$$\alpha(\epsilon) := \mathbb{E}(\rho(\epsilon)) = \tfrac{x(\epsilon)}{2-(1-\epsilon)x(\epsilon)}(1-\epsilon, 1-3\epsilon, 1-3\epsilon) - (0, 0, \tfrac{1}{2+(\epsilon\cdot x(\epsilon))^2})$$

of $L(\mathbf{u})$. Since $x(\epsilon) \to 1$ for $\epsilon \to 0$ we have

$$\alpha(0) := \lim_{\epsilon\to 0} \alpha(\epsilon) = (1, 1, \tfrac{1}{2}).$$

We could also do the easier computation $\alpha(0) = \mathbb{E}(\lim_{\epsilon\to 0} \rho(\epsilon))$ but the focus should be on $L(\mathbf{u})$ rather than $\mathcal{M}_3$. The limit $\alpha(0)$ is not an extremal point because it is the mid-point of the segment $s \subset L(\mathbf{u})$ between

$$\mathbb{E}((0,1,0)(0,1,0)^*) = (1,1,0) \quad \text{and} \quad \mathbb{E}((1,0,0)(1,0,0)^*) = (1,1,1).$$

Discontinuous maximum-entropy inference. We would like to point out that the maximum-entropy inference ρ^* is discontinuous at $\alpha(0)$ along the curve $\alpha(\epsilon)$. Namely, for $\epsilon \neq 0$ we have $\rho^*(\alpha(\epsilon)) = \rho(\epsilon)$ by Fact 5.1(2). The limit

$$\lim_{\epsilon\to 0} \rho^*(\alpha(\epsilon)) = \tfrac{1}{2}(1,1,0)(1,1,0)^*$$

is a pure state while $\rho^*(\alpha(0))$ has rank two. Indeed, we obtain

$$\rho^*(\alpha(0)) = p/2 \quad \text{for } p := (0,1,0)(0,1,0)^* + (1,0,0)(1,0,0)^*.$$

To see this, observe that the spectral projection corresponding to the maximal eigenvalue of u_1 equals p. Hence, by Fact 5.1(2), the exposed face of $L(\mathbf{u})$ consisting of the maximizers of the linear functional $L(\mathbf{u}) \to \mathbb{R}$, $\lambda \mapsto (1,0,0)^*\lambda$ has the pre-image $\mathcal{M}(pM_3p)$ under $\mathbb{E}|_{\mathcal{M}_3}$. Since $\alpha(0) = \mathbb{E}(p/2)$ and since $S(p/2) = \log(2)$ is the maximal value of the von Neumann entropy on $\mathcal{M}(pM_3p)$ we have $\rho^*(\alpha(0)) = p/2$.

Non-removability of the discontinuity. Further, we would like to point out that, by Prop. 3.2, the restricted maximum-entropy inference $\rho^*|_s$ is continuous on the segment s at $\alpha(0)$. This, together with the discontinuity at $\alpha(0)$ along the curve α proves that the discontinuity at $\alpha(0)$ is not removable from the restriction of ρ^* to the relative boundary of $L(\mathbf{u})$ (by changing only the value at $\alpha(0)$).

We will show that the discontinuity in Exa. 5.2 is a consequence of the fact that the extremal points $\alpha(\epsilon)$ converge to the point $\alpha(0)$ which lies in the relative interior of a higher-dimensional face. A convex body C is *stable* [34, 14] if the mid-point map

$$C \times C \to C, \quad (x,y) \mapsto \tfrac{1}{2}(x+y) \tag{5.2}$$

is open. The state space $\mathcal{M}_d$ is stable. Indeed, Lemma 3 in [38] proves that the map $\mathcal{M}_d \times \mathcal{M}_d \times [0,1]$, $(\rho,\sigma,\lambda) \mapsto (1-\lambda)\rho + \lambda\sigma$ is open. Prop. 1.1 in [14] then shows that $\mathcal{M}_d$ is stable.

Let us recall an equivalent statement of stability. Fact 5.3 is proved for example in Thm. 18.2 in [35].

Fact 5.3 (Face function)**.** For each point x in a convex set C there exists a unique face of C which contains x in the relative interior.

If x is a point in a convex set C then we denote the face of C containing x in its relative interior simply by $F(x)$, omitting C (which should be clear from the context). The *face function* of C is the set-valued map

$$C \to C, \quad x \mapsto F(x)$$

which has been studied for example in [25, 34]. A set-valued map $\Gamma : \widetilde{X} \to \widetilde{Y}$ between topological spaces $\widetilde{X}, \widetilde{Y}$ is *lower semi-continuous* at $x \in \widetilde{X}$ if for each open set G meeting $\Gamma(x)$ there exists a neighborhood N of x such that for all $x' \in N$ we have $G \cap \Gamma(x') \neq \emptyset$. The set-valued function Γ is *lower semi-continuous* if Γ is lower semi-continuous at every point of $\widetilde{X}$.

Fact 5.4 (Stable convex bodies)**.** If C is a convex body then the following are equivalent [34]:

(1) The convex body C is stable.

(2) The face function $x \mapsto F(x)$ of C is lower semi-continuous.

(3) The function $C \to \mathbb{N}_0$, $x \mapsto \dim(F(x))$ is lower semi-continuous.

Since extremal points have dimension zero, Fact 5.4(1) and (3) prove for any stable convex body that a limit of extremal points must be an extremal point. We now list some basic relations between the face functions of the convex bodies K and $L = f(K)$.

Lemma 5.5 (Linear images of faces)**.** *Let $w \in L$. Then:*

(1) *If $v \in f|_K^{-1}(w)$ then $f(F(v)) \subset F(w)$.*

(2) *If $v \in \mathrm{ri}(f|_K^{-1}(w))$ then $f(F(v)) = F(w)$.*

Proof: We prove (1) assuming $v \in f|_K^{-1}(w)$. The point v is a relative interior point of $F(v)$ by the definition of the face function. The relative interior of the linear image of a convex set is the linear image of the relative interior by [35], Thm. 6.6. So the relative interior of $f(F(v))$ is $f(\mathrm{ri}(F(v)))$. Hence $w = f(v)$ is a relative interior point of the convex set $f(F(v))$. Therefore, and since w lies in the face $F(w)$ of L, Thm. 18.1 in [35] proves (1).

We prove (2) assuming $v \in \mathrm{ri}(f|_K^{-1}(w))$. Recall that inverse images of faces are faces. So $G := f|_K^{-1}(F(w))$ is a face of K. As we have recalled in the previous paragraph, $f(\mathrm{ri}(G)) = \mathrm{ri}(f(G))$ holds so the affine space $f^{-1}(w)$ meets the relative interior of G. Hence, by [35], Coro. 6.5.1, the relative interior of $f|_K^{-1}(w) = f^{-1}(w) \cap G$ is the intersection of $f^{-1}(w)$ with $\mathrm{ri}(G)$. This shows that v lies in $\mathrm{ri}(G)$ and proves $G = F(v)$ which completes the proof. □

We are ready for the main result of this section.

Theorem 5.6. *Let $(w_i)_{i\in\mathbb{N}} \subset L$ converge to a point $w \in L$. We assume that* (a) *the convex body K is stable. We also assume that* (b) *a sequence $(v_i)_{i\in\mathbb{N}} \subset K$ converges to a point $v \in K$ such that $\mathbb{E}(v_i) = w_i$, $i \in \mathbb{N}$, and such that v lies in* $\mathrm{ri}(f|_K^{-1}(w))$. *Then the following statements hold.*

(1) *For all open subsets $O \subset L$ meeting $F(w)$ there exists $N \in \mathbb{N}$ such that for all $i \geq N$ we have $O \cap F(w_i) \neq \emptyset$.*

(2) *We have* $\dim F(w) \leq \liminf_{i\to\infty} \dim F(w_i)$.

Proof: We prove (1) assuming $O \subset L$ is an open set meeting $F(w)$. Since $f|_K$ is continuous $\widetilde{O} := f|_K^{-1}(O)$ is open. By the assumption (b) the point v lies in the relative interior of $f|_K^{-1}(w)$ so $f(F(v)) \supset F(w)$ holds by Lemma 5.5(2) and $\widetilde{O} \cap F(v) \neq \emptyset$ follows. By assumption (a) the convex body K is stable so the face function of K is lower semi-continuous by Fact 5.4(1) and (2). As $v = \lim_{i\to\infty} v_i$ holds there is $N \in \mathbb{N}$ such that for $i \geq N$ we have $\widetilde{O} \cap F(v_i) \neq \emptyset$. As $f(F(v_i)) \subset F(w_i)$ holds by Lemma 5.5(1) we get $O \cap F(w_i) \neq \emptyset$ for $i \geq N$. The statement (2) is an easy corollary of (1) for arbitrary convex bodies L. □

Let us discuss Thm. 5.6.

Remark 5.7. (1) Thm. 5.6 allows us to detect discontinuities of the maximum-entropy inference ρ^* in terms of the convex geometry of $L(\mathbf{u})$. We have seen in the paragraph of (5.2) that the state space $\mathcal{M}_d$ is stable while $\rho^*(\alpha) \in \mathrm{ri}\, \mathbb{E}|_{\mathcal{M}_d}^{-1}(\alpha)$ holds for all $\alpha \in L(\mathbf{u})$ by Lemma 5.8 in [45]. Thus the assumptions of Thm. 5.6 are fulfilled.

The Example 5.2 demonstrates explicitly a discontinuity of ρ^* at a point $\alpha(0)$ which is a limit of extremal points $\alpha(\epsilon)$ but not an extremal point itself.

(2) All assumptions of Thm. 5.6 are needed in general. Consider a convex body $K \subset X$ which is not stable, take $X = Y$ and the identity map $f : X \to Y$. Then the face function of $L = K$ is not lower semi-continuous by Fact 5.4(1) and (2), thereby contradicting Thm. 5.6(1). The assumption (b) is not met in Exa. 5.2 where the limit point $\rho(0) = \frac{1}{2}(1,1,0)(1,1,0)^*$ of $\rho(\epsilon) \in \mathcal{M}_3$ for $\epsilon \to 0$ is a relative boundary point of the Bloch ball $\mathbb{E}|_{\mathcal{M}_3}^{-1}(\alpha(0))$. In this example we have a jump from the dimension zero of $F(\alpha(\epsilon))$, $\epsilon \neq 0$, to the dimension one of $F(\alpha(0))$ which contradicts Thm. 5.6(2).

(3) Thm. 5.6(1) is in general stronger than Thm. 5.6(2) if the assumptions (a) and (b) of the theorem are ignored. This was pointed out in the work [34] in the example recalled in (5.1) where (1) fails at all points but the vertices of the segment between $(0,0,-1)$ and $(0,0,1)$ while (2) holds at all points but the mid-point of this segment. However we do not know whether the convex body in (5.1) is the linear image of a stable convex body so (1) and (2) could be equivalent under the assumptions of the theorem.

6. Irreducible Correlation

In this section we show that the discontinuity of the three-party irreducible correlation of three qubits, the correlation that can not be observed in two-party subsystems [30], can be detected *via* the face function of the convex body of two-party marginals.

The discontinuity which we 'detect' follows also from the well-known result [30] that almost every pure state of three qubits is uniquely specified by its two-party marginals among all states (pure or mixed). The only exceptions are the GHZ-like states [32]

$$\psi := \alpha|000\rangle + \beta|111\rangle, \qquad |\alpha|^2 + |\beta|^2 = 1, \alpha, \beta \in \mathbb{C} \tag{6.1}$$

and their local unitary transforms, that is vectors $(U_1 \otimes U_2 \otimes U_3)\psi$ where $U_1, U_2, U_3 \in M_2$ are unitaries.

A three-qubit system ABC is described by the algebra $M_8 \cong M_2 \otimes M_2 \otimes M_2$ with state space $\mathcal{M}_8 \cong \mathcal{M}(M_2 \otimes M_2 \otimes M_2)$. A *two-local Hamiltonian* is a sum of tensor product terms $a \otimes b \otimes c$ with at most two non-scalar factors $a, b, c \in M_2^{\mathrm{h}}$. In this section, we fix any spanning set $u_1, \ldots, u_r \in M_8^{\mathrm{h}}$, $r \in \mathbb{N}$, of the space $\mathcal{H}^{(2)}$ of two-local Hamiltonians and put $\mathbf{u} = (u_1, \ldots, u_r)$. Given any three-qubit state $\rho \in \mathcal{M}_8$, its *marginal* $\rho_{AB} \in \mathcal{M}_4$ on the AB subsystem is defined by

$$\langle \rho_{AB}, a \otimes b \rangle = \langle \rho, a \otimes b \otimes \mathbb{1}_2 \rangle, \qquad a, b \in M_2.$$

The marginals ρ_{AC}, ρ_{BC} are defined similarly. We denote by $\rho^{(2)} = (\rho_{AB}, \rho_{AC}, \rho_{BC})$ the vector of two-party marginals of ρ. For two states $\rho, \sigma \in \mathcal{M}_8$ the expected values of two-local Hamiltonians satisfy $\mathbb{E}_{\mathbf{u}}(\sigma) = \mathbb{E}_{\mathbf{u}}(\rho)$ if and only if the two-party marginals coincide, that is $\sigma^{(2)} = \rho^{(2)}$. Thus we identify the convex support $L(\mathbf{u})$ with respect to the spanning set $u_1, \dots, u_r$ of $\mathcal{H}^{(2)}$ and the set of two-party marginals, that is

$$L(\mathbf{u}) \cong \{\rho^{(2)} \mid \rho \in \mathcal{M}_8\}. \tag{6.2}$$

Using the identification (6.2) we define, as in (2.2), the maximum-entropy inference

$$\rho^* : L(\mathbf{u}) \to \mathcal{M}_8, \qquad \alpha \mapsto \operatorname{argmax}\{S(\rho) \in \mathcal{M}_8 \mid \rho^{(2)} = \alpha\}.$$

The *irreducible three-party correlation* [30] of ρ is defined as the difference of von Neumann entropies

$$C_3(\rho) := S(\rho^*(\rho^{(2)})) - S(\rho). \tag{6.3}$$

The definition of $C_3(\rho)$ is derived from the statistical inference view [23] of the maximum-entropy principle where $\rho^*(\rho^{(2)})$ is seen as the least informative state compatible with the two-party marginals $\rho^{(2)}$. Since ρ and $\rho^*(\rho^{(2)})$ are equal on every two-party subsystem of ABC, any discrepancy between them reveals additional information shared by ρ which can not be observed on any two-party subsystem. This information is called *irreducible three-party correlation* in [30] and is quantified by $C_3(\rho)$.

We remark that information is seen as a constraint on our beliefs in the context of inference [10] as opposed to the language usage in coding theory where information is a measure of unpredictability which is quantified, in the case of quantum information sources [8], in terms of von Neumann entropy.

The main point regarding continuity of C_3 is provided in Sec. 5.6 in [45]. Lemma 5.15(2) and Lemma 4.5 in [45] prove for all $\alpha \in L(\mathbf{u})$ that

$$\begin{gathered} \rho^* : L(\mathbf{u}) \to \mathcal{M}_8 \text{ is continuous at } \alpha \\ \Updownarrow \\ C_3 : \mathcal{M}_8 \to \mathbb{R} \text{ is continuous on } \mathbb{E}|_{\mathcal{M}_8}^{-1}(\alpha). \end{gathered} \tag{6.4}$$

The equivalence (6.4) allows us to apply convex geometric methods to detect discontinuities of C_3. In what follows, inspired by a model presented in Example 6 in [13], we prove existence of a discontinuity.

Example 6.1. We consider the two-local Hamiltonians

$$\begin{aligned} H_0 &:= \mathbb{1}_2 \otimes \sigma_3 \otimes \sigma_3 + \sigma_3 \otimes \mathbb{1}_2 \otimes \sigma_3 + \sigma_3 \otimes \sigma_3 \otimes \mathbb{1}_2 \\ H_1 &:= \sigma_1 \otimes \mathbb{1}_2 \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \sigma_1 \otimes \mathbb{1}_2 + \mathbb{1}_2 \otimes \mathbb{1}_2 \otimes \sigma_1 \end{aligned}$$

where σ_1 and σ_3 are Pauli matrices and for $\epsilon > 0$ we take

$$H(\epsilon) := H_0 + \epsilon H_1.$$

The maximal eigenvalue $\lambda(\epsilon) := 1 + \epsilon + 2\sqrt{1 - \epsilon + \epsilon^2}$ of $H(\epsilon)$ is non-degenerate. The positive number $s = s(\epsilon) := (\lambda(\epsilon) - 3)/3\epsilon$ which goes to zero for $\epsilon \to 0$ allows us to write $w(\epsilon) := (1, s, s, s, s, s, s, 1)$ for the corresponding eigenvector which defines the pure state $\rho(\epsilon) := w(\epsilon)w(\epsilon)^*/(2 + 6s^2)$ with AB-marginal

$$\rho(\epsilon)_{AB} = \tfrac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|) + \tfrac{1}{2+6s^2} \begin{pmatrix} -2s^2 & s^2+s & s^2+s & 2s \\ * & 2s^2 & 2s^2 & s^2+s \\ * & * & 2s^2 & s^2+s \\ * & * & * & -2s^2 \end{pmatrix} \in \mathcal{M}_4.$$

The symmetry of $H(\epsilon)$ shows $\rho(\epsilon)^{(2)} = (\rho(\epsilon)_{AB}, \rho(\epsilon)_{AB}, \rho(\epsilon)_{AB})$. Using the identification (6.2) we note from Fact 5.1(2) that $\rho(\epsilon)^{(2)}$ is an exposed point of the convex support $L(\mathbf{u})$ where $\mathbf{u} = (u_1, \ldots, u_r)$ spans the space of two-local Hamiltonians. The limit $\rho(0)^{(2)}$ of $\rho(\epsilon)^{(2)}$ for $\epsilon \to 0$ is the mid-point of the segment between the distinct marginals $|000\rangle\langle 000|^{(2)}$ and $|111\rangle\langle 111|^{(2)}$ and therefore $\rho(0)^{(2)}$ is not an extremal point of $L(\mathbf{u})$.

Out of curiosity we mention that $\rho(\epsilon)_{AB}$ has rank two for $0 < s < 1$ (non-zero eigenvalues $\frac{(s-1)^2}{2(3s^2+1)}$ and $\frac{5s^2+2s+1}{2(3s^2+1)}$). Although the extremal points of $\mathcal{M}_4$ are rank-one states this does not contradict the fact that $\rho(\epsilon)^{(2)}$ is an exposed point of $L(\mathbf{u})$ because $L(\mathbf{u}) \subsetneq \mathcal{M}_4 \times \mathcal{M}_4 \times \mathcal{M}_4$.

Let us turn to the irreducible correlation and its continuity. We have just seen that $\rho(0)^{(2)}$ is a limit of exposed points but not an extremal point itself. Hence Remark 5.7(1) shows that the maximum-entropy inference ρ^* is discontinuous at $\rho(0)^{(2)}$ and (6.4) proves that the irreducible correlation C_3 is discontinuous at some point in the fiber $\{\rho \in \mathcal{M}_8 \mid \rho^{(2)} = \rho(0)^{(2)}\}$.

This abstract existence result of a discontinuity is confirmed by the discontinuity of C_3 at the GHZ state $\frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ which follows directly from [30] and which we explain in detail. The projection

$$p := |000\rangle\langle 000| + |111\rangle\langle 111|$$

is the spectral projection corresponding to the maximal eigenvalue of H_0. So Fact 5.1(2) applied to $\mathbf{u}(\lambda) = H_0$ proves that $\mathcal{M}(pM_8p)$ is the inverse image of an exposed face of $L(\mathbf{u})$. Elements of the Bloch ball

$\mathcal{M}(pM_8p)$ can be written in the form

$$\begin{aligned}\sigma(x,y,z) := \tfrac{1}{2}\big(p &+ x\cdot(|000\rangle\langle 111| + |111\rangle\langle 000|)\\ &+ y\cdot(-i|000\rangle\langle 111| + i|111\rangle\langle 000|)\\ &+ z\cdot(|000\rangle\langle 000| - |111\rangle\langle 111|)\big)\end{aligned}$$

where $(x,y,z)\in\mathbb{R}^3$ lies in the three-ball, that is $x^2+y^2+z^2\leq 1$. The two-party marginal is

$$\sigma(x,y,z)^{(2)} = \tfrac{1}{2}(1+z)(|000\rangle\langle 000|^{(2)} + \tfrac{1}{2}(1-z)|111\rangle\langle 111|^{(2)}.$$

The maximum-entropy state

$$\rho^*(\sigma(x,y,z)^{(2)}) = \tfrac{1}{2}(1+z)(|000\rangle\langle 000| + \tfrac{1}{2}(1-z)|111\rangle\langle 111|$$

has von Neumann entropy $S(\rho^*(\sigma(x,y,z)^{(2)})) = H(\frac{1}{2}(1+z))$ where we use the function $H(\eta) := -\eta\log(\eta) - (1-\eta)\log(1-\eta)$, $\eta\in[0,1]$. In particular, for pure states $\psi := \alpha|000\rangle + \beta|111\rangle$, $\alpha,\beta\in\mathbb{C}$, $|\alpha|^2+|\beta|^2=1$ we get

$$C_3(\psi\psi^*) = H(|\alpha|^2)$$

which is strictly positive unless $|\alpha|=0$ or $|\alpha|=1$. The irreducible three-party correlation $C_3(\psi\psi^*)$ has the maximal value $\log(2)$ for states $\psi\psi^*$ where $\psi = \frac{1}{\sqrt{2}}(|000\rangle + e^{i\phi}|111\rangle)$, $\phi\in[0,2\pi)$.

On the other hand, ψ is approximated, for example, by vectors $\varphi := \alpha|000\rangle + \cos(\gamma)\beta|111\rangle + \sin(\gamma)\beta|001\rangle$ for real $\gamma\to 0$. For small $\gamma>0$ the vector φ is not a local unitary transform of a vector ψ because the two-party marginals of $\varphi\varphi^*$ are not identical. This implies [30], as we have recalled in (6.1), that $\varphi\varphi^*$ is uniquely determined by its two-party marginals. Hence $\varphi\varphi^*$ belongs to the maximum-entropy states $\rho^*(L(\mathbf{u}))$ and has zero irreducible three-party correlation. This proves discontinuity of C_3 at $\psi\psi^*$ for all $0<|\alpha|<1$. Analogous discontinuity statements hold for unitary transforms of vectors ψ.

7. Multiply Generated Round Boundary Points

In the sequel we study pairs of observables $u_1,u_2\in M_d^{\mathrm{h}}$, $d\in\mathbb{N}$, with $\mathbb{E}_{\mathbf{u}} : M_d^{\mathrm{h}}\to\mathbb{R}^2$ for $\mathbf{u}=(u_1,u_2)$ and where $\mathbb{E}_{\mathbf{u}}(\mathcal{M}_d) = L(\mathbf{u}) = W(\mathbf{u})$ is the numerical range (2.4). In this section we prove a sufficient condition for the openness of $\mathbb{E}|_{\mathcal{M}_d}$ in terms of unique pre-images and simplicial points. We will see that this condition works well for matrix sizes $d=3,4,5$ but has a limited meaning for $d\geq 6$.

In our earlier work [28] we call $z\in W(u_1+iu_2)\subset\mathbb{C}$ *singularly generated* if $x^*(u_1+iu_2)x = z$ holds for exactly one linearly independent unit vector $x\in\mathbb{C}^d$. Otherwise z is *multiply generated*. Since $\mathbb{E}|_{\mathcal{M}_d}$ is open at those points $\rho \in \mathcal{M}_d$ where $\mathbb{E}(\rho)$ is an interior point of the numerical range, a classification of boundary points is useful. A *corner point* is a point of $W(u_1, u_2) \subset \mathbb{R}^2$ which belongs to more than one supporting line of $W(u_1, u_2)$. A *flat boundary portion* is a non-trivial line segment lying in the boundary of $W(u_1, u_2)$. A boundary point of $W(u_1, u_2)$ which is no corner point and which does not belong to the relative interior of a flat boundary portion is called *round boundary point*.

Notice that every flat boundary portion is a sub-segment of a one-dimensional face of $W(u_1, u_2)$. Round boundary points exist only if the numerical range has dimension two.

Lemma 7.1. *If the dimension of $W(u_1, u_2)$ is two then every corner point is the intersection of two facets of $W(u_1, u_2)$. Without dimension restrictions, every point of $W(u_1, u_2)$ is either a round boundary point or a simplicial point but not both.*

Proof: Every corner point $\alpha \in W(u_1 + iu_2)$ is a *normal splitting eigenvalue*, see Sec. 13 in [24], that is $u_1 + iu_2$ is unitarily equivalent to a block diagonal matrix

$$\left[\begin{array}{c|c} \alpha & \\ \hline & B \end{array}\right]$$

with zeros on the off-diagonal. Since $W(u_1 + iu_2)$ is the convex hull of $W(B)$ and of α the first statement follows by induction. Going through the above classification of boundary points, the second assertion now follows easily. □

Remark 7.2 (Lattice theoretical proof of Lemma 7.1)**.** The numerical range $W(u_1, u_2)$ is the convex dual of an affine section of $\mathcal{M}_d$ [21, 42, 20]. Since all faces of this affine section are exposed, the lattice isomorphism (2) in [43] shows that all non-empty faces of normal cones of $W(u_1, u_2)$ are normal cones. In particular, if α is a corner point then the two boundary rays of its normal cone are normal cones of $W(u_1, u_2)$. The lattice isomorphism (1) in [43] now shows that α is an extremal point of two distinct one-dimensional faces of $W(u_1, u_2)$ which proves the claim.

Theorem 7.3. *The map $\mathbb{E}_{\mathbf{u}}|_{\mathcal{M}_d}$ is open on $\mathcal{M}_d$ except possibly at those states $\rho \in \mathcal{M}_d$ where $\mathbb{E}_{\mathbf{u}}(\rho)$ is a multiply generated round boundary point.*

Proof: If $\alpha \in W(u_1, u_2)$ is singularly generated then by Thm. 5 in [12] the fiber $\mathbb{E}|_{\mathcal{M}_d}^{-1}(\alpha)$ is a singleton. It is easy to prove and well-known in the theory of multi-valued maps [15] that $\mathbb{E}|_{\mathcal{M}_d}$ is open at singleton fibers. If α is a simplicial point then Prop. 3.2 proves that $\mathbb{E}|_{\mathcal{M}_d}$ is open on $\mathbb{E}|_{\mathcal{M}_d}^{-1}(\alpha)$. Otherwise, if α is not a simplicial point, then the second statement of Lemma 7.1 shows that α is a round boundary point. $\square$

The converse of Thm. 7.3 does not hold for $d \geq 4$, that is, $\mathbb{E}|_{\mathcal{M}_d}$ may be open on fibers of multiply generated round boundary points.

Example 7.4. An example inspired by Thm. 4.4 in [28] is

$$u_1 + iu_2 = \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \oplus \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} = \mathbb{1}_2 \otimes \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix}, \tag{7.1}$$

where the numerical range is the unit disk and all points on the unit circle S^1 are multiply generated round boundary points. Nevertheless $\mathbb{E}|_{\mathcal{M}_4} : \mathcal{M}_4 \to \mathbb{R}^2$ is open. A short computation with the unitary

$$v_\theta := \mathbb{1}_2 \otimes [\cos(\tfrac{\theta}{2})\mathbb{1}_2 - i\sin(\tfrac{\theta}{2})\sigma_3] \in M_2, \qquad \theta \in \mathbb{R},$$

and the Pauli matrix σ_3 shows

$$\mathbb{E}(v_\theta \rho v_\theta^*) = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix} \cdot \mathbb{E}(\rho), \qquad \rho \in \mathcal{M}_4.$$

The state space $\mathcal{M}_4$ is partitioned into the orbits of the group of unitaries $\{v_\theta \mid \theta \in [0, 2\pi)\}$. The orbit $\mathcal{O}(\rho)$ through any state ρ with $\mathbb{E}(\rho) \in S^1$ is homeomorphic to S^1 under $\mathbb{E}$. Hence $\mathbb{E}|_{\mathcal{O}(\rho)}$ is open at ρ and *a fortiori* $\mathbb{E}$ restricted to $\mathbb{E}|_{\mathcal{M}_4}^{-1}(S^1)$ is open at ρ. Now Thm. 4.3 proves that $\mathbb{E}|_{\mathcal{M}_4}$ is open at ρ. The openness of $\mathbb{E}|_{\mathcal{M}_4}$ at all other states of $\mathcal{M}_4$ follows from Prop. 3.2 applied to the interior of the unit disk.

To capture the non-generic direct sum form (7.1) we introduce a definition from [26]. A matrix $A \in M_d$ is *unitarily reducible* if A is unitarily equivalent to a matrix in block-diagonal form with at least two proper blocks. Otherwise A is *unitarily irreducible*.

Unitarily irreducible matrices have at most $d-3$ multiply-generated round boundary points when $d = 3, 4, 5$. See Thm. 3.2 in [28] for $d = 3$ and notice that every round boundary point is an extremal point. For $d = 4, 5$ see Thms. 4.1 and 5.7 in [28]. Since $\mathbb{E}|_{\mathcal{M}_2}$ is open by Fact 2.6 and since $\mathcal{M}_1$ is a singleton, Thm. 7.3 implies the following.

Corollary 7.5. *Let $d \leq 5$ and let $u_1 + iu_2$ be unitarily irreducible. Then there are at most* $\max\{0, d-3\}$ *points α of $W(u_1, u_2)$ such that $\mathbb{E}|_{\mathcal{M}_d}$ is not open on the fiber $\mathbb{E}|_{\mathcal{M}_d}^{-1}(\alpha)$.*

The maximum-entropy inference $\rho^* : W(u_1, u_2) \to \mathcal{M}_d$ is indeed discontinuous at the multiply generated round boundary point(s) of $W(u_1, u_2)$, if there are any, when $d = 4$ or 5 and when $u_1 + iu_2$ is unitarily irreducible. This happens because these points are isolated. So, approximating a multiply generated round boundary point α by singularly generated extremal points α_i we observe that $\rho^*(\alpha_i)$ has rank one while the rank of $\rho^*(\alpha)$ is at least two. This proves discontinuity of ρ^* at α.

It is known for matrix size $d \geq 6$ and irreducible matrix $u_1 + iu_2$ that $W(u_1, u_2)$ may have infinitely many multiply generated round boundary points. As was noticed earlier in [28], Sec. 6, this is closely connected to the failure of *Kippenhahn's conjecture*. On the other hand, one of us has recently shown [47] that for all $d \in \mathbb{N}$ the maximum-entropy inference $\rho^* : W(u_1, u_2) \to \mathcal{M}_d$ has at most finitely many discontinuities.

8. Numerical Range of 3 × 3 Matrices

In the numerical range approach, based on [24, 26, 36], we characterize points of discontinuity of $\rho^*(\alpha)$ depending on the type of shape of the numerical range of 3×3 matrices: unitarily irreducible — ovular, ellipse, with a flat portion on the boundary, and unitarily reducible — triangle, line segment, ellipse, and the convex hull of an ellipse and a point outside the ellipse.

See Example 4.18 in [45] for the problem of openness of $\mathbb{E}|_{\mathcal{M}(\mathcal{A})}$ for unitarily reducible $u_1 + iu_2$ and the C*-algebra $\mathcal{A} \subset M_3$ generated by $u_1 + iu_2$. Here we consider the full algebra M_3 and arbitrary 3×3 matrices.

Theorem 8.1. *Let $u_1, u_2 \in M_3^{\mathrm{h}}$. If $\mathbb{E}|_{\mathcal{M}_3}$ is not open on the fiber $\mathbb{E}|_{\mathcal{M}_3}^{-1}(z)$ of a point $z \in W(u_1 + iu_2)$ then after reparametrization* (2.5) *the matrix $u_1 + iu_2$ has the form*

$$A := \begin{bmatrix} 0 & 2 \\ 0 & 0 \end{bmatrix} \oplus [\,1\,]$$

and $W(A)$ is the unit disk in $\mathbb{C}$. The map $\mathbb{E}|_{\mathcal{M}_3}$ is open on $\mathcal{M}_3$ with the exception of the fiber $\mathbb{E}|_{\mathcal{M}_3}^{-1}(1)$ which is a three-dimensional ball where $\mathbb{E}|_{\mathcal{M}_3}$ is only open at the pure state $v_1 v_1^*$ for $v_1 := \frac{1}{\sqrt{2}}(1, 1, 0)$.

Proof. If $\mathbb{E}|_{\mathcal{M}_3}$ is not open on $\mathbb{E}|_{\mathcal{M}_3}^{-1}(z)$ then Thm. 7.3 shows that z is a multiply generated round boundary point. Thm. 3.2 in [28] shows then that $u_1 + iu_2$ is unitarily equivalent to a matrix $B \oplus [z]$ where B is a unitarily irreducible 2×2 matrix and z is a boundary point of the ellipse $W(u_1 + iu_2)$. This and (2.5) allow us to transform the matrix $u_1 + iu_2$ into the above matrix A. Now $W(u_1 + iu_2)$ is the unit disk and 1 is a multiply generated round boundary point. By Thm. 3.2 in

[28] all points $\alpha \neq 1$ on the unit circle S^1 are singularly generated, so the fiber $\mathbb{E}|_{\mathcal{M}_3}^{-1}(\alpha)$ is a singleton by Thm. 5 in [12]. At singleton fibers $\mathbb{E}|_{\mathcal{M}_3}$ is open. The map $\mathbb{E}|_{\mathcal{M}_3}$ is open on the fibers of all interior points of the unit disk, see Prop. 3.2, so it remains to examine the exceptional point $1 \in S^1$.

Since for any $\alpha \in S^1 \setminus \{1\}$ the fiber of α is a singleton we have $H(\alpha) = v_\alpha v_\alpha^*$ where $v_\alpha := \frac{1}{\sqrt{2}}(1, \alpha, 0)$. Choosing any $\rho_0 \in \mathbb{E}|_{\mathcal{M}_3}^{-1}(1)$ and maximizing the quadratic form $g_{\rho_0}(\rho) := -\langle \rho - \rho_0, \rho - \rho_0 \rangle$, $\rho \in \mathcal{M}_3$, gives $H(1) = \rho_0$. The restriction $H|_{S^1}$ is continuous at 1 if and only if $\rho_0 = v_1 v_1^*$. This, by Thm. 4.3, is also the condition that H is continuous at 1 and, by Fact 2.2, the condition that $\mathbb{E}|_{\mathcal{M}_3}$ is open at ρ_0. $\square$

The maximum-entropy states with respect to the transformed observables $u_1 = \sigma_1 \oplus 1$ and $u_2 = \sigma_2 \oplus 0$ in Thm. 8.1 are

$$\rho^*(1) = \begin{bmatrix} 1/4 & 1/4 \\ 1/4 & 1/4 \end{bmatrix} \oplus [\,1/2\,]$$

and

$$\rho^*(\alpha) = \begin{bmatrix} 1/2 & \overline{\alpha} \cdot 1/2 \\ \alpha \cdot 1/2 & 1/2 \end{bmatrix} \oplus [\,0\,], \qquad |\alpha| = 1, \quad \alpha \neq 1.$$

This proves discontinuity of ρ^* at $\alpha = 1$.

We conclude with a remark about several observables $u_1, \ldots, u_r \in M_3^{\mathrm{h}}$, $r \in \mathbb{N}$, and $\mathbf{u} = (u_1, \ldots, u_r)$.

Proposition 8.2. *Let F be a face of $L(\mathbf{u}) = \mathbb{E}(\mathcal{M}_3)$ and assume $0 < \dim(F) < \dim(L(\mathbf{u}))$. Then F is a Euclidean ball of dimension one, two or three, and all relative boundary points $w \in \mathrm{rb}(F)$ have singleton fibers $\mathbb{E}|_{\mathcal{M}_3}^{-1}(w)$.*

Proof: Let w be an extremal point of F. Then $\{w\} \subset F \subset L$ are faces of L, properly included into each other. Since inverse images of faces are faces, Fact 5.1(1) shows

$$\mathbb{E}|_{\mathcal{M}_3}^{-1}(F) = \mathcal{M}(p_1 M_3 p_1), \qquad \mathbb{E}|_{\mathcal{M}_3}^{-1}(\{w\}) = \mathcal{M}(p_2 M_3 p_2)$$

for projections $p_1 \succeq p_2$. By the assumption of strict dimension differences we get

$$3 = \mathrm{rank}(\mathbb{1}_3) > \mathrm{rank}(p_1) > \mathrm{rank}(p_2) \geq 1.$$

Thus $\mathrm{rank}(p_1) = 2$ holds and so $\mathbb{E}|_{\mathcal{M}_3}^{-1}(F)$ is a copy of the three-dimensional Euclidean Bloch ball. Now the claim follows easily. $\square$

Prop. 8.2 implies the following (for several observables, $r \in \mathbb{N}$).

Corollary 8.3. *Let F be a facet of $L(\mathbf{u}) = \mathbb{E}(\mathcal{M}_3)$. Then $\mathbb{E}|_{\mathcal{M}_3}$ is open on $\mathbb{E}|_{\mathcal{M}_3}^{-1}(F)$.*

An example where Coro. 8.3 gives new insights beyond Coro. 4.4 is the convex hull of the Steiner Roman surface, depicted in Fig. 10 in [4], which is a linear image of $\mathcal{M}_3$ and which has four disk facets.

9. Appendix

We recall a reduction of the state space in terms of the algebra of observables. The proof is from Sec. 3.4 in [42] and is reproduced here in a simpler setting.

For $d \in \mathbb{N}$ let us consider the parametrization of the hermitian pencil

$$\mathbf{u}(\theta) := \theta_1 u_1 + \cdots + \theta_r u_r, \qquad \theta \in \mathbb{R}^r$$

for observables $u_1, \ldots, u_r \in M_d^{\mathrm{h}}$. Let $\mathcal{A}(\mathbf{u})$ denote the real or complex *-algebra generated by the $d \times d$ identity matrix $\mathbb{1}_d$ and by $u_1, \ldots, u_r$. Recall that Minkowski's theorem asserts that a convex body is the convex hull of its extremal points. The statement of Straszewicz's theorem is that the closure of exposed points of a convex body contains all its extremal points. See e.g. Coro. 1.4.5 and Thm. 1.4.7 in [37] for these statements.

Lemma 9.1. *Any spectral projection of any matrix in the hermitian pencil $\{\mathbf{u}(\theta) \mid \theta \in \mathbb{R}^r\}$ belongs to $\mathcal{A}(\mathbf{u})$. The convex support of $\mathbf{u}$ is $L(\mathbf{u}) = \mathbb{E}(\mathcal{M}(\mathcal{A}(\mathbf{u})))$.*

Proof: Any spectral projection of $\mathbf{u}(\theta)$ for $\theta \in \mathbb{R}^r$ is a real polynomial in one variable evaluated at $\mathbf{u}(\theta)$. Therefore the spectral projection belongs to the algebra $\mathcal{A}(\mathbf{u})$.

Let α be an exposed point of $L(\mathbf{u})$. Then Fact 5.1(2) shows that there is $\theta \in \mathbb{R}^r$ such that the spectral projection p of $\mathbf{u}(\theta)$, corresponding to the largest eigenvalue of of $\mathbf{u}(\theta)$, yields

$$\mathbb{E}|_{\mathcal{M}_d}^{-1}(\alpha) = \mathcal{M}(pM_d p).$$

Since $p/\operatorname{tr}(p)$ belongs to the algebra $\mathcal{A} := \mathcal{A}(\mathbf{u})$, the image of the state space $\mathcal{M}(\mathcal{A})$ under $\mathbb{E}$ covers all exposed points of $L(\mathbf{u})$. Now Straszewicz's theorem implies that $\mathcal{M}(\mathcal{A})$ covers all extremal points of $L(\mathbf{u})$, and thus by Minkowski's theorem the whole $L(\mathbf{u})$. The converse inclusion is trivial because $\mathcal{A} \subset M_d$ holds. □

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