A Variation Principle for Ground Spaces

Workshop on Operator Theory, Complex Analysis, and Applications

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Abstract

A variation formula is presented for the ground space projections of a vector space of energy operators in a matrix *-algebra. We prove that the ground space projections are the greatest projections of the algebra under certain operator cone constraints. The formula is derived from lattice isomorphisms between normal cones and exposed faces of the state space of the algebra, and between ground space projections.

The vector space of local Hamiltonians is in the focus of quantum many-body physics. The variation formula will be demonstrated with two-local three-bit (commutative) Hamiltonians. A future goal is to understand the lattice of ground spaces of two-local three-qubit (non-commutative) Hamiltonians. Both its combinatorics and topology are unsettled issues.

Reference: `arXiv:1704.07675 [math-ph]`

(these slides are identical with those presented at the workshop, except for the present page which was added after the presentation)

Notation

- *-subalgebra $\mathcal{A}$ of M_n, the complex n-by-n matrices
  Hilbert-Schmidt inner product $\langle a, b \rangle = \mathrm{tr}(a^* b)$
  partial order $a \preceq b$ or $b \succeq a$ means that $b - a$ is positive semi-definite
- hermitian matrices $A = \{a \in \mathcal{A} : a^* = a\}$
  energy operators/Hamiltonians
- projection lattice $\mathcal{P}(\mathcal{A}) = \{p \in \mathcal{A} : p^2 = p^* = p\}$
  partially ordered by $\preceq$
- smallest eigenvalue $\lambda_0(a)$ of $a \in A$ ground state energy
- spectral projection $p_0(a) \in \mathcal{P}(\mathcal{A})$ onto eigenspace of $a \in A$
  corresponding to $\lambda_0(a)$ ground space projection

I) Motivation: Many-Body Physics

- $\mathcal{A} = \mathcal{B}^{\otimes N}$, N-fold tensor product of *-algebra $\mathcal{B}$
- a k-local Hamiltonian is a sum of terms $a_1 \otimes \cdots \otimes a_N \in A$ each summand having at most k non-scalar factors a_i
- vector space of k-local Hamiltonians $A_{(k)} \subset A$

Local Hamiltonian Problem
(condensed matter physics, quantum chemistry)

- given $a \in A_{(k)}$ and $(\xi - \eta) \propto 1/\mathrm{poly}(N)$, determine whether $\lambda_0(a) > \xi$ or $\lambda_0(a) < \eta$
- hard problem even on a quantum computer
(Zeng, Chen, Zhou, Wen `arXiv:1508.02595`)

II) Geometric Approach to Ground State Energy

- state space $\mathcal{M} = \{\rho \in \mathcal{A} : \rho \succeq 0, \mathrm{tr}(\rho) = 1\}$ of $\mathcal{A}$, set of mixed states or density matrices (convex compact set)

- linear subspace $U \subset A$,
  orthogonal projection $\pi : A \to A$ onto U

- $\lambda_0(u) = \min_{\rho \in \mathcal{M}} \langle \rho, u \rangle = \min_{a \in \pi(\mathcal{M})} \langle a, u \rangle$ for $u \in U$

$\lambda_0|_U$ is the support function of $\pi(\mathcal{M})$, that is the signed distance of the origin from supporting hyperplanes of $\pi(\mathcal{M})$

- $\pi(\mathcal{M}) \cong$ joint algebraic numerical range
  $\cong$ numerical range of $K + \mathrm{i}\, L$ if $\mathrm{span}(K, L, \mathbb{1}) = \mathrm{span}(U, \mathbb{1})$

- if $U = A_{(k)}$ is the space of k-local Hamiltonians,
  then $\pi(\mathcal{M}) \cong$ convex set of k-body marginals

III) Exposed Faces and Ground Space Projections

- Euclidean space A, convex subset $C \subset A$, linear subspace $U \subset A$, orthogonal projection $\pi : A \to A$ onto U

- an exposed face of C is either $\emptyset$ or a subset of the form $F_C(u) = \mathrm{argmin}_{x \in C} \langle x, u \rangle$ for some $u \in A$

- set of exposed faces $\mathcal{E}(C)$
  ordered by inclusion, $\mathcal{E}(C)$ is a complete lattice, infimum = intersection

Algebraic setting

- $\mathcal{P}(\mathcal{A}) \cong \mathcal{E}(\mathcal{M})$ (Kadison)
  isomorphism $\phi : \mathcal{P}(\mathcal{A}) \to \mathcal{E}(\mathcal{M})$
  $\phi(p) = \{\rho \in \mathcal{M} : s(\rho) \preceq p\}$ with support projection $s(\rho)$ of ρ

- ground space projections $\mathcal{P}(U) = \{p_0(u) : u \in U\} \cup \{0\}$

- $\mathcal{P}(U) \cong \mathcal{L}(U) \cong \mathcal{E}(\pi(\mathcal{M}))$
  lifted faces $\mathcal{L}(U) = \pi|_{\mathcal{M}}^{-1}(\mathcal{E}(\pi(\mathcal{M}))) \subset \mathcal{E}(\mathcal{M})$
  isomorphism $\pi \circ \phi : \mathcal{P}(U) \to \mathcal{E}(\pi(\mathcal{M}))$

IV) Variation Principle

positive cone $A^+ = \{a \in \mathcal{A} : a \succeq 0\}$,
complementary projection $p' = \mathbb{1} - p$ of $p \in \mathcal{P}(\mathcal{A})$

Definition. For $p \in \mathcal{P}(\mathcal{A})$ we define the pointed cone
$K(p) = p' A^+ p' \cap U = \{u \in U : p_0(u) \succeq p, u \succeq 0\}$

Theorem 1. (W. `arXiv:1704.07675 [math-ph]`)
Let $\mathbb{1} \in U$ and $p \in \mathcal{P}(\mathcal{A})$. Then $p \in \mathcal{P}(U)$ if and only if
$p = \bigvee\{q \in \mathcal{P}(\mathcal{A}) : K(q) = K(p)\}$.

Proof. use lattice isomorphisms (overleaf) + the expression
$N_{\mathcal{M}}(\rho) = \{u \in A : s(\rho) \preceq p_0(u)\} = \mathbb{1}\mathbb{R} + s(\rho)' A^+ s(\rho)'$
for the normal cone $N_{\mathcal{M}}(\rho)$ of the state space $\mathcal{M}$ at $\rho \in \mathcal{M}$ $\square$

Proof of Variation Principle: Normal Cones

- lifted faces $\mathcal{L} = \mathcal{L}(U) = \pi|_C^{-1}(\mathcal{E}(\pi(C))) \subset \mathcal{E}(C)$
- closure operation $\mathrm{cl}_\mathcal{L} : 2^C \to \mathcal{L}$, $X \mapsto \bigcap\{F \in \mathcal{L} : X \subset F\}$

Lemma. Let $X \subset C$. Then $X \in \mathcal{L}$ if and only if $X = \bigvee\{G \in \mathcal{E}(C) : \mathrm{cl}_\mathcal{L}(G) = \mathrm{cl}_\mathcal{L}(X)\}$.

- normal cone $N_C(x) = \{u \in A : \langle y - x, u \rangle \geq 0\}$ of C at x

Theorem. Let $|\pi(C)| > 1$ and $X \subset C$ convex. Then $X \in \mathcal{L}$ iff $X = \bigvee\{G \in \mathcal{E}(C) : N_C(G) \cap U = N_C(X) \cap U\}$.

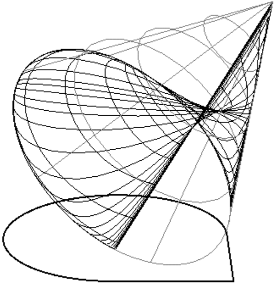
Proof. lattice isomorphisms $\mathcal{L} \cong \mathcal{E}(\pi(C)) \cong \{\text{normal cones of } \pi(C)\}$,
for convex $X \subset C$ the normal cone is $N_{\pi(C)}(\pi(X)) = N_C(X) \cap U$ □

V) Examples of Bizarre Topology of $\mathcal{P}(U)$

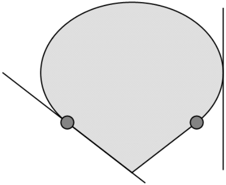
real *-algebra $\mathcal{A} = \mathrm{span}\{\sigma_1 \oplus 0, \sigma_2 \oplus 0, \mathrm{i}\,\sigma_3 \oplus 0, 0 \oplus 1\}$,
Pauli matrices $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$,
and curve of pure states $\rho_\alpha = \frac{1}{2}(\mathbb{1} + \sin(\alpha)\sigma_1 + \cos(\alpha)\sigma_2)$

(W. and Knauf JMP '12)

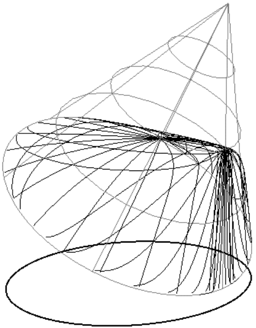
Example a) $U = \mathrm{span}\{\sigma_1 \oplus 1, \sigma_2 \oplus 1\}$
$\mathcal{P}(U) = \{\rho_\alpha \oplus 0 : \alpha \in]\frac{\pi}{2}, 2\pi[\,\} \cup \{\rho_0 \oplus 1, 0 \oplus 1, \rho_{\pi/2} \oplus 1\}$



the missing closure points $\rho_0 \oplus 0$ and $\rho_{\pi/2} \oplus 0$ of $\mathcal{P}(U)$ correspond to non-exposed points of $\pi(\mathcal{M})$



Example b) $U = \text{span}\{\sigma_1 \oplus 0, \sigma_2 \oplus 1\}$
$\mathcal{P}(U) = \{\rho_\alpha \oplus 0 : \alpha \in]0, 2\pi[\,\} \cup \{\rho_0 \oplus 1\}$



the missing closure point $\rho_0 \oplus 0$ of $\mathcal{P}(U)$ causes a discontinuity of the maximum-entropy inference map

$$\rho^* : \pi(\mathcal{M}) \to \mathcal{M}, x \mapsto \underset{\rho \in \mathcal{M}, \pi(\rho) = x}{\text{argmax}} \; S(\rho)$$

where $S(\rho) = -\operatorname{tr} \rho \log(\rho)$ is the von Neumann entropy

discontinuities of ρ^* were studied in operator theory
(Rodman, Spitkovsky, Szkoła, W. JMP '16)
and physics in the context of quantum phase transitions
(Chen, Ji, Li, Poon, Shen, Yu, Zeng, Zhou New J. Phys. '15)

VI) Coatoms

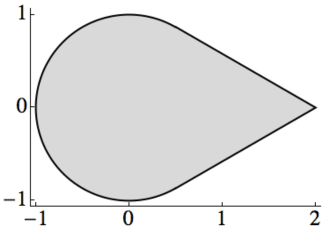
- a coatom of $\mathcal{P}(U)$ is a maximal element of $\mathcal{P}(U) \setminus \{\mathbb{1}\}$
- $\mathcal{P}(U)$ is coatomistic, that is all elements are infima of coatoms (W. `arXiv:1606.03792 [math.MG]`, W. JCA '12)

Theorem 2. Let $\mathbb{1} \in U$, $|\pi(\mathcal{M})| > 1$, and $p \in \mathcal{P}(U)$. Then p is a coatom of $\mathcal{P}(U)$ if and only if $K(p)$ is a ray.

Notice: $\mathcal{P}(U) \cong \mathcal{E}(\pi(\mathcal{M}))$ may not be atomistic!

Example: numerical range of $K + \mathrm{i}\, L$ for

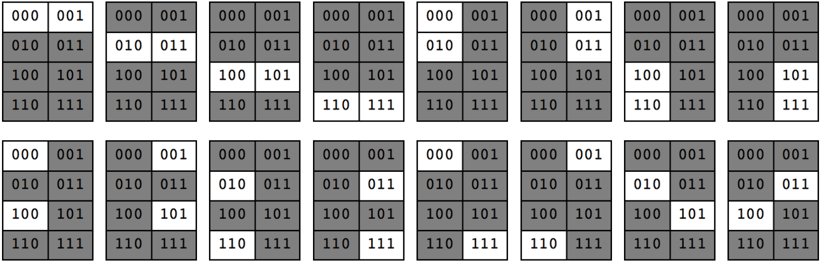
$$K = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & -\mathrm{i} & 0 \\ \mathrm{i} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



VII) Example 2-local 3-bit Hamiltonians

- (commutative) three-bit algebra $\mathcal{A} = (\mathbb{C}^2)^{\otimes 3} \cong \{X \to \mathbb{C}\}$ with 3-bit configuration space $X = \{0,1\} \times \{0,1\} \times \{0,1\}$

- the coatoms of $\mathcal{P}(A_{(2)})$ are easily computable from Theorems 1 and 2, they are



- the lattice $\mathcal{P}(A_{(2)})$ is visualizable on the complete bipartite graph $K_{4,4}$

Open Problems

- find a direct algebraic proof of Theorem 1
- compute the coatoms of $\mathcal{P}(A_{(2)})$ for the (non-commutative) three-qubit algebra $\mathcal{A} = M_2 \otimes M_2 \otimes M_2$
- compute the closure of the lattice $\mathcal{P}(A_{(2)})$ for $\mathcal{A} = M_2 \otimes M_2 \otimes M_2$

  $\mathcal{P}(A_{(2)})$ is not closed (in the norm topology) for $\mathcal{A} = M_2 \otimes M_2 \otimes M_2$, see Example 8.1 of Rodman, Spitkovsky, Szkoła, W. JMP ’16

Thank you for the attention