A Variation Principle for Ground Spaces

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Notation

- $\mathcal{A} \subset M_n$ *-subalgebra, inner product $\langle a, b \rangle = \mathrm{tr}(a^* b)$
- hermitian matrices $A = \{a \in \mathcal{A} : a^* = a\}$
  (energy operators/Hamiltonians)
- projection lattice $\mathcal{P}(\mathcal{A}) = \{p \in \mathcal{A} : p^2 = p^* = p\}$
- smallest eigenvalue $\lambda_0(a)$ of $a \in A$ (ground state energy)
- 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 Systems

- $\mathcal{A} = \mathcal{B}^{\otimes N}$, n-fold tensor product of $\mathcal{B}$
- 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 tensor factors
- 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 (see for example the book by Zeng et al. `arXiv:1508.02595`)

ground state problems have a natural geometry

- state space $C_{\mathcal{A}} = \{\rho \in \mathcal{A} : \rho \succeq 0, \mathrm{tr}(\rho) = 1\}$ of $\mathcal{A}$
  $a \preceq b$ or $b \succeq a$ means that $b - a$ is positive semi-definite ($a, b \in \mathcal{A}$)
- projection $\pi : A \to A$ onto $A_{(k)}$
- for $a \in A_{(k)}$: $\lambda_0(a) = \min_{\rho \in C_{\mathcal{A}}} \langle \rho, a \rangle = \min_{b \in \pi(C_{\mathcal{A}})} \langle b, a \rangle$

GOAL: study geometry of $\pi(C_{\mathcal{A}})$ (set of k-body marginals)

- this problem is closely related to study the lattice of ground space projections $\mathcal{P}(A_{(k)}) = \{p_0(u) : u \in A_{(k)}\} \cup \{0\}$

II) Exposed Faces

- convex subset $C \subset A$ (Euclidean space), subspace $U \subset A$, $\pi : A \to A$ projection onto U
- an exposed face of C is either $\emptyset$ or a subset of the form $F_C(u) = \operatorname{argmin}_{x \in C} \langle x, u \rangle$ for some $u \in A$
- lattice of exposed faces $\mathcal{E}(C)$ (ordered by inclusion) is a complete lattice with infimum equal intersection
- lifted faces $\mathcal{L} = \pi|_C^{-1}(\mathcal{E}(\pi(C))) \subset \mathcal{E}(C)$
- 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 $X = \bigvee\{G \in \mathcal{E}(C) : \mathrm{cl}_{\mathcal{L}}(G) = \mathrm{cl}_{\mathcal{L}}(X)\}$.

III) Normal Cones

- (inner) normal cone $N_C(x) = \{u \in A : \langle y - x, u\rangle \geq 0\}$ of C at $x \in C$
- $N_C(\emptyset) = A$ and $N_C(X) = N_C(x)$ for a non-empty convex subset $X \subset C$ with relative interior point x

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

Pf. lattice isomorphisms $\mathcal{E}(\pi(C)) \cong \mathcal{L}$, $\mathcal{E}(\pi(C)) \cong \{$normal cones of $\pi(C)\}$, and normal cones $N_{\pi(C)}(\pi(X)) = N_C(X) \cap U$ $\square$

IV) Ground Space Projections

- exposed faces of $C_{\mathcal{A}} \cong$ projections of $\mathcal{A}$ (Kadison)

  Pf. use $\phi(p) = \{\rho \in C_{\mathcal{A}} : s(\rho) \preceq p\}$ with $s(\rho)$ support projection of ρ $\square$

- vector space of hermitian matrices $U \subset A \subset \mathcal{A}$, lattice of ground space projections $\mathcal{P}(U) = p_0(U) \cup \{0\}$

- positive cone $A^+ = \{a \in \mathcal{A} : a \succeq 0\}$, we define for $p \in \mathcal{P}(\mathcal{A})$ and $p' = \mathbb{1} - p$ the cone

$$K(p) = p' A^+ p' \cap U = \{u \in U : p_0(u) \succeq p, u \succeq 0\}$$

Theorem 2. Let $\mathbb{1} \in U$ and $p \in \mathcal{P}(\mathcal{A})$. Then $p \in \mathcal{P}(U)$ if and only if $p = \bigvee\{q \in \mathcal{P}(\mathcal{A}) : K(q) = K(p)\}$.

Pf. $\mathcal{P}(U) = \phi^{-1}(\mathcal{L})$, $N_{C_{\mathcal{A}}}(\rho) = \{u \in A : s(\rho) \preceq p_0(u)\} = \mathbb{1}\mathbb{R} + s(\rho)' A^+ s(\rho)'$ $\square$

V) Coatoms of the Lattice of Ground Space Projections

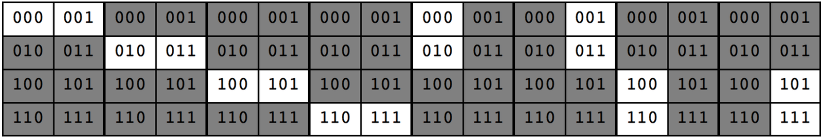
- a coatom of $\mathcal{P}(U)$ is a maximal element of $\mathcal{P}(U) \setminus \{\mathbb{1}\}$
- $\mathcal{P}(U)$ is coatomistic, that is every element is an infimum of coatoms (`arXiv:1606.03792 [math.MG]`, also W. 2012)

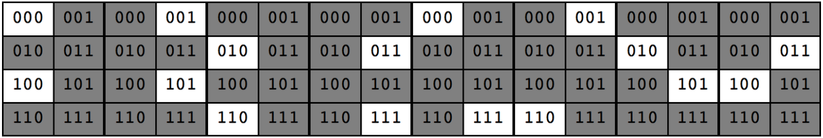
  Pf. $\mathcal{P}(U) \cong \mathcal{E}(\pi(C_{\mathcal{A}}))$, the polar of $\pi(C_{\mathcal{A}})$ is a spectrahedron, its exposed face lattice is atomistic by Minkowski's theorem $\square$

Theorem 3. Let $\mathbb{1} \in U$, $|\pi(C_{\mathcal{A}})| > 1$, and $p \in \mathcal{P}(U)$. Then p is a coatom of $\mathcal{P}(U)$ if and only if $K(p)$ is a ray.

VI) 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 2 and 3, here they are





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

Open Problems

- (non-commutative) three-qubit algebra
  $\mathcal{A} = M_2 \otimes M_2 \otimes M_2 \cong M_8$
- can you compute the coatoms of $\mathcal{P}(A_{(2)})$ for the three-qubit algebra?
- the lattice $\mathcal{P}(A_{(2)})$ is not closed (in the norm topology), see Example 8.1 of Rodman, Spitkovsky, Szkoła, W. (2016)
- can you compute the closure of $\mathcal{P}(A_{(2)})$ for the three-qubit algebra?

Thank you for the attention

General refrence `arXiv:1704.07675 [math-ph]`