On Lattices of Ground Spaces

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49 Symposium on Mathematical Physics
Toruń, Poland
June 17–18, 2017

Notation

- *-subalgebra $\mathcal{A}$ of M_n, the complex n-by-n matrices
  Hilbert-Schmidt inner product $\langle a, b \rangle = \operatorname{tr}(a^* b)$
  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
- 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 $\mathcal{B}$
- 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 Meaning of 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 $U \subset A$, projection $\pi : A \to A$ onto U

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

$\lambda_0|_U$ 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

- 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

- 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 $F_C(u) = \text{argmin}_{x \in C} \langle x, u \rangle$ for some $u \in A$
- set of exposed faces $\mathcal{E}(C)$, ordered by inclusion, is a complete lattice whose infimum is the intersection
- $\mathcal{E}(\mathcal{M}) \cong \mathcal{P}(\mathcal{A})$ (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 $\mathcal{P}(U) = \{p_0(u) : u \in U\} \cup \{0\}$
- $\mathcal{E}(\pi(\mathcal{M})) \cong \mathcal{P}(U)$
  isomorphism $\pi \circ \phi : \mathcal{P}(U) \to \mathcal{E}(\pi(\mathcal{M}))$

IV) The Bizarre Topology of $\mathcal{P}(U)$

$\mathcal{P}(U) = \{\lim_{\beta\to\infty} \frac{e^{-\beta u}}{\mathrm{tr}(e^{-\beta u})} : u \in U\} \cup \{0\}$ is not closed!

- despite the bizarre topology of $\mathcal{P}(U)$, information geometry extends from states of full support to non-maximal support

Information Geometry. (full support: Petz, Nagaoka 90's)

Gibbs family $\mathcal{F} = \{\frac{e^{u}}{\mathrm{tr}(e^{u})} : u \in U\}$

if $\rho, \sigma, \tau \in \mathcal{M}$, $\sigma, \tau \in \mathcal{F}$ and $(\rho - \sigma) \perp U$, then

- $S(\rho,\tau) = S(\rho,\sigma) + S(\sigma,\tau)$ Pythagorean Theorem
- $S(\rho,\sigma) < S(\rho,\tau)$ if $\sigma \neq \tau$ Projection Theorem

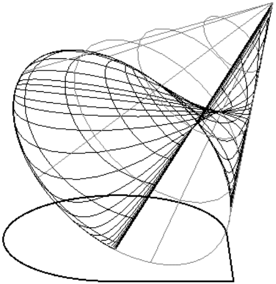
with relative entropy $S(\rho,\sigma) = \mathrm{tr}\,\rho(\log(\rho) - \log(\sigma))$

- extend $\mathcal{F}$ by limits $\lim_{\beta\to\infty} \frac{e^{u-\beta v}}{\mathrm{tr}(e^{u-\beta v})}$ $u, v \in U$, and certain other limit points of $\mathcal{F}$ (W. and Knauf JMP '12, W. JCA '14)

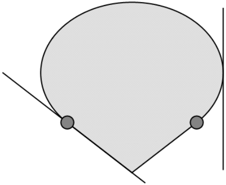
Examples. $\mathcal{A} = \text{span}\{\sigma_1 \oplus 0, \sigma_2 \oplus 0, \mathrm{i}\,\sigma_3 \oplus 0, 0 \oplus 1\}$ real *-algebra, $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}$, $\sigma_3 = \begin{pmatrix}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

a) $U = \text{span}\{\sigma_1 \oplus 1, \sigma_2 \oplus 1\}$

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

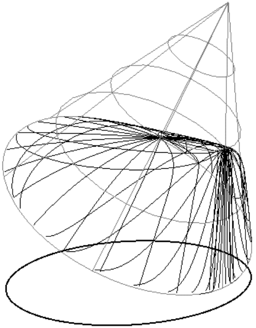


the missing closure points $\rho_0 \oplus 0$ and $\rho_{\pi/2} \oplus 0$ correspond to non-exposed points of $\pi(\mathcal{M})$



b) $U = \mathrm{span}\{\sigma_1 \oplus 0, \sigma_2 \oplus 1\}$

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



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

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

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

notice that $\mathcal{F} \subset \mathrm{image}(\rho^*)$

discontinuities of ρ^* for k-local Hamiltonians $U = A_{(k)}$ were discussed in the context of quantum phase transitions (Chen, Ji, Li, Poon, Shen, Yu, Zeng, Zhou New J. Phys. '15)

V) Sufficient Condition for Discontinuity of ρ^*

face function $F : \pi(\mathcal{M}) \to 2^{\pi(\mathcal{M})}$,
$x \mapsto \bigcup\{\text{segment } s \subset \pi(\mathcal{M}) : x \in \text{relative interior of } s\}$

Theorem 1. (Rodman, Spitkovsky, Szkoła, W. JMP '16)
If $(x_i) \subset \pi(\mathcal{M})$ converges to x and $\rho^*(x) = \lim_{i\to\infty} \rho^*(x_i)$, then $\dim\ F(x) \leq \liminf_{i\in\mathbb{N}} \dim\ F(x_i)$.

Example a) $H_\epsilon = -K - \epsilon L$ for $K = \mathbb{1} \otimes \sigma_3 \otimes \sigma_3 +$ cycl. perm. and $L = \sigma_1 \otimes \mathbb{1} \otimes \mathbb{1} +$ cycl. perm.

- for small $\epsilon > 0$ the ground space projection $p_0(H_\epsilon)$ has rank one, so $\pi(p_0(H_\epsilon))$ is an exposed point of $\pi(\mathcal{M})$
- $\lim_{\epsilon \searrow 0} p_0(H_\epsilon) = |GHZ\rangle\langle GHZ|$ and $\pi(|GHZ\rangle\langle GHZ|)$ is the midpoint of the segment $\pi(\{\rho \in \mathcal{M} : s(\rho) \preceq |000\rangle\langle 000| + |111\rangle\langle 111|\})$

Theorem 1 $\implies$ ρ^* has no continuous extension from $\pi(p_0(H_\epsilon))_{\epsilon>0}$ to $\epsilon = 0$

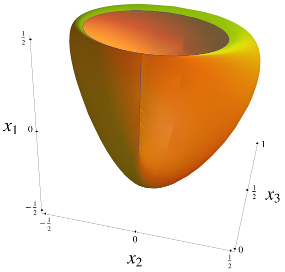
- unless it is unitarily equivalent to $\alpha|000\rangle + \beta|111\rangle$, $|\psi\rangle \in (\mathbb{C}^2)^{\otimes 3}$ is uniquely determined by its 2-body marginals (Linden, Popescu, Wootters PRL '02), so ρ^* is continuous at $\pi(|\psi\rangle\langle\psi|)$

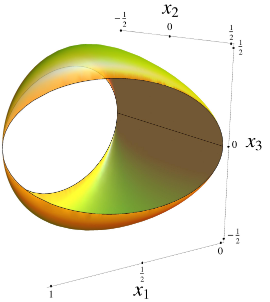
Example b) Joint algebraic numerical range of $A_1, A_2, A_3 \in M_3$

$$W(A_1, A_2, A_3) = \{(\langle \rho, A_1 \rangle, \langle \rho, A_2 \rangle, \langle \rho, A_3 \rangle) : \rho \in \mathcal{M}\}$$

$W(A_1, A_2, A_3) \cong \pi(\mathcal{M})$ for $U = \mathrm{span}\{A_1, A_2, A_3\}$

$A_1 = \frac{1}{2}\begin{pmatrix} 1&0&0\\0&0&1\\0&1&0 \end{pmatrix}, A_2 = \frac{1}{2}\begin{pmatrix} 0&0&1\\0&0&0\\1&0&0 \end{pmatrix}, A_3 = \begin{pmatrix} 0&0&0\\0&0&0\\0&0&1 \end{pmatrix}; \; A_1 = \begin{pmatrix} 0&0&0\\0&0&0\\0&0&1 \end{pmatrix}, A_2 = \frac{1}{2}\begin{pmatrix} 0&1&0\\1&0&0\\0&0&0 \end{pmatrix}, A_3 = \frac{1}{2}\begin{pmatrix} 0&0&1\\0&0&0\\1&0&0 \end{pmatrix}$





(Szymański, W., Życzkowski arXiv:1603.06569 [math.FA])

VI) Variation Principle

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

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

an analysis of normal cones of $\pi(\mathcal{M})$ yields

Theorem 2. (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 $p = \bigvee\{q \in \mathcal{P}(\mathcal{A}) : K(q) = K(p)\}$.

VII) Coatoms

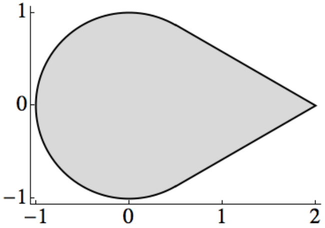
- a coatom of $\mathcal{P}(U)$ is a maximal element of $\mathcal{P}(U) \setminus \{\mathbb{1}\}$
- $\mathcal{P}(U)$ is coatomistic, every element of $\mathcal{P}(U)$ is an infimum of coatoms (W. `arXiv:1606.03792 [math.MG]`, W. JCA '12)

Theorem 3. 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: $\mathcal{P}(U) \cong \mathcal{E}(\pi(\mathcal{M}))$ is not atomistic!

Example: numerical range $\{(\langle \rho, A_1 \rangle, \langle \rho, A_2 \rangle) : \rho \in \mathcal{M}\}$ of

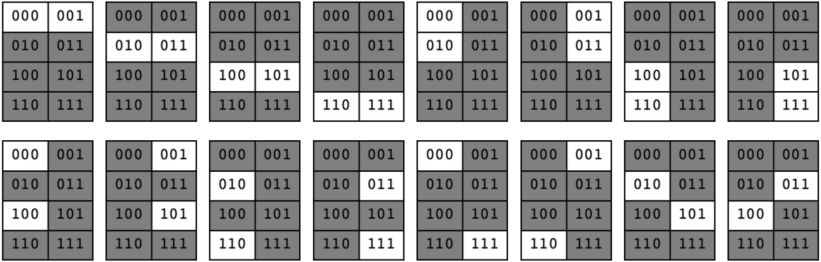
$$A_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$



VIII) 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, 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 $M_2 \otimes M_2 \otimes M_2 \cong M_8$

- can you compute the coatoms of $\mathcal{P}(A_{(2)})$ if $\mathcal{A}$ is the three-qubit algebra?
- the lattice $\mathcal{P}(A_{(2)})$ is not closed in the norm topology if $\mathcal{A}$ is the three-qubit algebra (Example 8.1 of Rodman, Spitkovsky, Szkoła, W. JMP '16)
- can you compute the closure of $\mathcal{P}(A_{(2)})$ if $\mathcal{A}$ is the three-qubit algebra?

Thank you for the attention