A new signature of quantum phase transitions from the numerical range

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speaker Stephan Weis

Centre for Quantum Information and Communication

Université libre de Bruxelles, Belgium

joint work with Ilya M. Spitkovsky

New York University Abu Dhabi, United Arab Emirates

Abstract

Predicting quantum phase transitions by signatures in finite models has a long tradition. Here we consider the numerical range W of a finite dimensional one-parameter Hamiltonian, which is a planar projection of the convex set of density matrices. We propose the new geometrical signature of non-analytic points of class C^2 on the boundary of W. We prove that a discontinuity of a maximum-entropy inference map occurs at these points, a pattern which was earlier fostered as a signature of quantum phase transitions. More precisely, we reduce both phenomena to higher energy level crossings with the ground state energy.

Reference: `arXiv:1703.00201 [math-ph]`

These slides are identical to those presented at the ILAS 2017 workshop. Additional whiteboard drawings were sketched during the talk at ILAS 2017.

Overview

1. energy operators and quantum phase transitions
2. numerical range W, boundary ∂W as an envelope
3. boundary ∂W as a manifold, smoothness of ∂W
4. maximum-entropy inference
5. conclusion

1. energy operators and quantum phase transitions

- one-parameter Hamiltonian $H(g) = H_0 + g \cdot H_1$
  ground state energy of $H(g)$ = smallest eigenvalue of $H(g)$
  arbitrary hermitian d-by-d matrices $H_0, H_1 \in M_d$

- statistical mechanics: often $M_d = \bigotimes_{i \in \Lambda} M_2$, qubits on a lattice Λ with next-neighbour interactions $H(g)$

- quantum phase transition: ground state phenomenon of $H(g)$ in the thermodynamic limit $|\Lambda| \to \infty$ (see e.g. Sachdev)
  - non-analyticity of the ground state energy
  - energy level crossings with the ground state energy
  - long-range correlations of the ground state

finite systems $|\Lambda| < \infty$ signal a quantum phase transition

in the focus of this talk: differentiability order of ground state energy, and

1. geometry of projections of the set of density matrices
   $\mathcal{M}_d = \{\rho \in M_d \mid \rho \succeq 0, \mathrm{tr}(\rho) = 1\}$
2. strong variation / discontinuity of inference maps

references about quantum phase transitions in this context

1. 3D projections of $\mathcal{M}_d$ (also separable) and ruled surfaces:
   Zauner, Draxler, Vanderstraeten, Haegeman, Verstraete (2016)
   Chen, Guo, Ji, Poon, Yu, Zeng, Zhou, (2017)
2. strong variation / discontinuity of inference maps:
   Arrachea, Canosa, Plastino, Portesi, Rossignoli (1992)
   Chen, Ji, Li, Poon, Shen, Yu, Zeng, Zhou (2015)

we study

- 2D projections W of $\mathcal{M}_d$ and non-analytic boundary points
- discontinuity of the maximum-entropy inference map $W \to \mathcal{M}_d$,
  studied earlier by W., Knauf (2012)

notation

$$\mathrm{Re}(X) = \tfrac{1}{2}(X + X^*), \quad \mathrm{Im}(X) = \tfrac{1}{2\,\mathrm{i}}(X - X^*), \quad X \in M_d$$

$$A(\theta) = \cos(\theta) H_0 + \sin(\theta) H_1 = \mathrm{Re}(e^{-\mathrm{i}\,\theta} A), \quad A = H_0 + \mathrm{i}\, H_1$$

$\lambda(\theta) =$ smallest eigenvalue of $A(\theta)$, *ground state energy*

$$H(g) = H_0 + g \cdot H_1 = \sqrt{1 + g^2} \cdot A(\theta), \quad \theta = \arctan(g)$$

the maximal order of differentiability of the ground state energy of H at $g \in \mathbb{R}$ equals that of λ at $\arctan(g)$

$\Longrightarrow$ study $\lambda(\theta)$ instead of the ground state energy of $H(g)$

2. numerical range and its boundary as an envelope

numerical range $W = W(A) = \{\langle x|Ax\rangle \mid x \in \mathbb{C}^d, \langle x|x\rangle = 1\}$

compact, convex subset of $\mathbb{C}$ (Hausdorff, Toeplitz)

support function $h_W(u) = \min_{z\in W}\langle z, u\rangle, \quad u \in \mathbb{C}$

distance of supporting lines from origin, scalar product $\langle a, b\rangle = \mathrm{Re}\langle a|b\rangle$

Lemma. $\lambda(\theta) = h_W(e^{\mathrm{i}\,\theta}), \quad \theta \in \mathbb{R}$

Proof. let $x, y \in \mathbb{C}^d$ be unit vectors. if x is a ground state, i.e. $A(\theta)x = \lambda(\theta)x$, then $\lambda(\theta) = \langle x|A(\theta)x\rangle \leq \langle y|A(\theta)y\rangle = \langle y|\,\mathrm{Re}(e^{-\mathrm{i}\,\theta}A)y\rangle = \mathrm{Re}\langle e^{\mathrm{i}\,\theta}|\langle y|Ay\rangle\rangle = \langle e^{\mathrm{i}\,\theta}, \langle y|Ay\rangle\rangle$. now minimize over y. □

geometric meaning of ground state energy

$\lambda(\theta)$ is the signed distance of the origin from supporting lines of W

smoothness assumptions

let ∂W be a C^2-manifold of $\mathbb{C}$. the *Gauß map* sends $z \in \partial W$ to the inner unit normal vector of W at z,

Gauß map $\quad u_W : \partial W \to S^1$

we assume further that u_W is a C^1-diffeomorphism.
then the inverse $x_W = u_W^{-1}$ exists,

reverse Gauß map $\quad x_W : S^1 \to \partial W$

- W is strictly convex since the domain of x_W is S^2
- reverse Gauß map x_W parametrizes ∂W as the envelope of the supporting lines of W
  (the tangent of ∂W at z is the supporting line of W at z)

these smoothness assumptions are not restrictive (discussion follows)

exploring the reverse Gauß map

Lemma. reverse Gauß map = gradient of support function

$$x_W(u) = \nabla h_W(u),\ u \in S^1$$

Proof. this is a general property of convex bodies. let $u, v \in \mathbb{C}$.

- $\langle \nabla h_W(u), u \rangle = h_W(u)$ since h_W is homogeneous (Euler's theorem)
- $\langle \nabla h_W(u), v \rangle \geq h_W(v)$ since $-h_W$ is sublinear $\square$

Problem: x_W is a suboptimal parametrization of ∂W

λ is C^k at $\theta \iff \partial W$ is a C^k manifold at $x_W(e^{i\theta})$ (proof sketch follows)

but $x_W : S^1 \to \partial W$ is only of order C^{k-1} at $e^{i\theta}$

- x_W and λ are related by $x_W(e^{i\theta}) = \nabla h_W(e^{i\theta}) = e^{i\theta}(\lambda(\theta) + i\,\lambda'(\theta))$
- differential geometry of ∂W was studied by Gutkin, Jonckheere, Karow (2004)
- we relate finite maximal orders of differentiability of ∂W and λ

3. numerical range and its boundary as a manifold

Solution: maximal orders of differentiability of ∂W and λ match through the dual convex body

dual convex body $W^* = \{u \in \mathbb{C} \mid 1 + \langle u, z\rangle \geq 0, \forall z \in W\}$

radial function $r_{W^*}(u) = \max\{r \geq 0 \mid r \cdot u \in W^*\} = -1/h_W(u)$

Proof sketch of solution.

Schneider, *Convex Bodies: The Brunn-Minkowski Theory*, 2014

a) let 0 be an inner point of W and W^* and let h_W be C^k,

then $S^1 \to \partial W^*$, $u \mapsto u \cdot r_{W^*}(u)$ is a C^k-parametrization of ∂W^*,

$\implies \partial W^*$ is a C^k manifold

b) ∂W^* is a C^k-manifold $\implies h_{W^*}$ is C^k

c) replace W with W^* and repeat a) and b)

$\implies \partial W$ at $x_W(e^{\mathrm{i}\,\theta})$ and λ at θ have the same order of differentiability

smoothness of ∂W

Lemma. ∂W is a C^2-manifold and u_W a diffeomorphism,
up to finitely many points / segments

- radius of curvature of ∂W at $z \in \partial W$

  $\rho(z) = \liminf_{\xi \to 0} \frac{\xi^2}{2f(\xi)}$, where $(\xi, f(\xi))$ parametrizes ∂W from a supporting line of ∂W at z

  if $\rho(z) = 0$ then z is a corner point of W and an intersection of two segments in ∂W

  (Farid '95, Salinas and Velasco '01, Spitkovsky 2000, Hansmann 2015)

- if z is a non-exposed point, then ∂W is a C^1-manifold at z
- if z is in the relative interior of a boundary segment of W, then ∂W is an analytic manifold at z

otherwise $z = x_W(e^{i\theta})$ and ∂W is a C^2-manifold at z
with finite $\rho(z) = -\lambda(\theta) - \lambda''(\theta) > 0$ and $(\mathrm{d}x_W)_{e^{i\theta}}(i\, e^{i\theta}) = -i\, e^{i\theta}\rho(z) \neq 0$

correspondence of maximal orders of differentiability

Lemma. let ∂W be a C^2-manifold at $z = x_W(e^{i\theta})$ and u_W a diffeomorphism at z.

a) ∂W is analytic at $z \iff \lambda$ is analytic at θ.

b) in case of non-analyticity,

the maximal order of differentiability of ∂W at z

is the maximal order of differentiability of λ at θ

three cases:

1. λ analytic at θ, no crossing
2. λ analytic at θ, with crossing
3. λ non-analytic at θ, with crossing, and the maximal order of differentiability of λ at θ for even ≥ 2

4. maximum-entropy inference

- *state space* $\mathcal{M}_d = \{\rho \in M_d \mid \rho \succeq 0, \mathrm{tr}(\rho) = 1\}$
- *von Neumann entropy* $S(\rho) = -\mathrm{tr}\,\rho \log(\rho)$
  (measure of disorder)
- recall that $W = W(A) = \{\mathrm{tr}(\rho A) \mid \rho \in \mathcal{M}_d\}$
- define maximum-entropy inference map
  $\rho^* : W \to \mathcal{M}_d$, $z \mapsto \mathrm{argmax}\{S(\rho) \mid \mathrm{tr}(\rho A) = z\}$

Lemma (Continuity analysis I). the map ρ^* is continuous at $z \in W$ if z is an interior point of W, a corner point of W, or a relative interior point of a boundary segment of W

Continuity analysis at round points

- the following lemma applies to non-exposed points z of W, by replacing derivatives of λ with directional derivatives
- there are analytic curves $x_k : \mathbb{R} \to \mathbb{R}^d$, and $\lambda_k : \mathbb{R} \to \mathbb{R}$, $k = 1, \ldots, d$, such that for all $\theta \in \mathbb{R}$ we have $A(\theta)x_k(\theta) = \lambda_k(\theta)x_k(\theta)$ and $\{x_k(\theta)\}_k$ is an orthogonal basis of $\mathbb{C}^d$, Rellich (1954)

Lemma (Continuity analysis II).

let ∂W is a C^2-manifold at $z = x_W(e^{\mathrm{i}\,\theta})$. then

$$\rho^*(z) = \tfrac{1}{N(\theta)} \sum |x_k(\theta)\rangle\langle x_k(\theta)|,$$

summation over $k \in I(\theta) := \{\, \ell \mid \lambda_\ell(\theta) = \lambda(\theta), \lambda'_\ell(\theta) = \lambda'(\theta)\,\}$

and ρ^* is continuous at z iff the functions $(\lambda_k)_{k \in I(\theta)}$ are mutually equal (proof: u_W is a diffeomorphism at z)

5. conclusion

if ∂W is localy at z a non-analytic C^2-manifold,
then ρ^* is discontinuous at z

remarks

- non-analytic C^2 points of ∂W indicate some but not all discontinuities of ρ^*

- let ∂W be locally at $z = x_W(e^{\mathrm{i}\,\theta})$ a C^2-manifold.
  then ∂W is analytic at z if and only if there is a function λ_k such that $\lambda_k = \lambda$ locally at θ

  $\Longrightarrow$ the non-analytic C^2 points of ∂W are the points where the inverse numerical range map fails to be weakly continuous,
  Leake, Lins, Spitkovsky (2014)

questions

1) 3D projections.

which boundary configurations of a 3D projection of $\mathcal{M}_d$ generate a non-analytic C^2 point on the boundary of a 2D projection ?

2) separable numerical range.

Puchała, Miszczak, Gawron, Dunkl, Holbrook, Życzkowski (2012)

$$\operatorname{conv}\{\operatorname{tr}(A\rho\otimes\sigma)\mid \rho,\sigma\in\mathcal{M}_2\},\qquad A\in M_4$$

study differential and algebraic geometry of its boundary

Thank you for the attention