# A new signature of quantum phase transitions from the numerical range <br> talk at the conference 

Entropy 2018:
From Physics to Information Sciences and Geometry
University of Barcelona, Spain
May 15th, 2018
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

## Overview

1. Ground Energy
2. Convex Geometry
3. Numerical Range
4. Results
5. Conclusion

## Part I <br> Ground Energy

## Quantum Phase Transitions

are characterized in terms of

1) long-range correlation in ground state
2) non-analytic ground energy
3) geometry of reduced density matrices

Zauner-Stauber et al. New J. Phys. 18 (2016), 113033
\& Chen et al. Phys. Rev. A 93 (2016), 012309
4) strong variation / discontinuity of MaxEnt maps

Arrachea et al. Phys. Rev. A 45 (1992), 7104
\& Chen et al. New J. Phys. 17 (2015), 083019
this talk clarifies in the finite-dimensional setting relationships between 2), 3), 4) and certain open mapping properties

## Differentiability of Ground Energy

one-parameter Hamiltonian $H(g)=H_{0}+g \cdot H_{1}, \quad g \in \mathbb{R}$
angular representation $A(\theta)=\cos (\theta) H_{0}+\sin (\theta) H_{1}, \theta \in\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$
ground energy $\lambda(X)=$ minimal eigenvalue of $X$

## Observation

$\lambda \circ H$ is $C^{k} /$ analytic at $\tan (\theta) \Longleftrightarrow \lambda \circ A$ is $C^{k} /$ analytic at $\theta$
focus on ground energy $\lambda(\theta)=\lambda \circ A(\theta)$
advantage: reduced density matrices and MaxEnt maps are easier described in angular coordinates

## Part II <br> Convex Geometry

## Convex Geometry

$K \subset \mathbb{C} \cong \mathbb{R}^{2}$ compact convex
support function
$\tilde{h}_{K}: \mathbb{C} \rightarrow \mathbb{R}, \tilde{h}_{K}(u)=\min _{z \in K}\langle z, u\rangle$
exposed face $F(u)=\operatorname{argmin}_{z \epsilon K}\langle z, u\rangle$
$\tilde{h}_{F(u)}(v)=\tilde{h}_{K}^{\prime}(u ; v)=$ directional
derivative $=\lim _{t>0} \frac{1}{t}\left(\tilde{h}_{K}(u+t v)-\tilde{h}_{K}(u)\right)$
end-points of exposed face, $u \in S^{1}$
$x_{ \pm}(u)=u \tilde{h}_{K}(u) \pm u^{\perp} \tilde{h}_{K}^{\prime}\left(u ; \pm u^{\perp}\right) \in \partial K$
using $h_{K}(\theta)=\tilde{h}_{K}\left(e^{i \theta}\right)$,
$x_{ \pm}\left(e^{i \theta}\right)=e^{\mathrm{i} \theta}\left(h_{K}(\theta) \pm \mathrm{i} h_{K}^{\prime}(\theta ; \pm 1)\right) \in \partial K$
$x_{ \pm}$restricted to $u \in S^{1}$ with $x_{+}(u)=x_{-}(u)$ is the reverse Gauss map $x_{ \pm}(u)=\nabla \tilde{h}(u)$ which parametrizes $\partial K$ as an envelope

## Part III Numerical Range

## Numerical Range

density matrices $D_{n}=\left\{\rho \in M_{n}: \rho \geq 0, \operatorname{tr}(\rho)=1\right\}$

$$
\text { numerical range } \begin{aligned}
W & =\left\{\langle\psi| H_{0}+\mathrm{i} H_{1}|\psi\rangle:\langle\psi \mid \psi\rangle=1\right\} \\
& =\left\{\operatorname{tr} \rho\left(H_{0}+\mathrm{i} H_{1}\right): \rho \in D_{n}\right\}
\end{aligned}
$$

$W$ is the set of expected values of $H_{0}$ and $H_{1}$ (reduced density matrices)

Theorem 1 (Toeplitz) $\quad h_{W}(\theta)=\lambda \circ A(\theta)=\lambda(\theta)$
Math. Z. 2 (1918), 187
von Neumann entropy $S(\rho)=-\operatorname{tr} \rho \log (\rho), \rho \in D_{n}$ maximum-entropy inference map (MaxEnt map)

$$
\rho^{*}: W \rightarrow D_{n}, \quad z \mapsto \operatorname{argmax}\left\{S(\rho): \operatorname{tr} \rho\left(H_{0}+\mathrm{i} H_{1}\right), \rho \in D_{n}\right\}
$$

## Numerical Range - Diagonal Matrices

$$
\begin{aligned}
& H_{0}=\operatorname{diag}\left(E_{0}^{1}, \ldots, E_{0}^{n}\right) \text { and } H_{1}=\operatorname{diag}\left(E_{1}^{1}, \ldots, E_{1}^{n}\right) \\
& W=\operatorname{conv}\left\{E_{0}^{1}+\mathrm{i} E_{1}^{1}, \ldots, E_{0}^{n}+\mathrm{i} E_{1}^{n}\right\} \\
& A(\theta)=\operatorname{diag}\left(E_{0}^{1} \cos (\theta)+E_{1}^{1} \sin (\theta), \ldots, E_{0}^{n} \cos (\theta)+E_{1}^{n} \sin (\theta)\right)
\end{aligned}
$$



- $W$ is a polytope
- $\lambda$ is piecewise harmonic
- $x_{+}$and $x_{-}$are piecewise constant
- flat boundary portions of $W$ $\cong$ non-differentiable points of $\lambda$
- $\rho^{*}$ is continuous


## Numerical Range - Non-Commutative

we assume $\operatorname{dim}(W)=2 \Leftarrow\left[H_{0}, H_{1}\right] \neq 0$
analytic curves $\lambda_{1}(\theta), \ldots, \lambda_{n}(\theta)$ and ONB 's $\left|\psi_{k}(\theta)\right\rangle_{k=1}^{n}$ such that

$$
\boldsymbol{A}(\theta)=\sum_{k=1}^{n} \lambda_{k}(\theta)\left|\psi_{k}(\theta)\right\rangle\left\langle\psi_{k}(\theta)\right|
$$

Rellich, IMM-NYU 2, New York: New York University, 1954

- $\lambda$ is piecewise analytic
- the maximal order of differentiability of $\lambda$ is even at non-analytic points
max. order 0

max. order 2



## Numerical Range - Continuity of Inference

$\rho^{*}$ is analytic on the interior of $W, W^{\circ} \ni z \mapsto e^{\mu_{1} H_{1}+\mu_{2} H_{2}} / \operatorname{tr}\left({ }^{\prime \prime}\right)$, if $z=x_{+}\left(e^{i \theta}\right)$ then

$$
\begin{aligned}
\rho^{*}(z)= & \text { maximally mixed state on } \\
& \operatorname{span}\left\{\left|\psi_{k}(\theta)\right\rangle: \lambda_{k}(\theta)=\lambda(\theta), \lambda_{k}^{\prime}(\theta)=\lambda^{\prime}(\theta ;+1)\right\}
\end{aligned}
$$

- the maps $x_{+}, x_{-}: S^{1} \rightarrow \partial W$ cover all extreme points of $W$
- $\left.\rho^{*}\right|_{\partial W}$ may be discontinuous at extreme points of $W$ because of $C^{2}$ smooth eigenvalue crossings with the ground energy $\lambda$
- $\left.\rho^{*}\right|_{F(u)}$ is continuous on flat boundary portions $F(u) \subset \partial W$ of $W$
- for $z \in \partial W:\left.\rho^{*}\right|_{\partial W}$ is continuous at $z \Longleftrightarrow \rho^{*}$ is continuous at $z$
- discontinuities of $\rho^{*}$ are irremovable because $\rho^{*}(W) \subset \overline{\rho^{*}\left(W^{\circ}\right)}$, Wichmann JMP 4 (1963), 884
- discontinuities of $\left.\rho^{*}\right|_{\partial w}$ may be removable


## Numerical Range - Open Mappings

## definitions

a map $\alpha: X \rightarrow Y$ between topological spaces is open at $x \in X$ if $\alpha$ maps neighborhoods of $x$ to neighborhoods of $\alpha(x)$
numerical range map $f:\{|\psi\rangle:\langle\psi \mid \psi\rangle=1\} \rightarrow W,|\psi\rangle \mapsto\langle\psi| H_{0}+\mathrm{i} H_{1}|\psi\rangle$
expected value map $\mathbb{E}: D_{n} \rightarrow W, \rho \mapsto \operatorname{tr} \rho\left(H_{0}+\mathrm{i} H_{1}\right)$
the inverse numerical range map $f^{-1}$ is strongly (resp. weakly) continuous at $z \in W$ if for all (resp. for at least one) $|\psi\rangle \in f^{-1}(z)$ the map $f$ is open at $|\psi\rangle$

Noticeable: Openness of linear maps on state spaces of $C^{*}$-algebras are studied since the 70's (Lima, Vesterstrøm, O'Brian), with applications to quantum information theory: Shirokov, Izvestiya: Math. 76 (2012), 840

## Part IV Results

## Smoothness of $\lambda$, geometry of $W$, continuity of $\rho^{*}$

Let $z=x_{+}\left(e^{\mathrm{i} \theta}\right)=x_{-}\left(e^{\mathrm{i} \theta}\right)$ be not a corner point: the statements in each column are equivalent

| $\lambda$ is analytic locally at $\theta$ |  | $\lambda$ is $C^{2 k}$ but not $C^{2 k+1}$ <br> locally at $\theta, k \geq 1$ |
| :---: | :--- | :---: |
| $\lambda(\theta)=\lambda_{k}(\theta)=\lambda_{l}(\theta)$ <br> $\lambda^{\prime}(\theta)=\lambda_{k}^{\prime}(\theta)=\lambda_{l}^{\prime}(\theta)$ <br> $\Rightarrow \lambda_{k}=\lambda_{l}$ | $\exists k: \lambda=\lambda_{k}$ locally at $\theta$ | $\nexists k: \lambda=\lambda_{k}$ locally at $\theta$ |
| $\partial W$ is an analytic manifold locally at $z$ |  | $\partial W$ is a $C^{2 k}$ but <br> not a $C^{2 k+1}$ manifold <br> locally at $z, k \geq 1$ |
| $\rho^{*}$ is continuous at $z$ | $\rho^{*} l_{\partial W}$ has a <br> removable <br> discontinuity at $z$ | $\rho^{*} l_{2 w}$ has an <br> irremovable <br> discontinuity at $z$ |

Notice: $S^{1} \rightarrow \partial W, e^{\mathrm{i} \theta} \mapsto x_{ \pm}(\theta)=e^{\mathrm{i} \theta}\left(\lambda(\theta)+\mathrm{i} \lambda^{\prime}(\theta)\right)$ is only $C^{2 k-1}$ if $\lambda$ is $C^{2 k}$ !

## Open Mapping Conditions

Let $z \in W$ be arbitrary: the statements in each column are equivalent

| $\rho^{*}$ is continuous at $z$ | $\left.\rho^{*}\right\|_{\partial w}$ has a <br> removable <br> discontinuity at $z$ | $\left.\rho^{*}\right\|_{\partial w}$ has an <br> irremovable <br> discontinuity at $z$ |
| :---: | :---: | :---: |
| $f^{-1}$ is strongly <br> continuous at $z$ | $f^{-1}$ is weakly but not <br> strongly continuous <br> at $z$ | $f^{-1}$ is not weakly <br> continuous at $z$ |
| $\mathbb{E}$ is open at $\rho^{*}(z)$ | $\mathbb{E}$ is not open at $\rho^{*}(z)$ |  |

## Part V Conclusion

## Summary: <br> Geometry and inference approach to the smoothness of the ground energy of a one-parameter Hamiltonian

## References:

Weis and Knauf, Entropy distance: New quantum phenomena, JMP 53 (2012), 102206

Leake et al., Inverse continuity on the boundary of the numerical range, Linear and Multilinear Algebra 62 (2014), 1335

Rodman et al., Continuity of the maximum-entropy inference: Convex geometry and numerical ranges approach, JMP 57 (2016), 015204

Spitkovsky and Weis, A new signature of quantum phase transitions from the numerical range, arXiv:1703.00201 [math-ph]

Thank you

