PES: Robust Analytic Continuation Methods for Green's Functions

Projection, Estimation and Semidefinite relaxation

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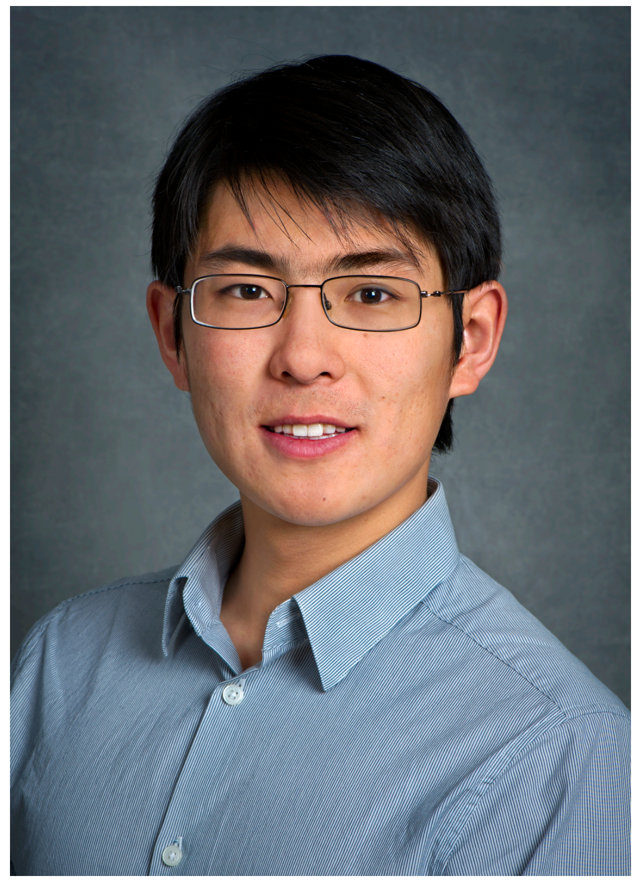
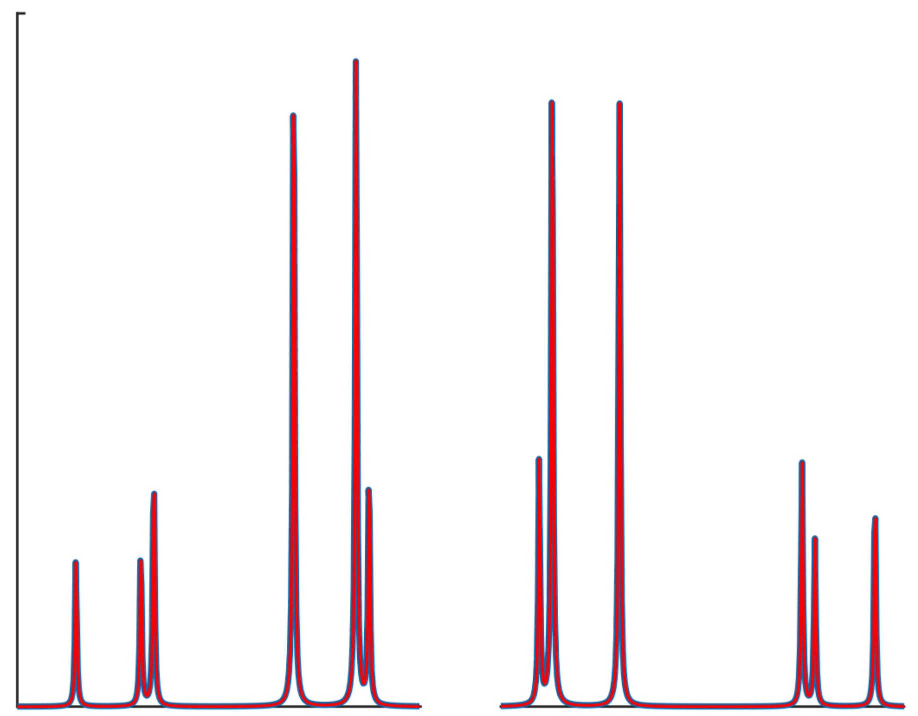


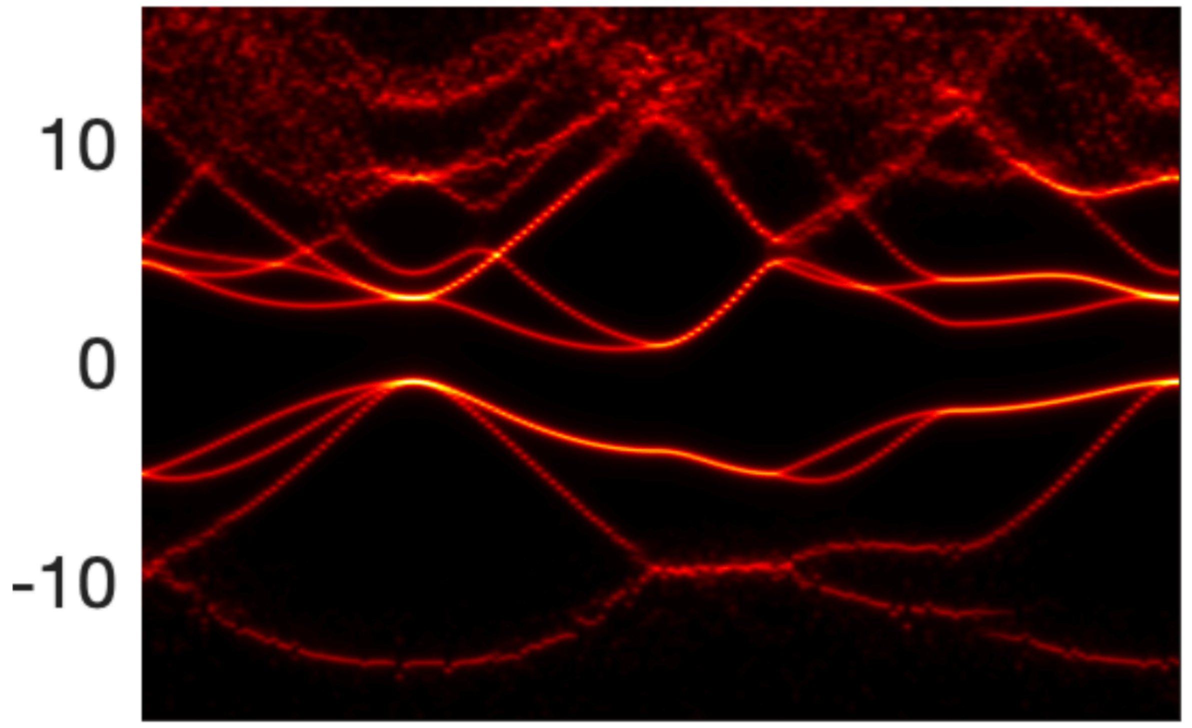
Lin Lin (UC Berkeley)

Emanuel Gull (U Michigan)

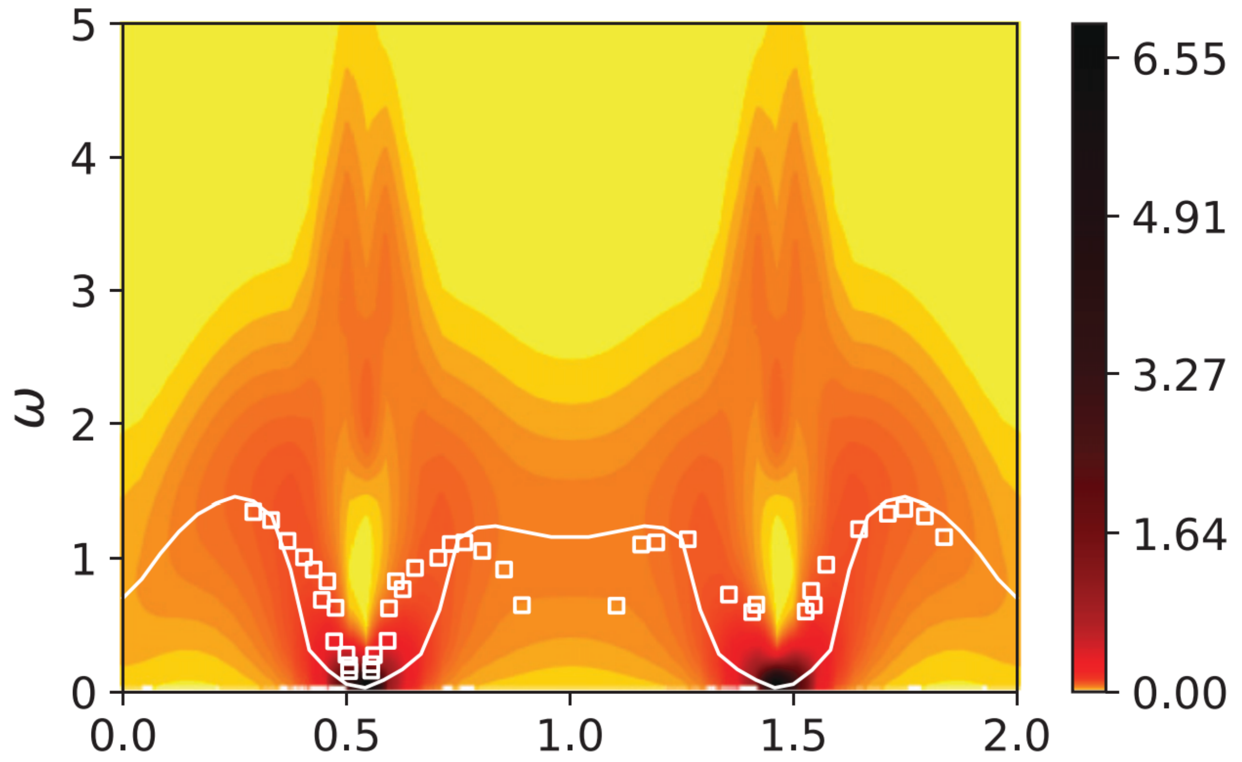
Why Analytic Continuation?



Spectral functions



k resolved spectral functions



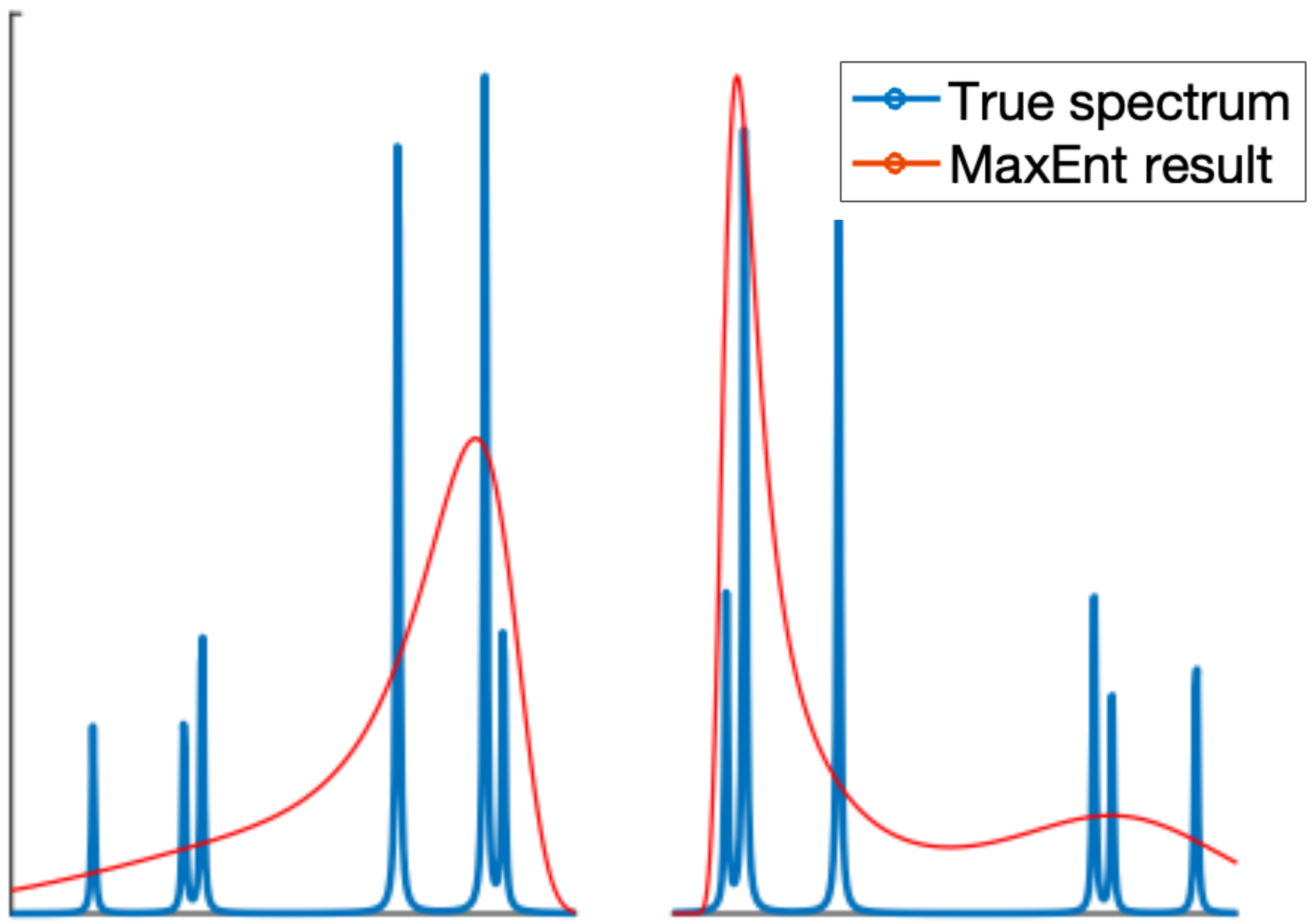
Susceptibility

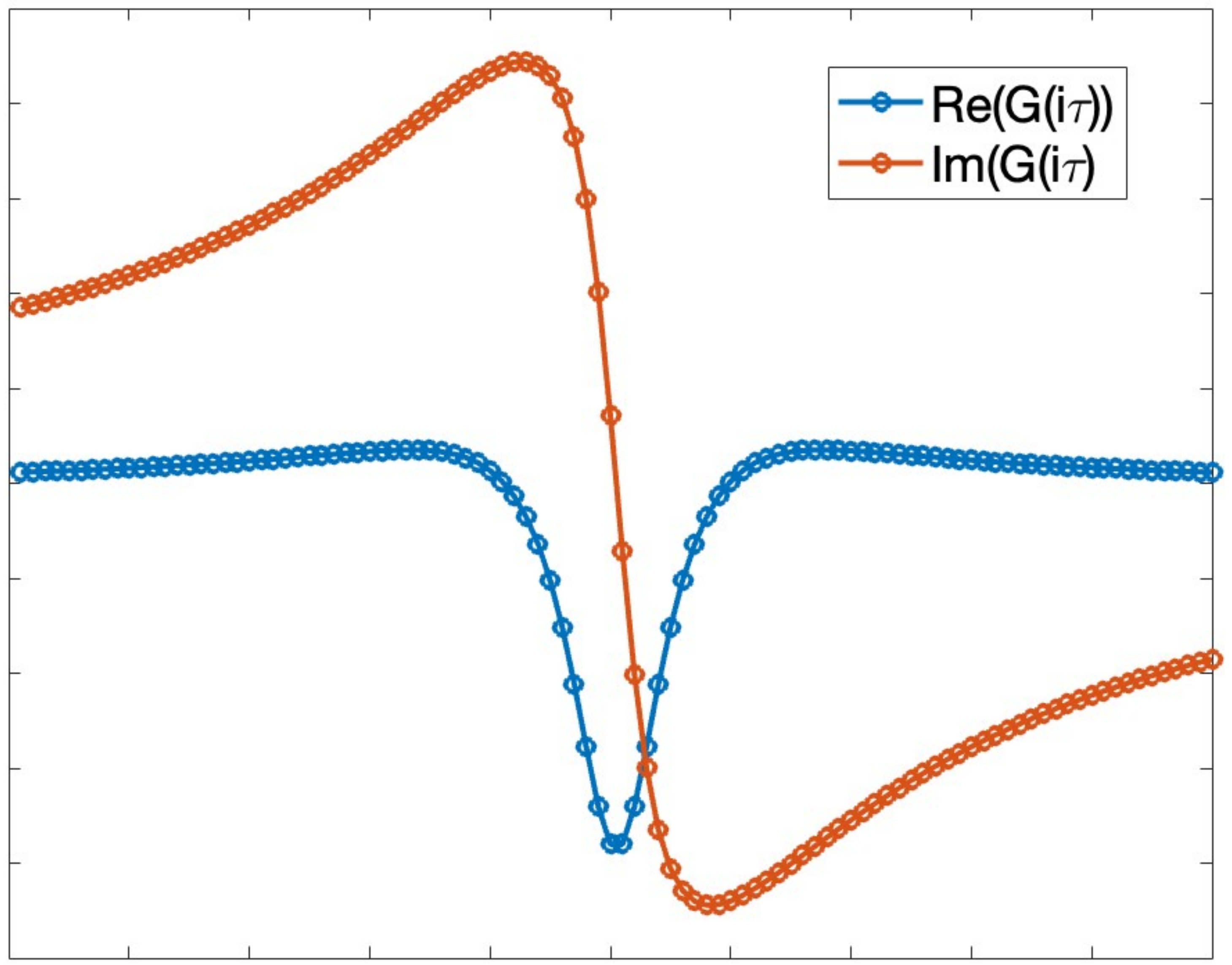
- Analytic continuation has wide applications in studying strongly correlated systems.
- Instead of doing *expensive* **real-time** calculations, ...
- We do **imaginary-time** calculations, ...
- Then perform **analytic continuation** from ***imaginary*** to ***real*** axis.

Z. Huang, E. Gull, L. Lin, Robust analytic continuation of Green's functions via projection, pole estimation, and semidefinite relaxation, ***Phys. Rev. B*** 107, 075151, 2023
Y. Yu, S. Li, S. Iskakov, and E. Gull, Magnetic phases of the anisotropic triangular lattice Hubbard model, ***Phys. Rev. B*** 107 (7), 075106, 2023

- Previous methods:
  - **Padé approximants** (Baker et al, 1996; Schott et al, 2016; ...)
  - **Maximum entropy (MaxEnt)** (Bryan, 1990; Asakawa et al 2001; Levy et al, 2017; ...)
  - **Stochastic analytic continuation and its variants** (Sandvik, 1998; Vafayi et al 2007; ...)
  - **Sparse modeling** (Otsuki, 2017; Yoshimi, 2019; ...)
  - **Machine learning approaches** (Yoon, 2018; Fournier, 2020; ...)

Shortcomings of Analytic Continuation Approach



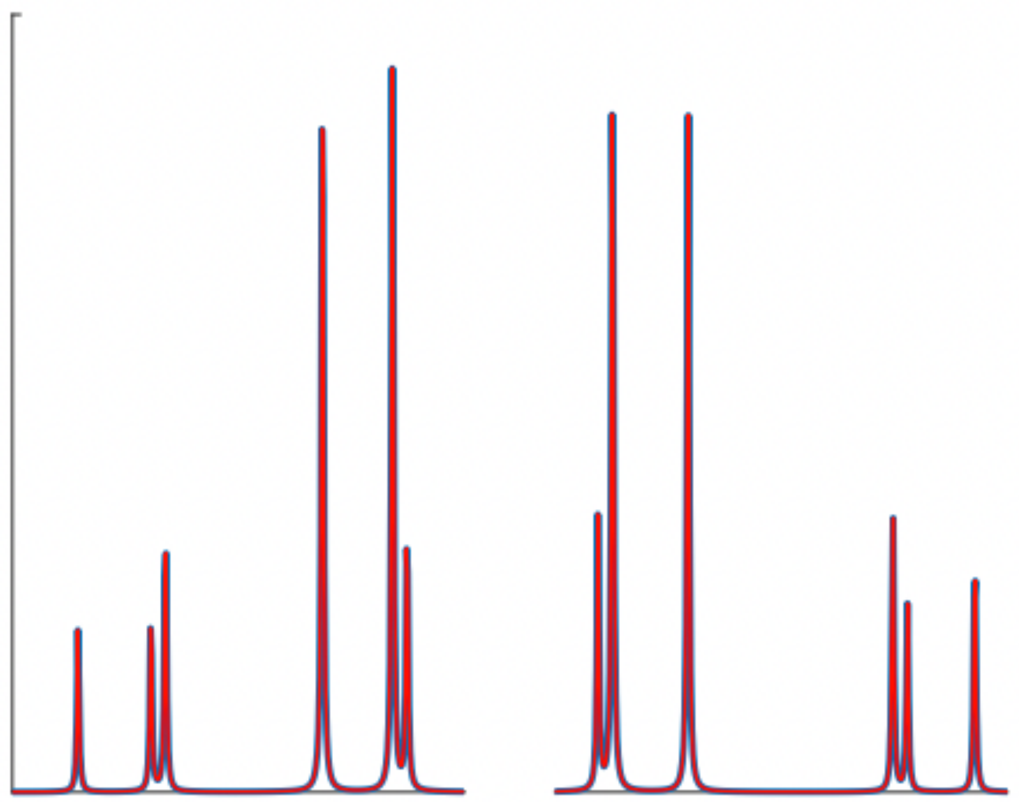


- **Imaginary-time** data → **Real-time** data: **ill-posed**!
  - **Solutions non-unique! (But only one of them is true.)**
  - **e.g. Maximum entropy** loses sharp features, loses multiple features, loses high frequency information.
- Obtaining imaginary-time data might be easier, but analytic continuation is hard. There is **NO** free lunch!

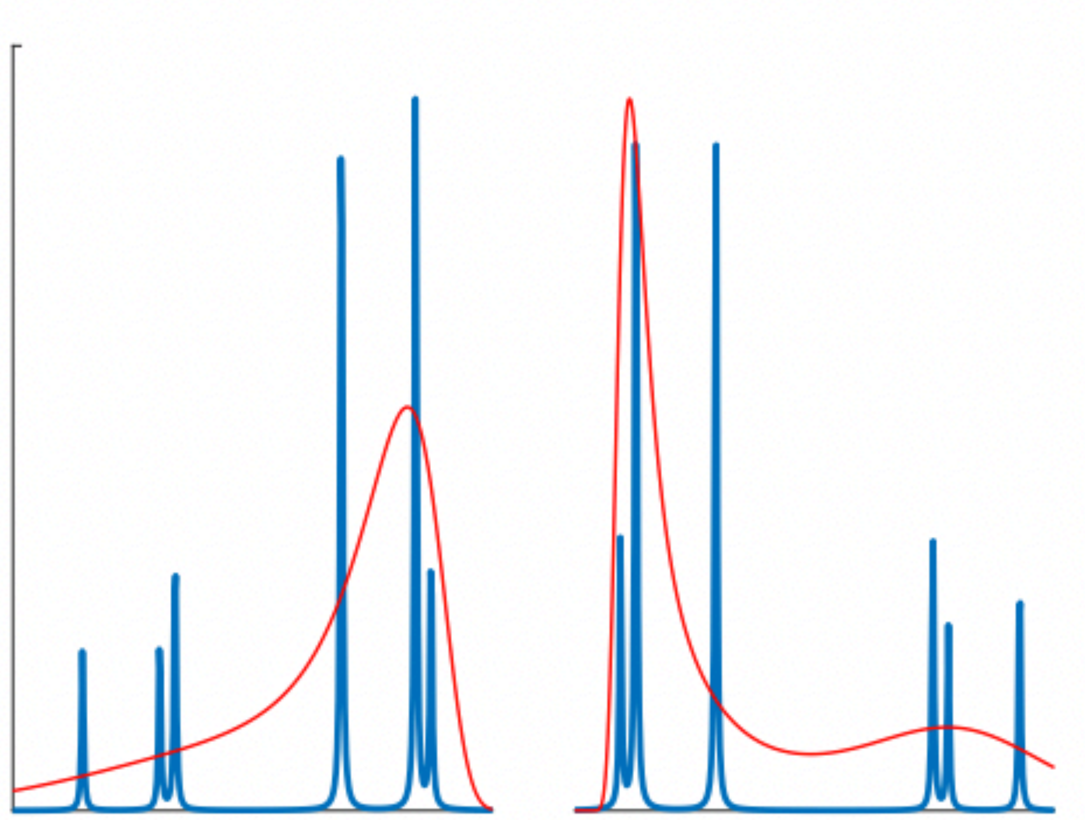
Nevanlinna/Carathéodory Continuation

- Observation: not all complex functions could be Green's functions!
- Green's functions are ***Herglotz-Nevanlinna*** functions.
  Based on this *analytic* structure, **Nevanlinna** and **Carathéodory** methods are proposed.
- A huge improvement over previous methods!

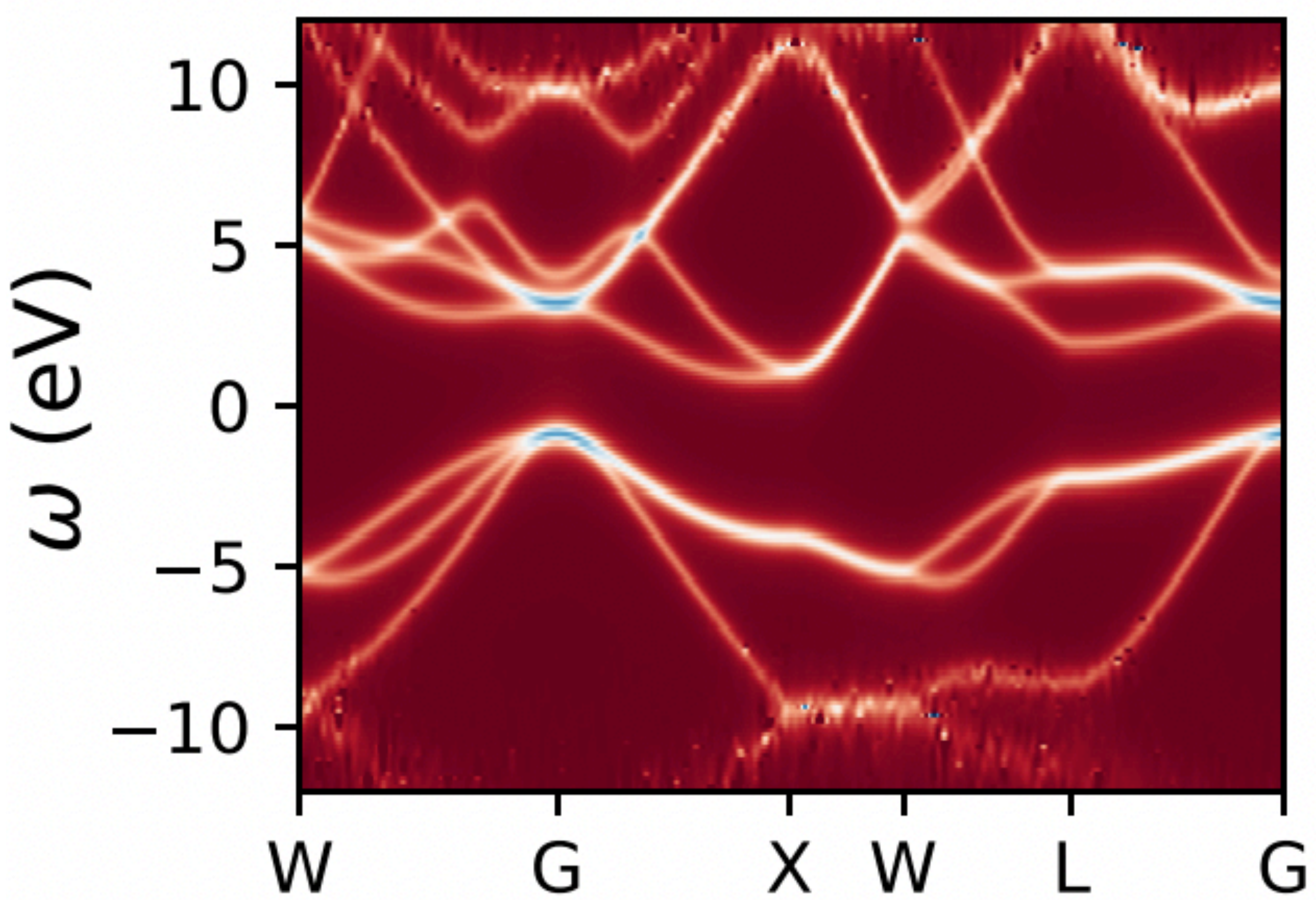
Nevanlinna for Hubbard dimer



MaxEnt for Hubbard dimer



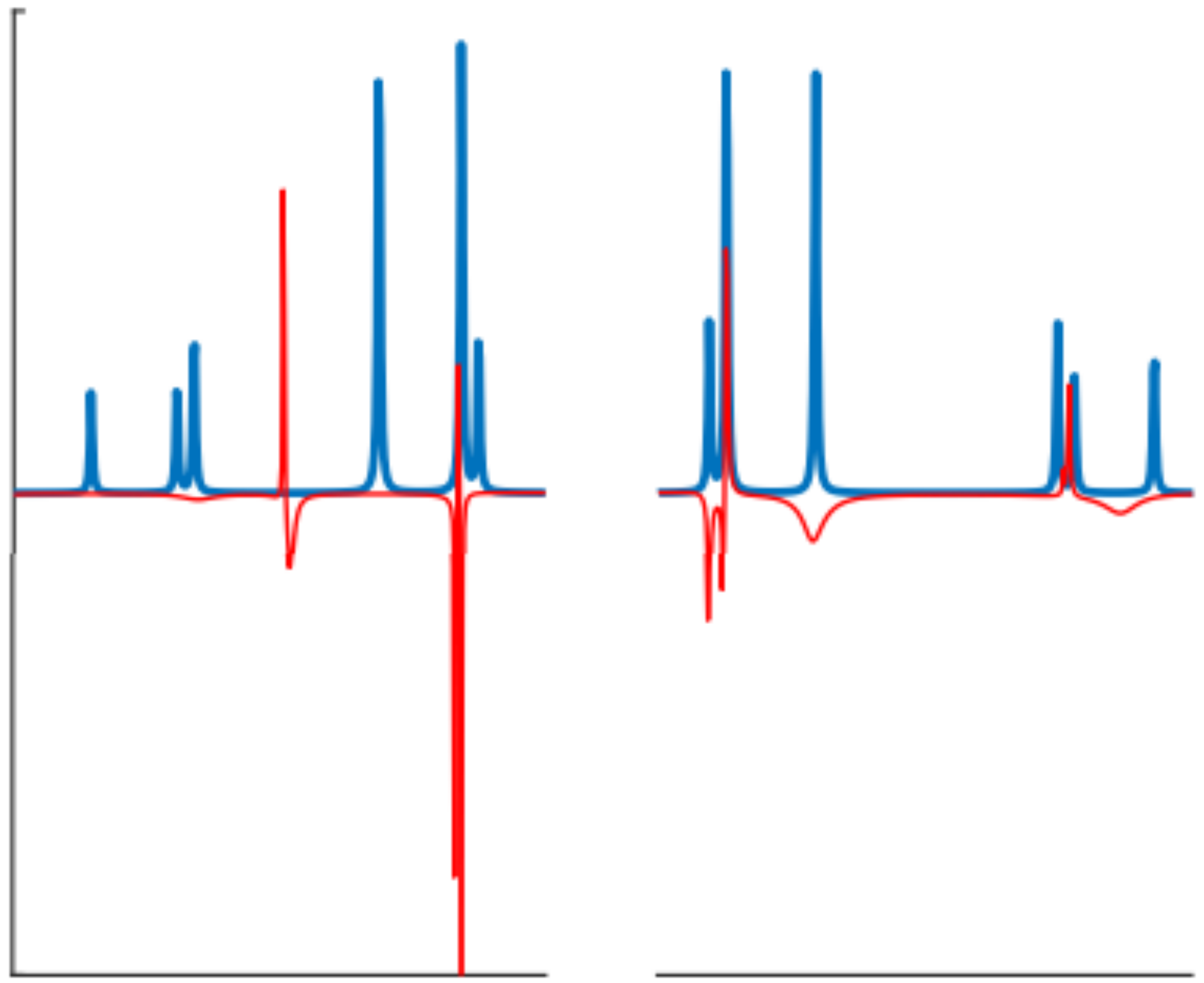
SIlicon band structure



J. Fei, C.N. Yeh and E. Gull, Nevanlinna analytical continuation. ***Phys. Rev. Lett***, *126*(5), 056402, 2021
J. Fei, C.N. Yeh, D.Zgid and E. Gull, Analytical continuation of matrix-valued functions: Carathéodory formalism. ***Phys. Rev. B***, *104*(16), 165111, 2021

Numerical instability of Nevanlinna/Carathéodory

Carathéodory method for Hubbard dimer data with noise level 4e-6

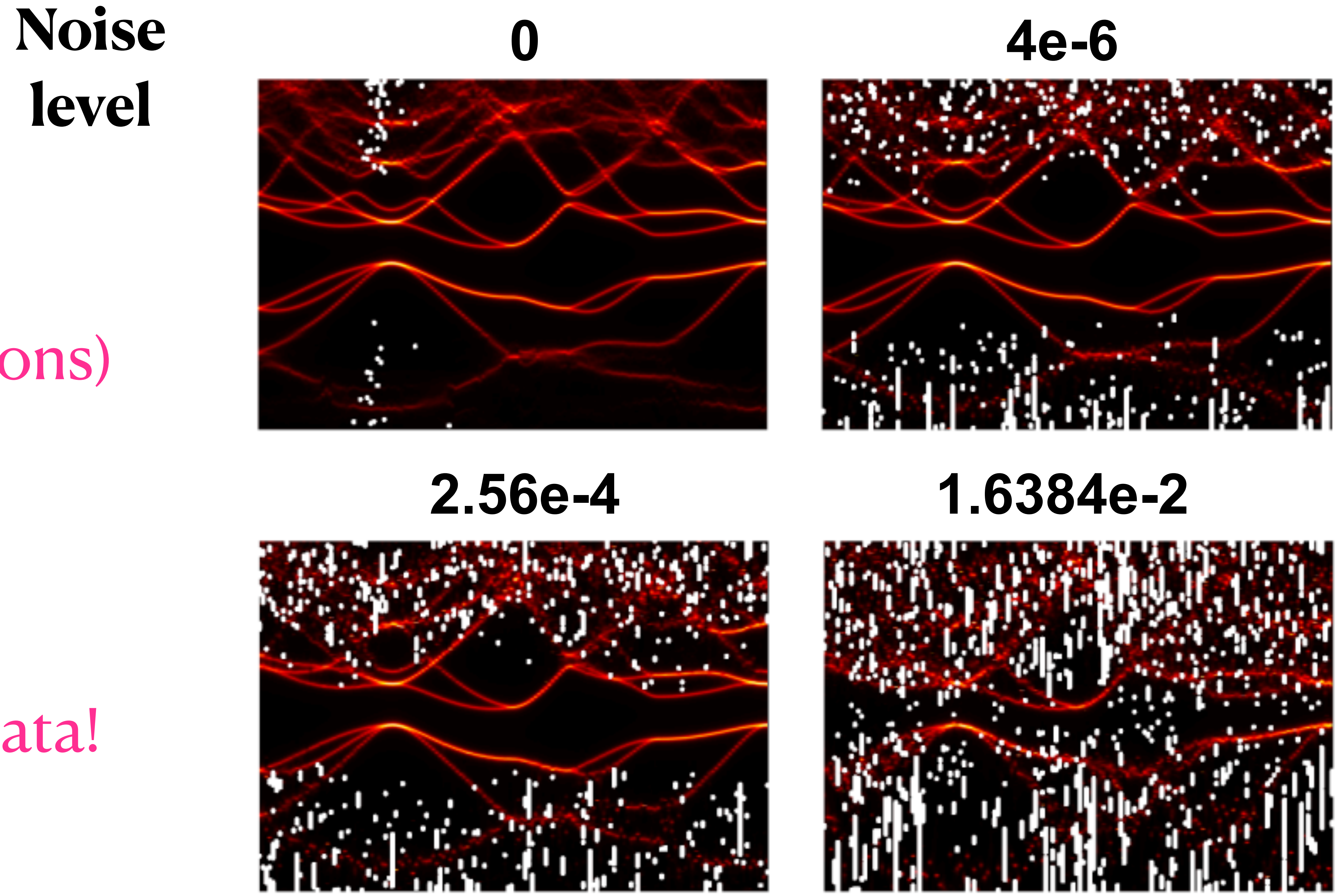


Noncausality
(negative spectral functions)

Problematic for **noisy** data!

Extended arithmetic required

Band structure from Nevanlinna

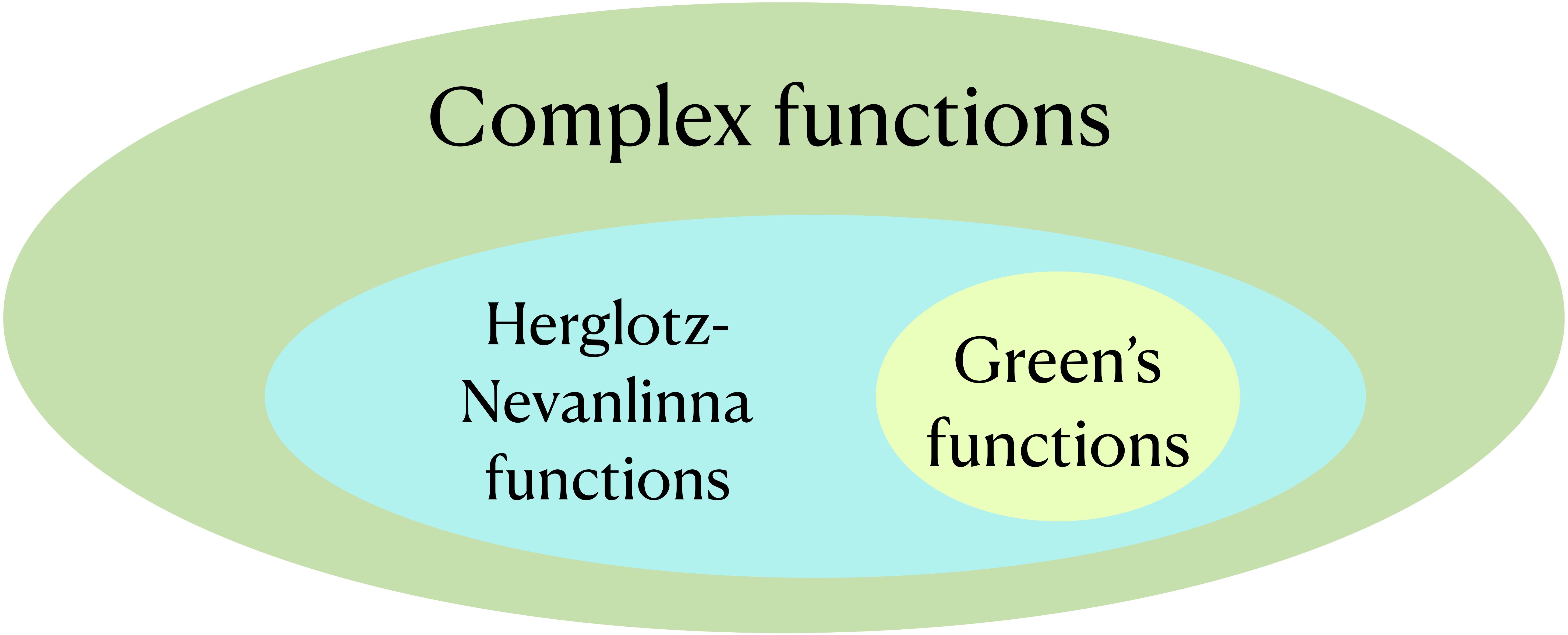


White markers correspond to a negative value of spectral function.

Z. Huang, E. Gull, L. Lin, Robust analytic continuation of Green's functions via projection, pole estimation, and semidefinite relaxation, **Phys. Rev. B**, 107, 075151, 2023

Our approach: make full use of the causal space

- Green's functions are Herglotz-Nevanlinna functions.
- Not **all** Herglotz-Nevanlinna functions are Green's functions!
- Key: making **full** use of the **causal space** of Green's functions.
- Nevanlinna/Caratheodory outperforms previous methods because they make ***some*** use of the **causal space**.



Z. Huang, E. Gull, L. Lin, Robust analytic continuation of Green's functions via projection, pole estimation, and semidefinite relaxation, **Phys. Rev. B**, 107, 075151, 2023

How to make make **full** use of the **causal space**?

- What is causal space?
- $G(z)$ is in the **causal space** if it has the following structure:

$$\mathbb{G}(z) = \sum_{l=1}^{N_p} \frac{\mathbb{X}_l}{z - \lambda_l}$$

  - $\{\lambda_l\}_{l=1}^{N_p}$ are real-valued poles;
  - $\{\mathbb{X}_l\}_{l=1}^{N_p}$ are **rank-1 semidefinite** matrices.
- This structure could be directly derived from **Lehmann's representation**.
- **Semidefinite relaxation** **(SDR)**: drop rank-1 constraint. ***Only*** require $\mathbb{X}_l$ to be semidefinite.
- **Semidefinite programming** **(SDP)**: if given $\{\lambda_l\}_{l=1}^{N_p}$, $\mathbb{X}_l$ could be found from SDP solvers.
- This approach was used previously in DMFT calculations.

C. Mejuto-Zaera, L. Zepeda-Nunez, M. Lindsey, N. Tubman, K. B. Whaley, L. Lin, Efficient hybridization fitting for dynamical mean-field theory via semi-definite relaxation, Phys. Rev. B, 101, 035143, 2020.

How to make make **full** use of the **causal space**?

- To kick off the **semidefinite relaxation step**, we need a very accurate initial estimate of poles in practice.
- Hence we need an **estimation step** of poles. We use AAA algorithm to do this.

Y. Nakatsukasa, O. Sète, and L. Trefethen. The AAA algorithm for rational approximation. **SIAM J. Sci. Comput** 40.3, 2018

- How to deal with noisy data?
- Noisy data do not belong in the causal space.
- Hence the **projection step**, which projects the noisy data onto the causal space.

- Combining all, we have PES method for analytic continuation:
  - **Projection onto causal space** + **Estimation of poles** + **Semidefinite relaxation**

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Results: Hubbard-dimer

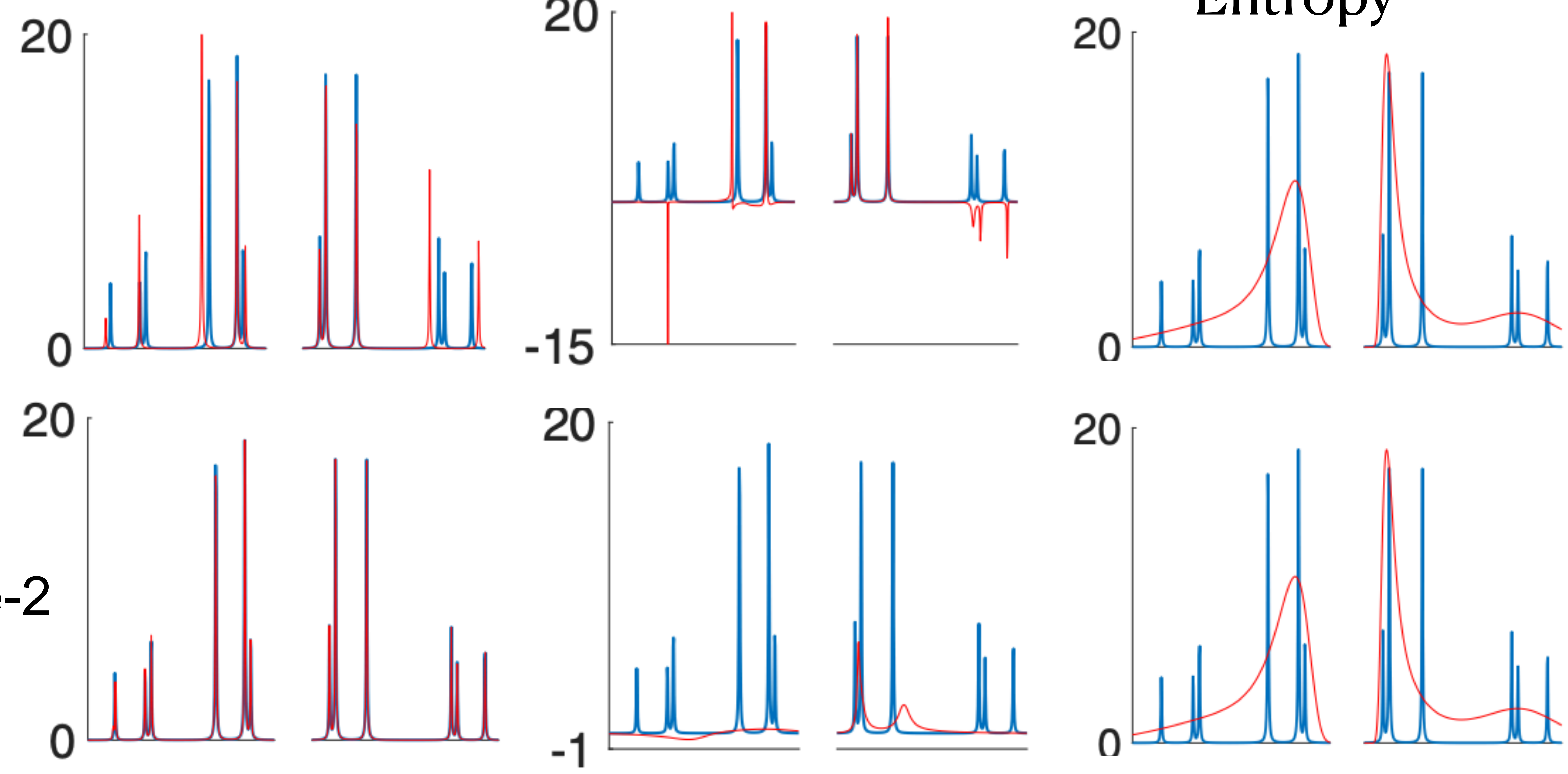
Spectral functions

PES | Caratheodory | Maximum Entropy

Noise level

4e-6

1.6384e-2



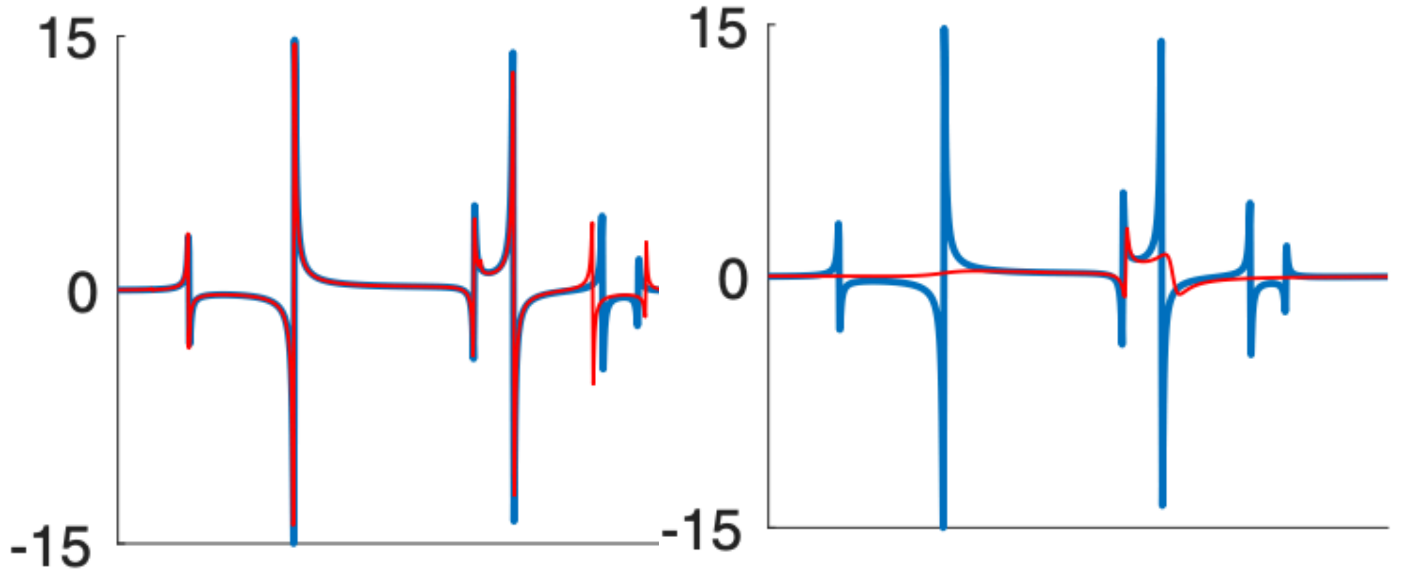
Small noise: almost **exactly recover**.

Large noise: correct **band gaps** and low energy information.

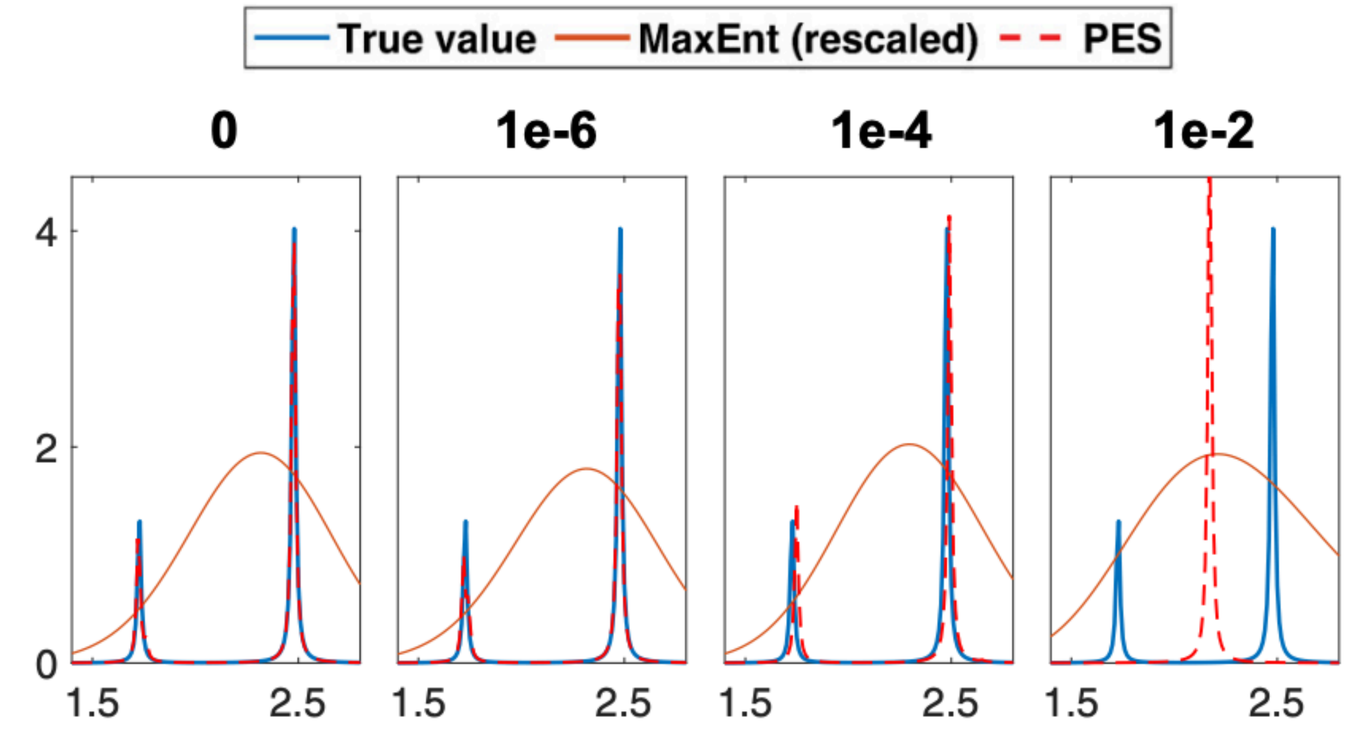
blue line: true value
red line: results from analytic continuation

Nondiagonal elements also available!

PES | Caratheodory



Bosonic functions also applicable!



Spin susceptibility

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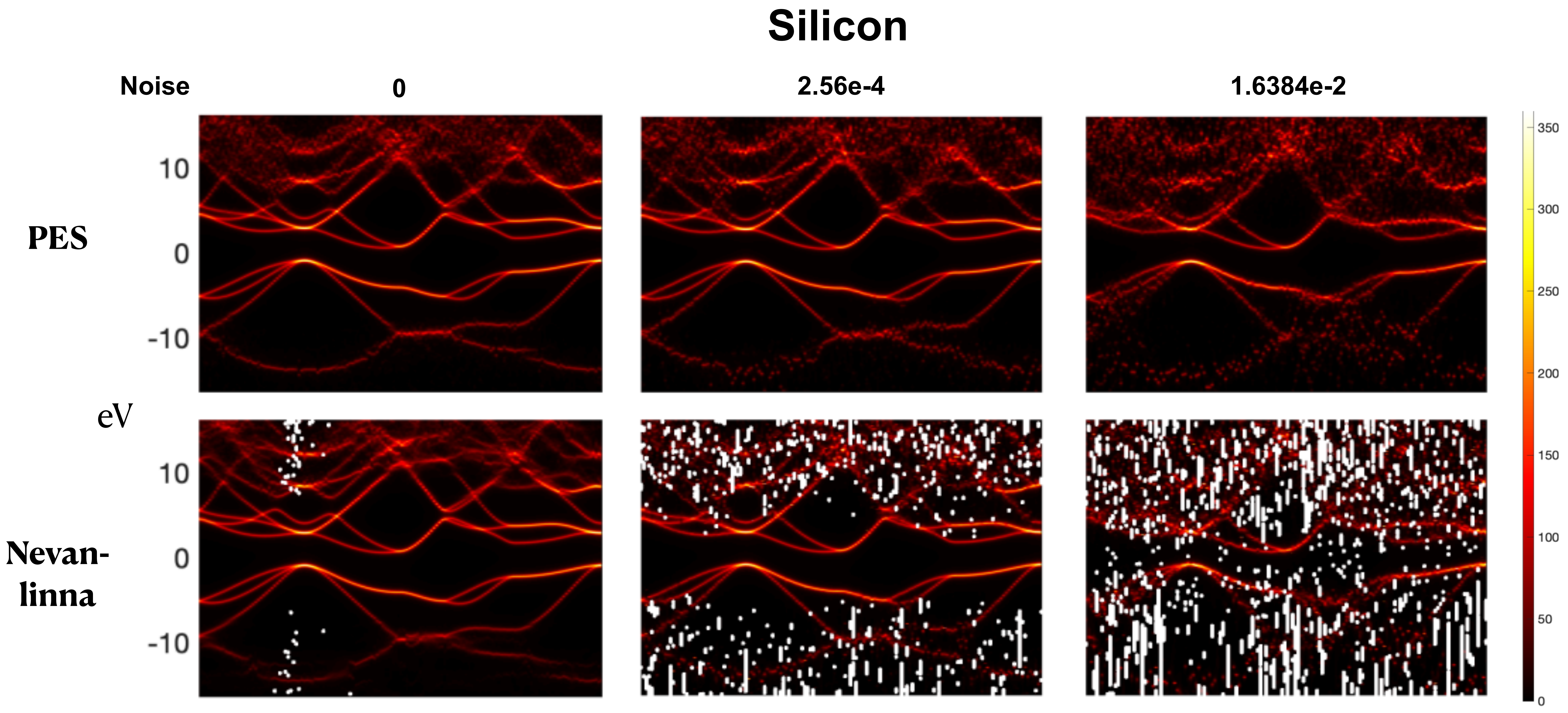
Band structures, to test the method for complicated cases



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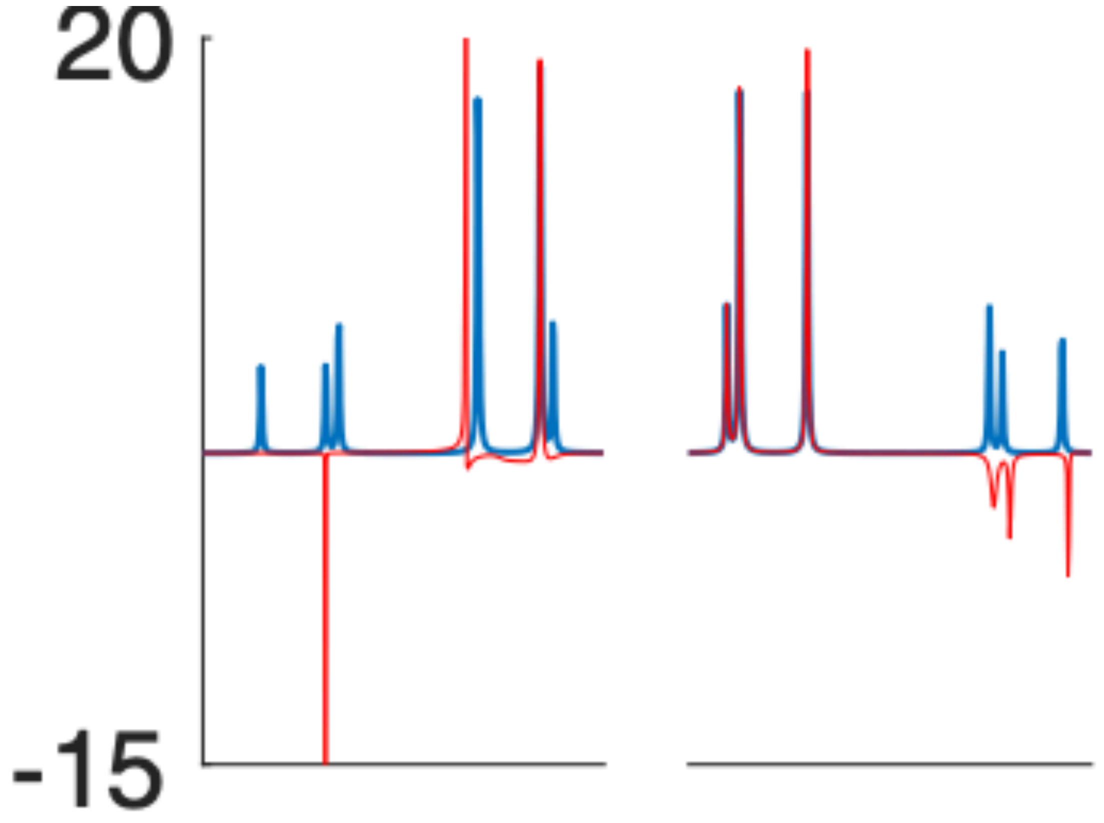
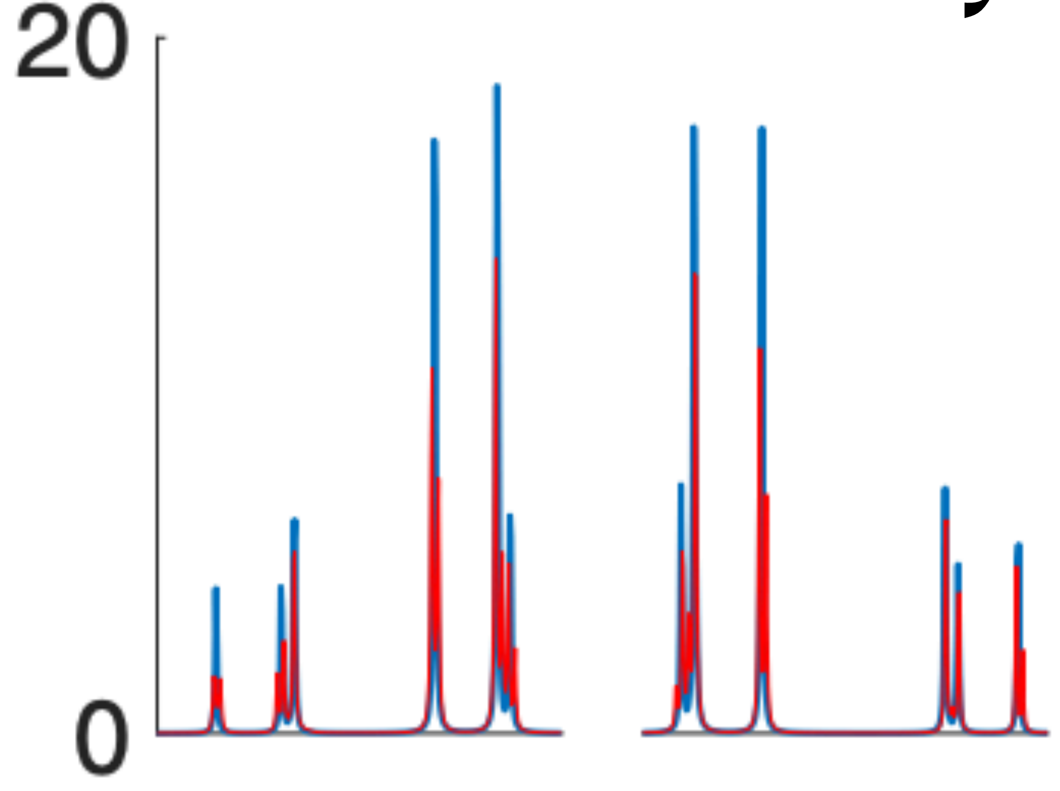
We also find a way to *systematically* improve the numerically unstable methods: applying them on *projected* data instead of noisy data!

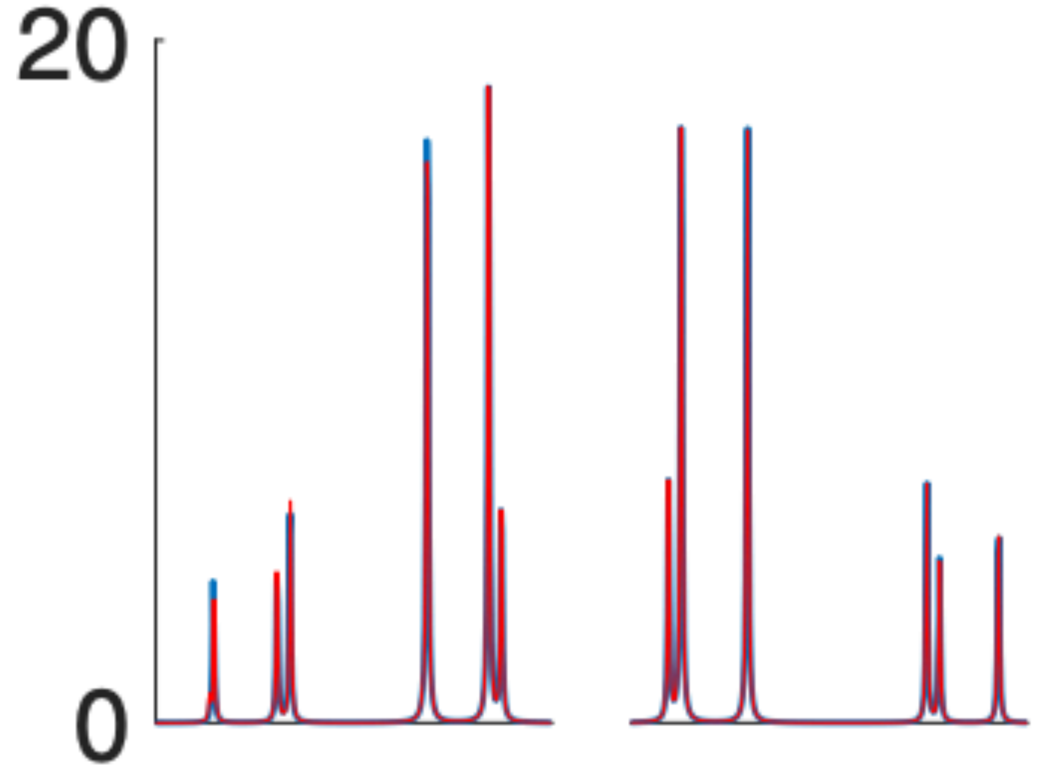
Caratheodory



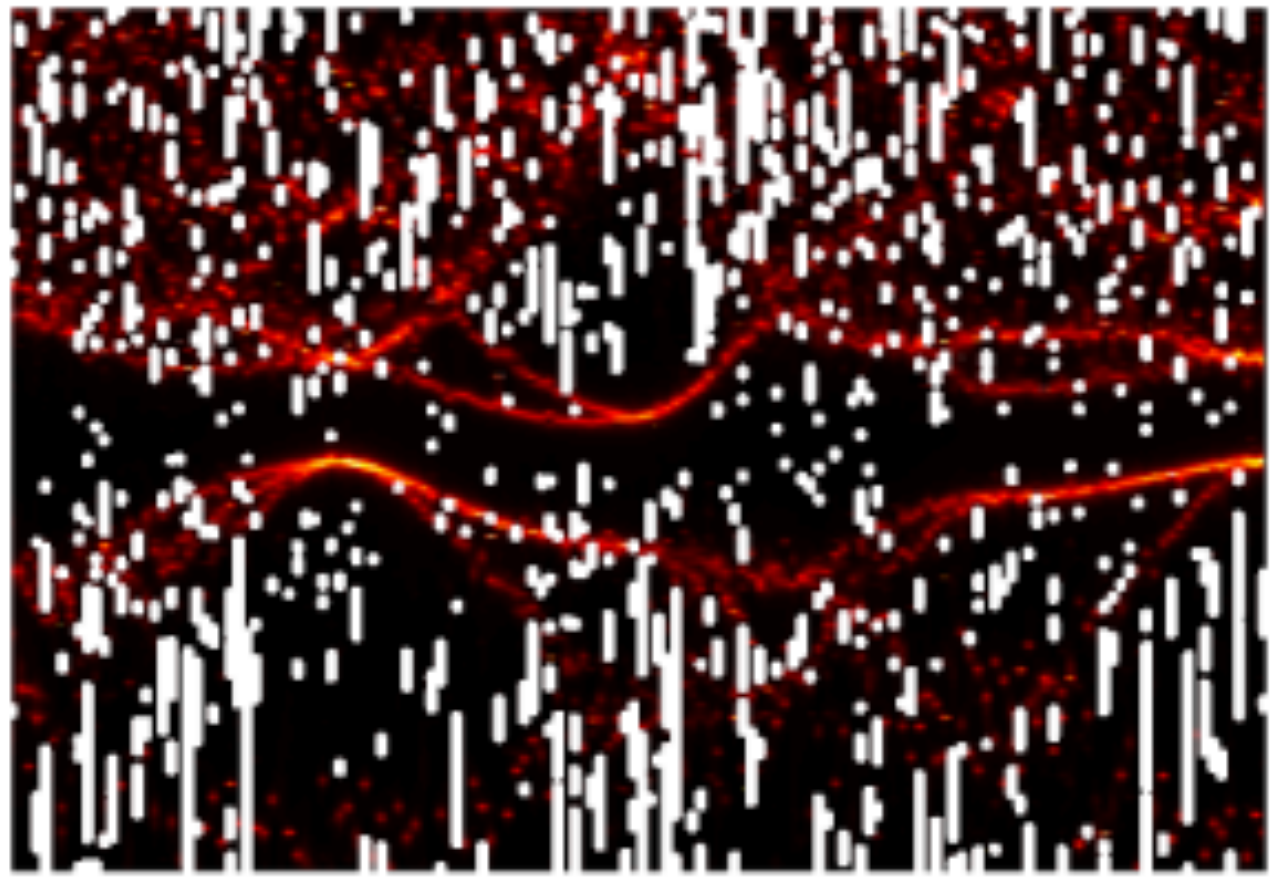
Projection+
Caratheodory



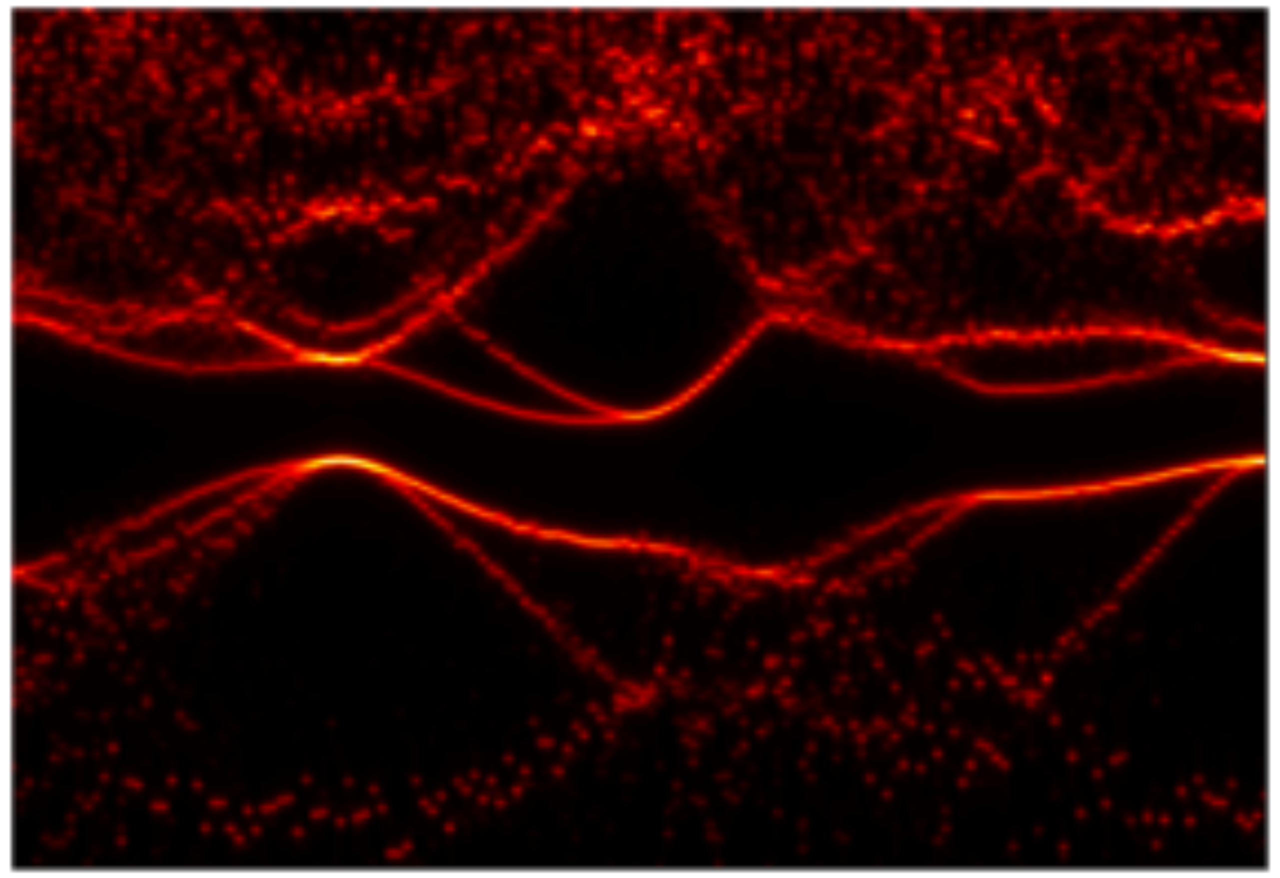
PES



Nevanlinna



Projection+
Nevanlinna



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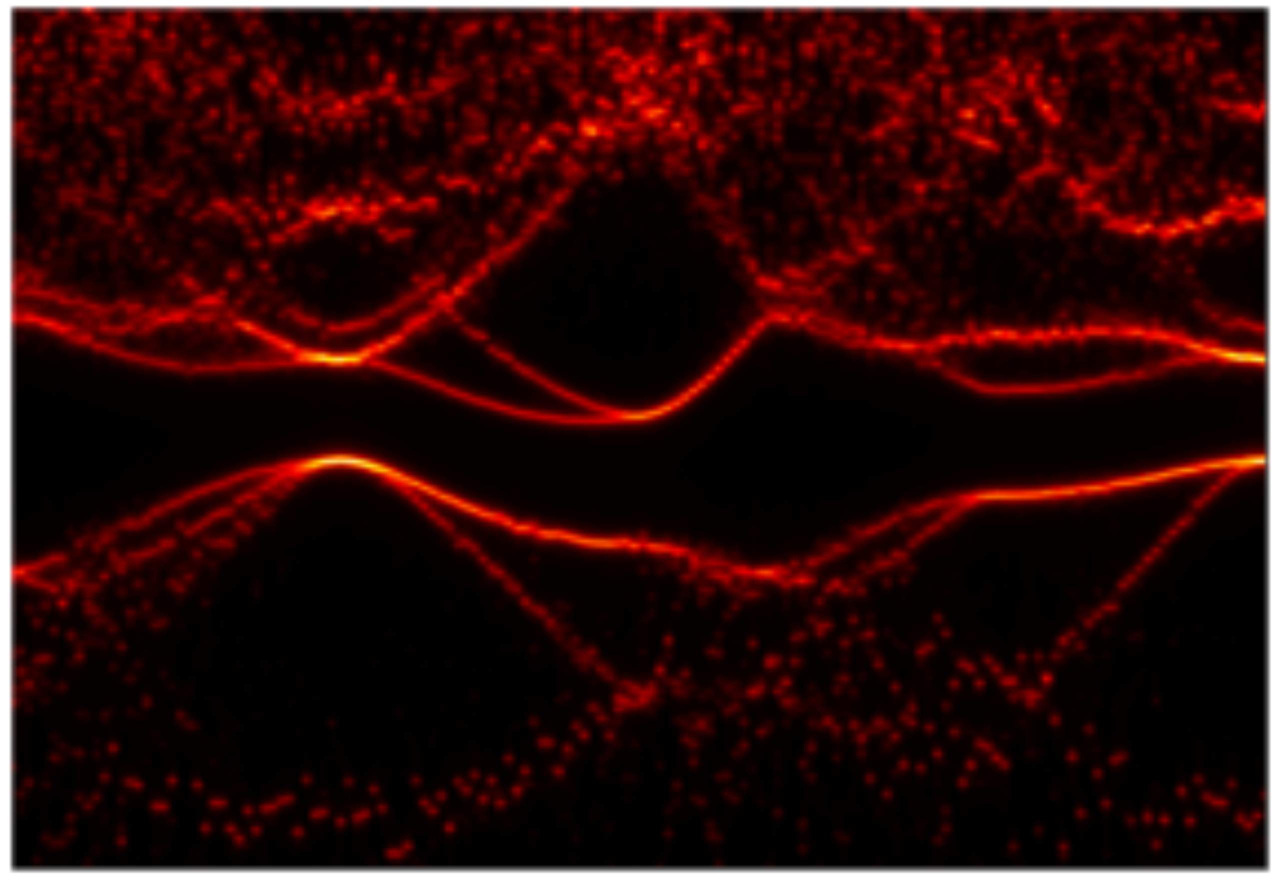

Conclusion

Method	Noise robustness	Calculation precision requirement	Sharp features	Causality
This paper	✓	Double	✓	✓
Nevanlinna and Carathéodory	✗	Extended	✓	✓ if clean ✗ if noisy
MaxEnt	✓	Double	✗	✓
Padé	✗	Extended	✓	✗

- **Z. Huang**, E. Gull, L. Lin, Robust analytic continuation of Green's functions via projection, pole estimation, and semidefinite relaxation, **Phys. Rev. B**, 107, 075151, 2023
- Software available on **GitHub**: **https://github.com/Hertz4/PES**
- Software also available as **supplementary material** on PRB website.
- Contact me at hertz@berkeley.edu !

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