## **PES: Robust Analytic Continuation Methods for Green's Functions Projection, Estimation** and Semidefinite relaxation

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## Why Analytic Continuation?



- 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



Susceptibility



- Previous methods:
  - Padé approximants (Baker et al, 1996; Schott et al, 2016; ...)
  - Levy et al, 2017; ...)
  - 1998; Vafayi et al 2007; ...)
  - Sparse modeling (Otsuki, 2017; Yoshimi, 2019; ...)
  - Machine learning approaches (Yoon, 2018; Fournier, 2020; ...)

• Maximum entropy (MaxEnt) (Bryan, 1990; Asakawa et al 2001;

## Stochastic analytic continuation and its variants (Sandvik,

## **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



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

MaxEnt for Hubbard dimer

Silicon band structure



## Numerical instability of Nevanlinna/Carathéodory

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



### **Extended** arithmetic required

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

### **Band structure from Nevanlinna**

Noise level



2.56e-4



**4e-6** 

1.6384e-2





### White markers correspond to a negative value of spectral function.







# 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

**Complex functions** 

Herglotz-Nevanlinna functions

Green's functions





## 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:

 $\mathbb{G}(z) =$ 

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

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

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?

- 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:

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

### • To kick off the semidefinite relaxation step, we need a very accurate initial estimate

### Projection onto causal space + Estimation of poles + Semidefinite relaxation



## Results: Hubbard-dimer

### **Spectral** functions



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

analytic continuation

### Nondiagonal elements also available!



### **Bosonic** functions also applicable!



## Band structures, to test the method for complicated cases Silicon



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



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

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### Nevanlinna





### Projection+ Caratheodory



### Projection+ Nevanlinna



PES



Method	Noise robustness	Calculation precision requirement	Sharp features	Causality	
This paper	$\checkmark$	Double	$\checkmark$	$\checkmark$	
Nevanlinna and Carathéodory	×	Extended	$\checkmark$	<ul><li>✓ if clean</li><li>✗ if noisy</li></ul>	
MaxEnt	$\checkmark$	Double	×	$\checkmark$	
Padé	×	Extended	$\checkmark$	×	

- Z. Huang, E. Gull, L. Lin, <u>Robust analytic continuation of Green's functions via</u>
- Software available on GitHub: <u>https://github.com/Hertz4/PES</u>
- Software also available as supplementary material on PRB website.
- Contact me at <u>hertz@berkeley.edu</u>!





## Conclusion

# projection, pole estimation, and semidefinite relaxation, Phys. Rev. B, 107, 075151, 2023

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