From Mathematics to Algorithms—Obtaining Spectral Information from Real- and Imaginary-Time Response Functions

Emanuel Gull

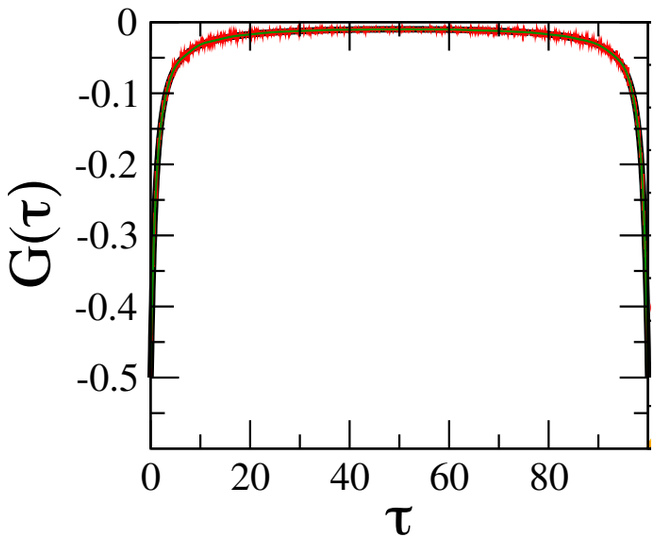
University of Michigan

Jani Fei, Chia-Nan Yeh, Dominika Zgid, Lei Zhang, Yang Yu, Lex Kemper, Chao Yang

Funding by NSF QIS (for Prony fitting) and DOE SciDAC (for projections)

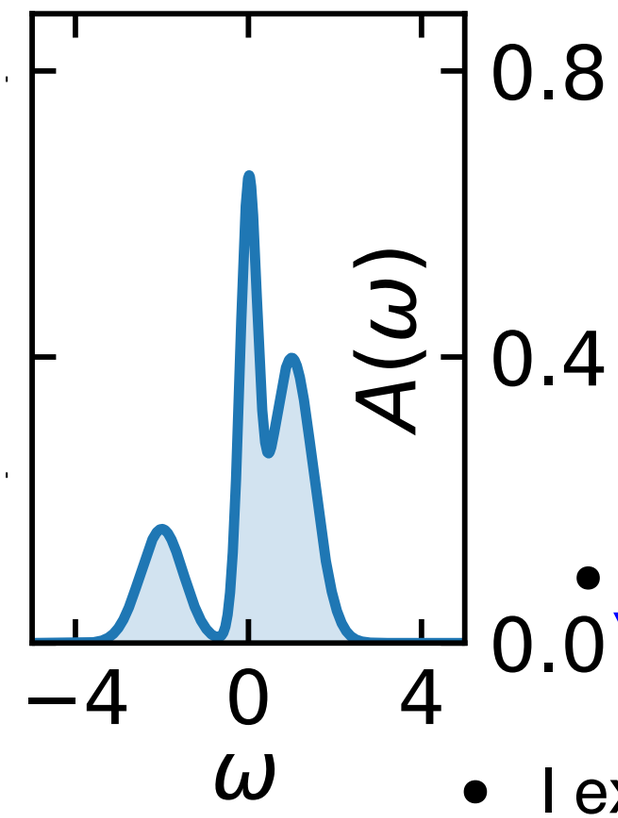
Obtaining spectral functions

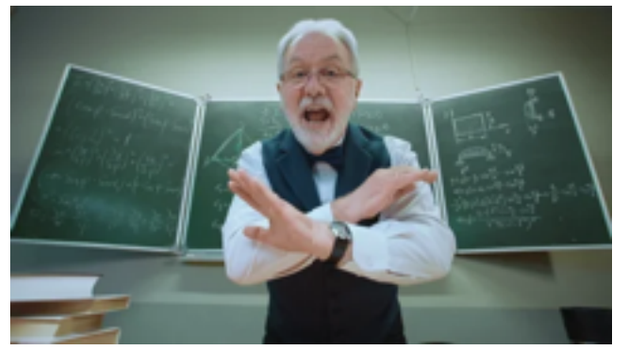
- Here's a correlation function!



- Give me the spectrum!

- Spectrum looks like this!





- Do you believe it?
- Why?
- Which feature?
- Can you exclude this scenario?
- I expect to see a bump around here. Can you give me the right spectrum?

This talk: 3 approaches

Can we put the AC problem on a rigorous mathematical footing?

Is there such a thing as ‘control’ & systematics, can we get ‘better’ continuations for better data? How about noise?

If time permits: Other things we can do with math, such as denoising & extending data

None of this is difficult, mostly 1920s math

…all of it comes with open source codes (MIT license). Test it with your own data. Ask me for help to get started!

…There will be translation problems between Condensed Matter & Nuclear / High Energy / Astro. Ask!

I will mostly limit to positive fermion spectral functions but bosons/anomalous/matrix-valued extensions are straightforward.

Obtaining spectral functions

- Well-known problem with finite-temperature field theories: analytic continuation to the real axis to obtain spectral functions is ill conditioned.

$$G(i\omega_n) = -\frac{1}{\pi}\int \frac{\mathrm{Im}G(\omega)d\omega}{i\omega_n - \omega}$$

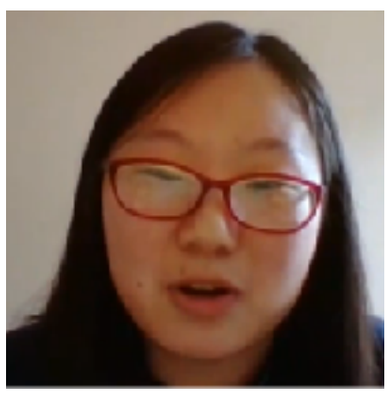
$$A(\omega) = \frac{-1}{\pi}\mathrm{Im}G(\omega)$$

$$G(i\omega_n) = K(i\omega_n, \omega)G(\omega)$$

$$\downarrow$$

$$G(\omega) = [K(i\omega_n, \omega)]^{-1}G(i\omega_n)$$

- Little progress can be made where data is noisy. However, when data is accurate, progress is possible…



Jiani Fei

- Green's functions satisfy mathematical ('Nevanlinna') properties

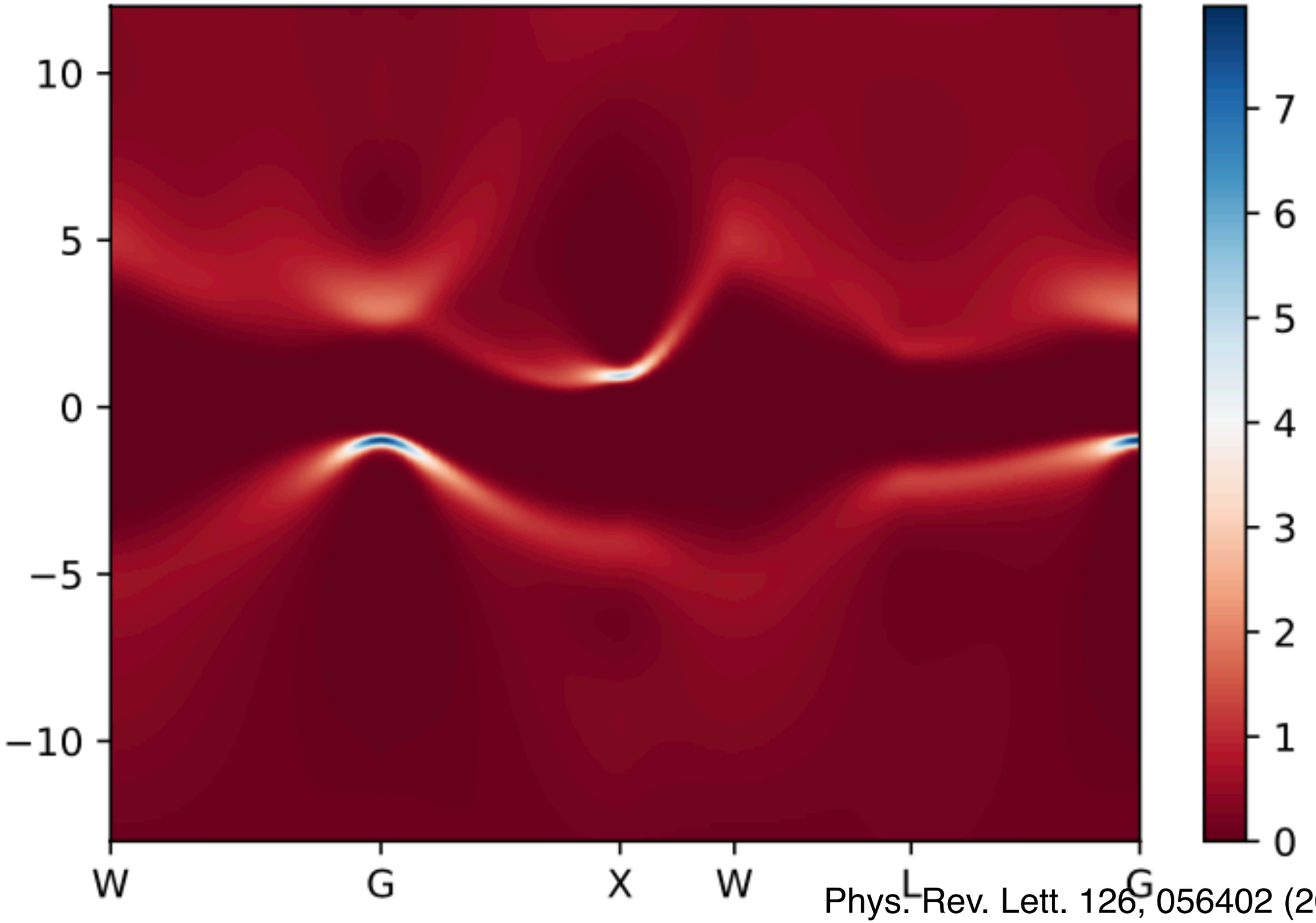
$$\mathrm{Im}\ G_\gamma(z) \leq 0 \quad \text{for} \quad z \in \mathbb{C}^+$$

- It is possible (and rather straightforward) to construct a numerical method that satisfies these mathematical properties
- Doing so vastly constrains the solution space and yields much better continuations.

Phys. Rev. Lett. 126, 056402 (2021)

Obtaining spectral functions

Si, 6x6x6 lattice, self-consistent GW



Phys. Rev. Lett. 126, 056402 (2021)

Green's functions & Lehmann Representation

Lehmann representation

$$G_\gamma(z) = \frac{1}{Z}\sum_{m,n}\frac{|\langle m|c_\gamma^\dagger|n\rangle|^2}{z+E_n-E_m}(e^{-\beta E_n}+e^{-\beta E_m})$$

G coincides with Matsubara Green's function on imaginary axis, with retarded Green's function just above real axis. Define

$$A = \frac{1}{Z}|\langle m|c_\gamma^\dagger|n\rangle|^2(e^{-\beta E_b}+e^{-\beta E_m}) > 0$$

For

$$z = x+iy$$

$$S = \frac{A}{(x+E_n-E_m)+iy} = \frac{A(x+E_n-E_m-iy)}{(x+E_n-E_m)^2+y^2}$$

$$\mathrm{Im}S = \frac{-Ay}{(x+E_n-E_m)^2+y^2}$$

And therefore for any Green's function, independent of the system:

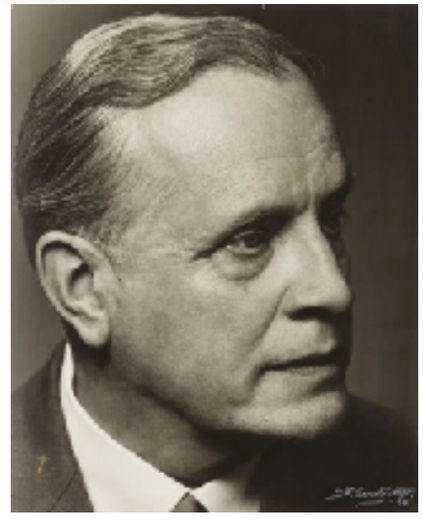
$$\mathrm{Im}\ G_\gamma(z) \leq 0 \quad \text{for} \quad z \in \mathbb{C}^+$$

Phys. Rev. Lett. 126, 056402 (2021)

Nevanlinna and Schur functions

Nevanlinna functions are functions with a positive imaginary part on the upper half of the complex plane.

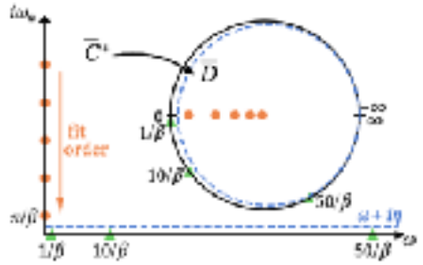
$$\mathcal{N}G = -G$$ Is a Nevanlinna function



Rolf Nevanlinna

The invertible Möbius transform h maps the upper half plane to the unit disk

$$h(z) : z \to \frac{z-i}{z+i}$$



$$\mathcal{D} = \{z : |z| < 1\};$$

$$\overline{\mathcal{D}} = \{z : |z| \leq 1\}$$

Nevanlinna functions can be mapped onto Schur functions: Schur functions map the open unit disk D to the closed unit disk D (‘contractive’ functions). Every Schur function has a continued fraction expansion that can be recursively defined.

Combine mapping to contractive functions with Schur’s continued fraction expansion to obtain an intrinsically causal expansion for Green’s functions

Phys. Rev. Lett. 126, 056402 (2021)

The Schur algorithm

Input data $f(Y_i) = C_i \quad i = 1,2,\ldots,M \qquad Y_i = i\omega_n \in \mathcal{C}^+ \text{ and } C_i \in \mathcal{C}^+$

Contractive interpolant.

$$\theta(Y_i) = \lambda_i = h(C_i) = \frac{C_i - i}{C_i + i} \quad i = 1,2,\ldots,M$$

Start the interpolation by constructing an interplant through Y_1. Express this contractive interpolant as a function that is zero at Y_1, and a constant λ_1:

We want $\theta(Y_1) = \lambda_1 \quad |\lambda_1| < 1$

Functional form $\theta(z) = \dfrac{\phi(z) + \lambda_1}{\lambda_1^* \phi(z) + 1}$ Where $\phi(z) = \dfrac{z - Y_1}{z - Y_1^*}\theta_1(z)$

Such that $\phi \in \mathrm{B} \text{ and } \phi(Y_1) = 0$

Issai Schur

J. Schur, Uber potenzreihen, die im innern des einheitskreises beschränkt sind, Journal für die reine und angewandte Mathematik **1918**, 122 (1918).

Note that $\theta_1(z)$ is now an arbitrary contractive function. Express it as a sum of a function that is λ_2 at Y_2 and an arbitrary contractive function. Express that one as the sum of a function that is λ_3 at Y_3 and an arbitrary contractive function, iterate and repeat for all interpolation points.

This will result in an expression for **all possible interpolants** in terms of a remaining arbitrary Schur/Nevanlinna function. We will use this freedom later.

Phys. Rev. Lett. 126, 056402 (2021)

The Pick criterion: existence of interpolants

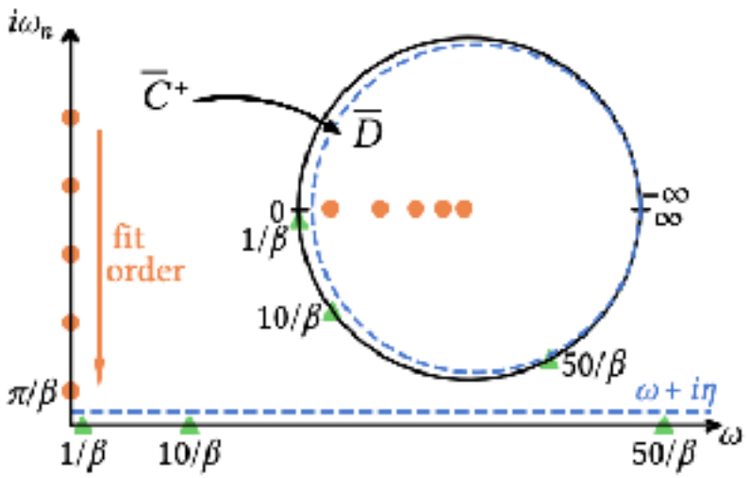
If $g(x_i) = y_i \quad (x_i \in \mathcal{D}, y_i \in \overline{\mathcal{D}})$

Then a Schur interpolant to g can be found iff the Pick matrix is positive semi-definite. It has a unique solution if furthermore the Pick matrix is singular.

$$P_{ij} = \left[\frac{1 - y_i y_j^*}{1 - x_i x_j^*} \right]$$

Georg A. Pick

G. Pick, Über die beschränkungen analytischer funktionen, welche durch vorgegebene funktionswerte bewirkt werden- ber die beschränkungen analytischer funktionen, welche durch vorgegebene funktionswerte bewirkt werden, Math. Ann. **78**, 270 (1917).

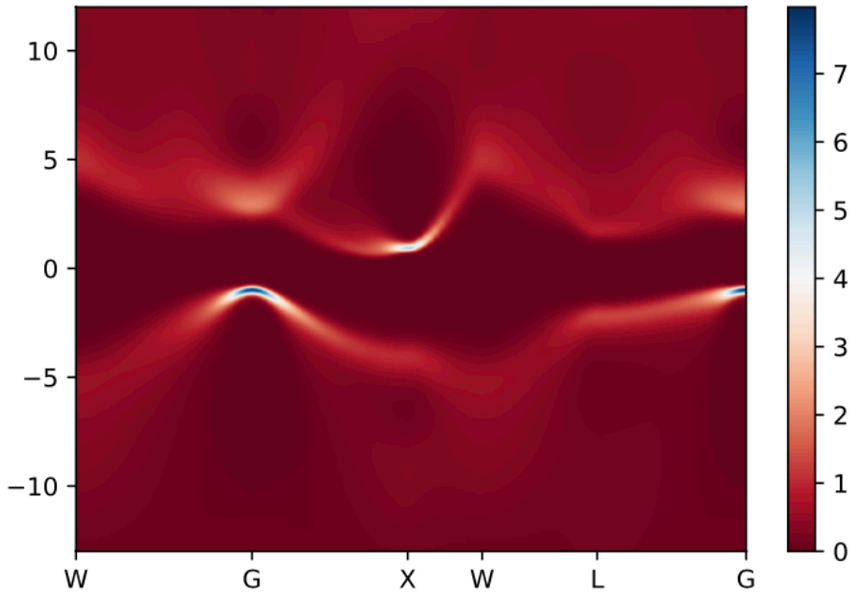


Provides a straightforward check on any input data. Transform the data to the unit circle, evaluate Pick matrix, check if it has negative eigenvalues. If it does, there WILL NOT be a positive spectral function.

Interesting observation: Monte Carlo data never fulfills this criterion. GW data only if very well converged and not too many interpolation points. Synthetic benchmark data shows very high precision at high frequency needed to make it work. Sign of the very constrained nature of Nevanlinna/Schur function space.

Phys. Rev. Lett. 126, 056402 (2021)

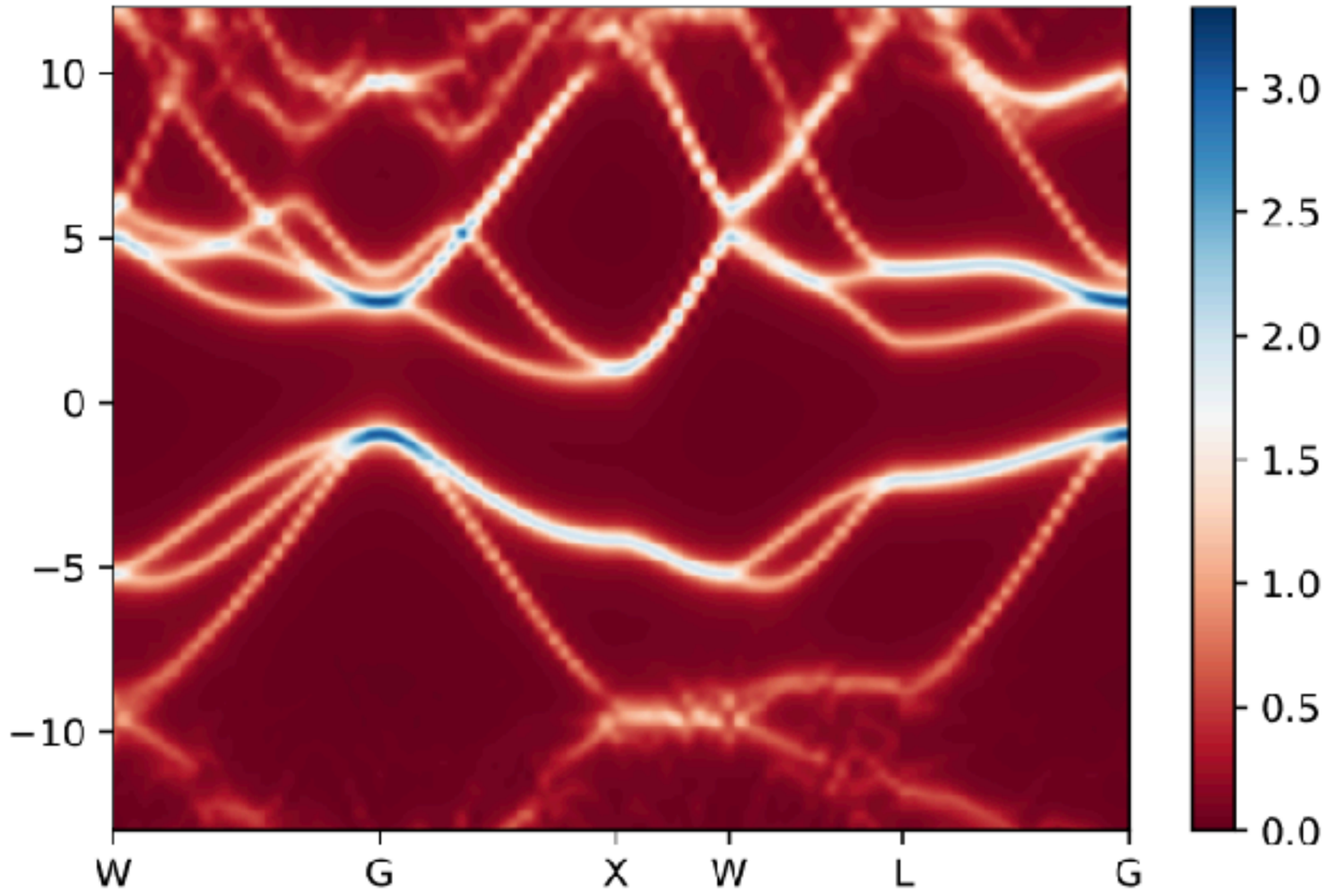
Old Technology vs Nevanlinna



Maxent, orbital- and k-resolved

Band structure is visible, individual bands can be separated

Both continuations operating on same input data!



Nevanlinna, orbital- and k-resolved

Fully self-consistent GW of Si, no quasiparticle or similar approximations, analytic continuation of fully interacting Green's function.

Analytic continuation

Phys. Rev. Lett. 126, 056402 (2021)

Constructing Approximate Nevanlinna functions

- While mathematically interesting, Nevanlinna continuation is not useful for noisy data. Even semi-analytic data is only accurate to ~14 digits.

- Don’t need interpolation. Need an approximation

- Traditional knowledge: lots of functions consistent within error bars, let’s pick the smoothest

- Claim here: We need a **new optimality criterion**. Let’s pick the function with the **least information** in it.

- Every Schur (Nevanlinna) function has a continued fraction expansion. Every continued fraction expansion can be written as a pole expansion. Let’s pick the pole expansion with the **fewest poles** that is **consistent with the data** and has the **right analytics**.

arXiv:2312.10576

Pole Representation

$$G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l},$$

$\xi_l \in \mathbb{C}$ denote M pole locations

$A_l \in \mathbb{C}$ the corresponding complex weights

- Provide G at points z in the upper half of the complex plane (or on the real axis), together with tolerance. Algorithm needed to find minimal M and corresponding pole locations and weights.

- Question related to an old applied Math / signal processing problem (1796, Gaspard de Prony)

$$\left| G_k - \sum_{i=0}^{K-1} w_i \gamma_i^k \right| \leq \varepsilon \text{ for all } 0 \leq k \leq 2N$$

- Interpolation of a function by a sequence of decaying exponential terms. Appropriate truncation leads to stable numerical algorithm.

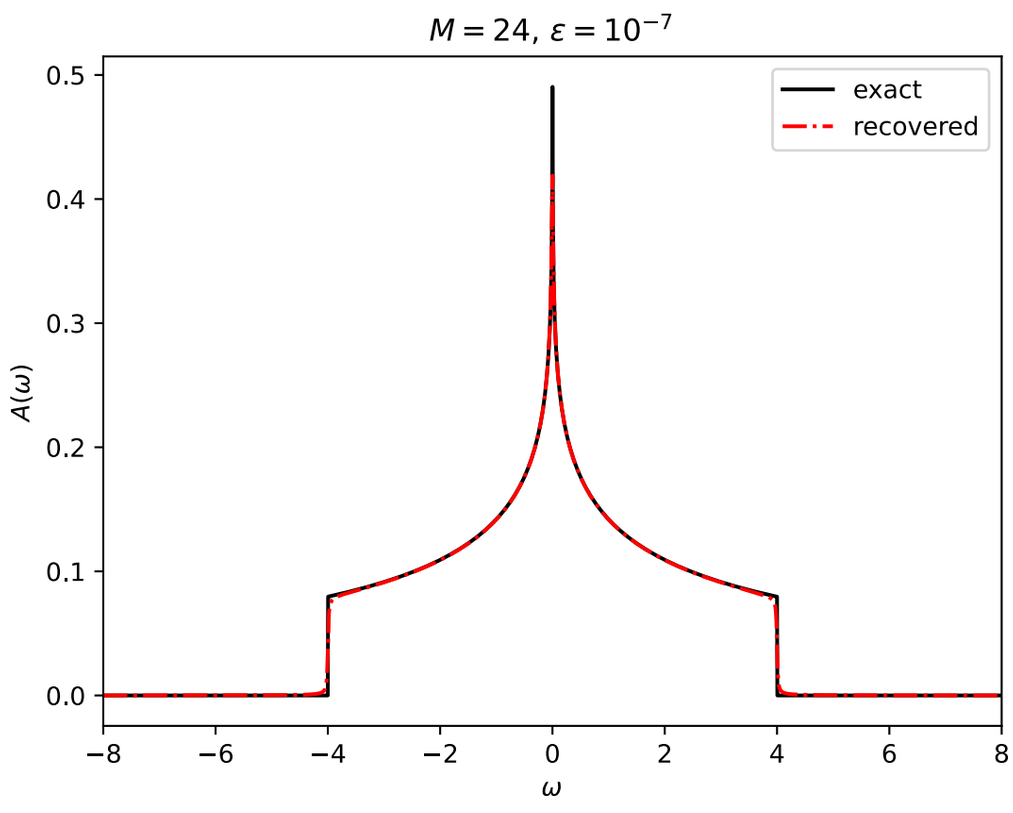
arXiv:2312.10576

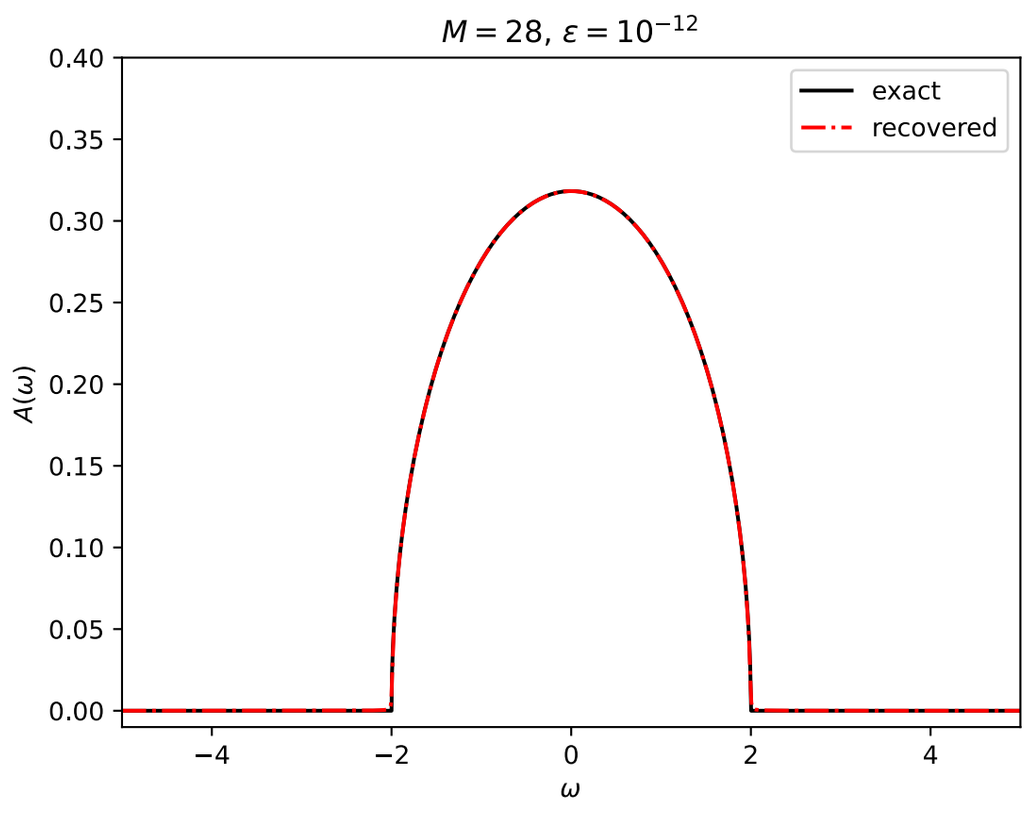
How compact is this approximation?

$$G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l},$$

$\xi_l \in \mathbb{C}$ denote M pole locations

$A_l \in \mathbb{C}$ the corresponding complex weights





- Data given on the real axis, approximated by pole approximation

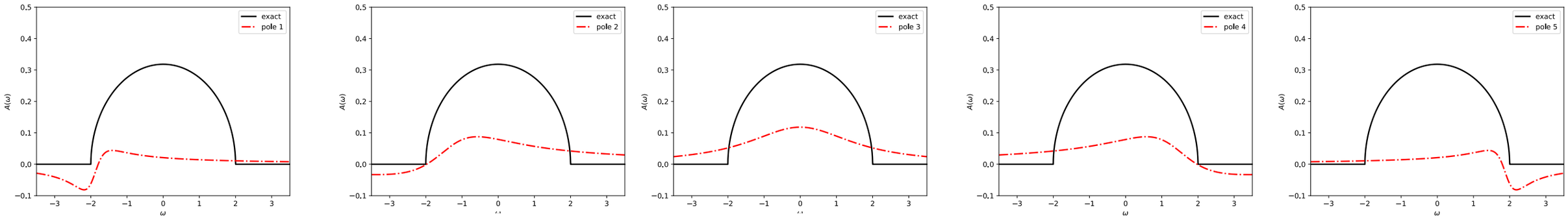
arXiv:2312.10576

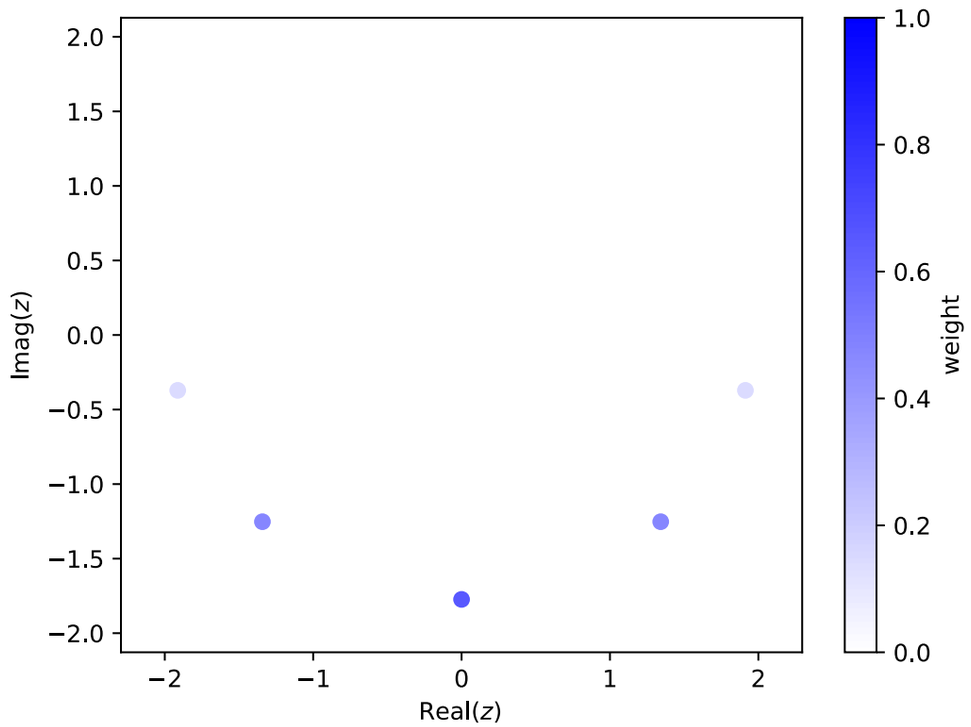
How compact is this approximation?

$$G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l},$$

$\xi_l \in \mathbb{C}$ denote M pole locations

$A_l \in \mathbb{C}$ the corresponding complex weights





arXiv:2312.10576

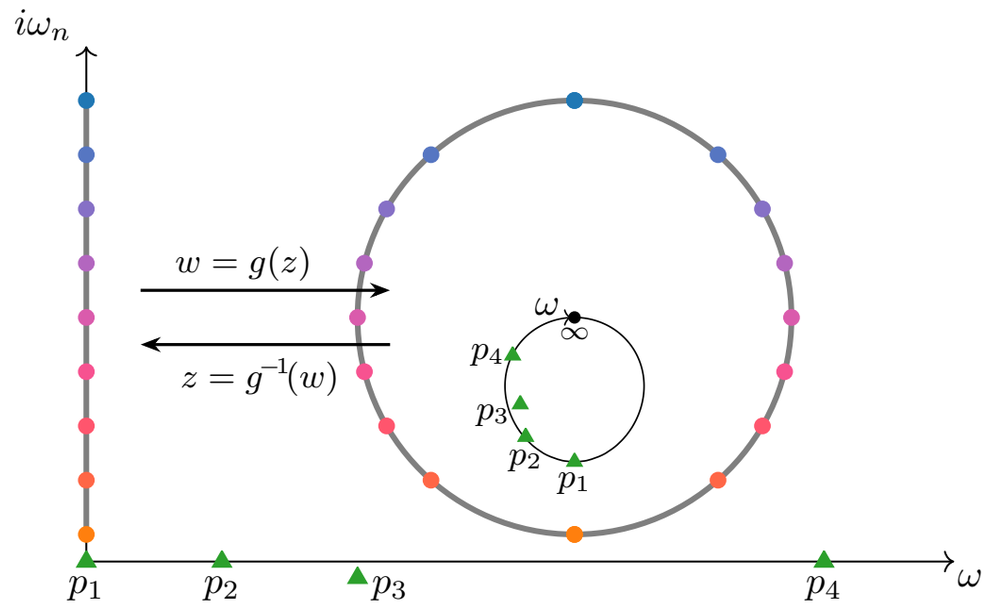
Prony AC in a nutshell

- Smooth approximation on imaginary axis (first Prony)

$$\left| G_k - \sum_{i=0}^{K-1} w_i \gamma_i^k \right| \leq \varepsilon \text{ for all } 0 \leq k \leq 2N$$

- Joukowsky transform to unit circle

$$\begin{cases} w = g(z) & = z_\mathrm{s} - \sqrt{z_\mathrm{s}^2 + 1} \text{ with } z_\mathrm{s} = \frac{z - i\omega_\mathrm{m}}{\Delta\omega_\mathrm{h}} \\ z = g^{-1}(w) & = \frac{\Delta\omega_\mathrm{h}}{2}(w - \frac{1}{w}) + i\omega_\mathrm{m} \end{cases}$$



- Calculation of moments (quadrature)

$$h_k := \frac{1}{2\pi i} \int_{\partial \bar{D}} \tilde{G}(w) w^k dw$$

- Residue theorem for poles says

$$h_k = \sum_l \tilde{A}_l \tilde{\xi}_l^k, \ k \geq 0 \ .$$

- Residue theorem for poles is a Prony problem

$$h_k = \sum_l \tilde{A}_l \tilde{\xi}_l^k, \ k \geq 0 \ .$$

- Transform poles back after mapping

$$\xi_l = g^{-1}(\tilde{\xi}_l) = \frac{\Delta\omega_\mathrm{h}}{2}(\tilde{\xi}_l - \frac{1}{\tilde{\xi}_l}) + i\omega_\mathrm{m} \ ,$$

$$A_l = \mathrm{Res}[G(z), \xi_l] = \frac{\Delta\omega_\mathrm{h}}{2}(1 + \frac{1}{\tilde{\xi}_l^2})\tilde{A}_l \ .$$

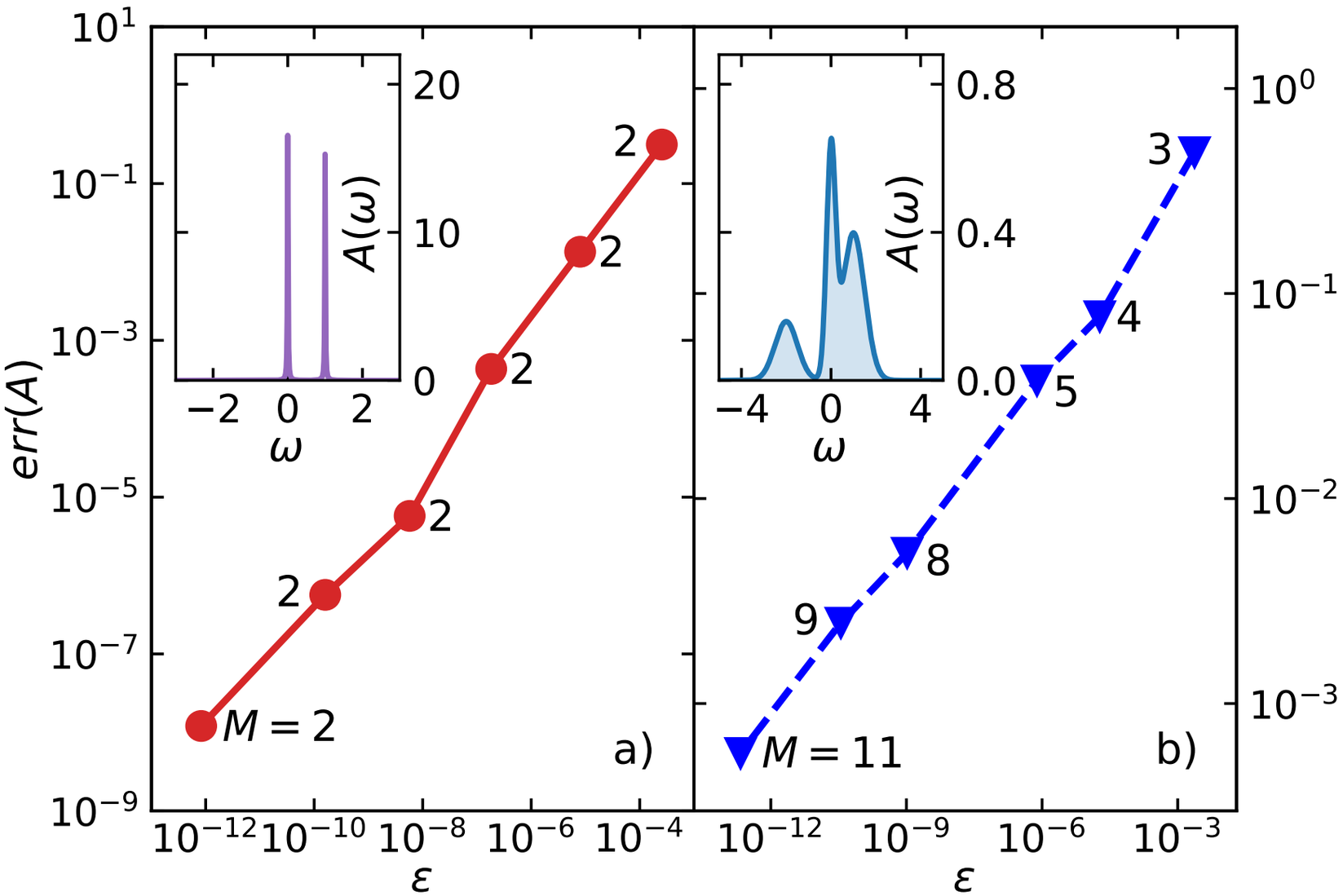
- All poles inside unit circle, so moments decay quickly

arXiv:2312.10576

Prony Analytic Continuation

$$G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l},$$

FIG. 2. Integrated real axis error $err(A) = \int_{\mathbb{R}} d\omega |A - A_{\text{cont}}|$ for the discrete (left) and continuous (right) case as a function of control parameter ε. Also indicated is the number of poles M. Inset: spectrum $A(\omega)$. Other parameters are $\beta = 200$, $n_0 = 30$ (left) and 0 (right), $\Delta n = 1$ and $N_\omega = 2001$.



- Data given on the imaginary axis, continued by Prony approximation

arXiv:2312.10576

Prony representation

$$G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l},$$

- Data given on the imaginary axis, continued by Maximum Entropy, Stochastic Analytic Continuation, and Prony approximation

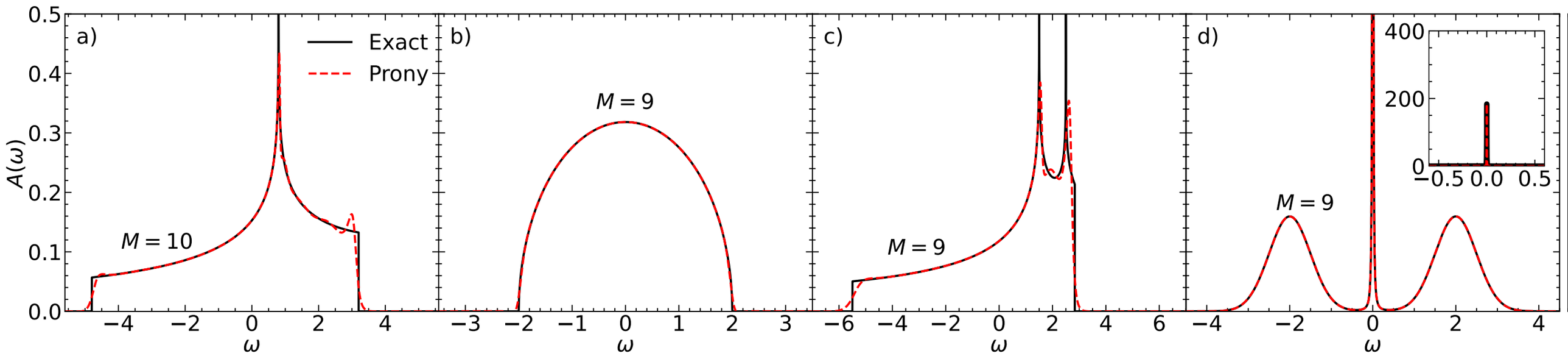


FIG. 3. Continuation of continuous spectral functions. From left to right: tight binding density of states of 2d square lattice with nearest- and next-nearest neighbor hopping. Semicircular density of states. Tight-binding density of states of the anisotropic triangular lattice. 'Kondo'-like spectral function. Shown are the exact input $A(\omega)$ in black, a continuation with Maximum Entropy (blue), SOM (purple), and a Prony fit (this method) in red. Maximum Entropy parameters fine-tuned to yield best spectra possible.

arXiv:2312.10576

Prony representation

$$G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l},$$

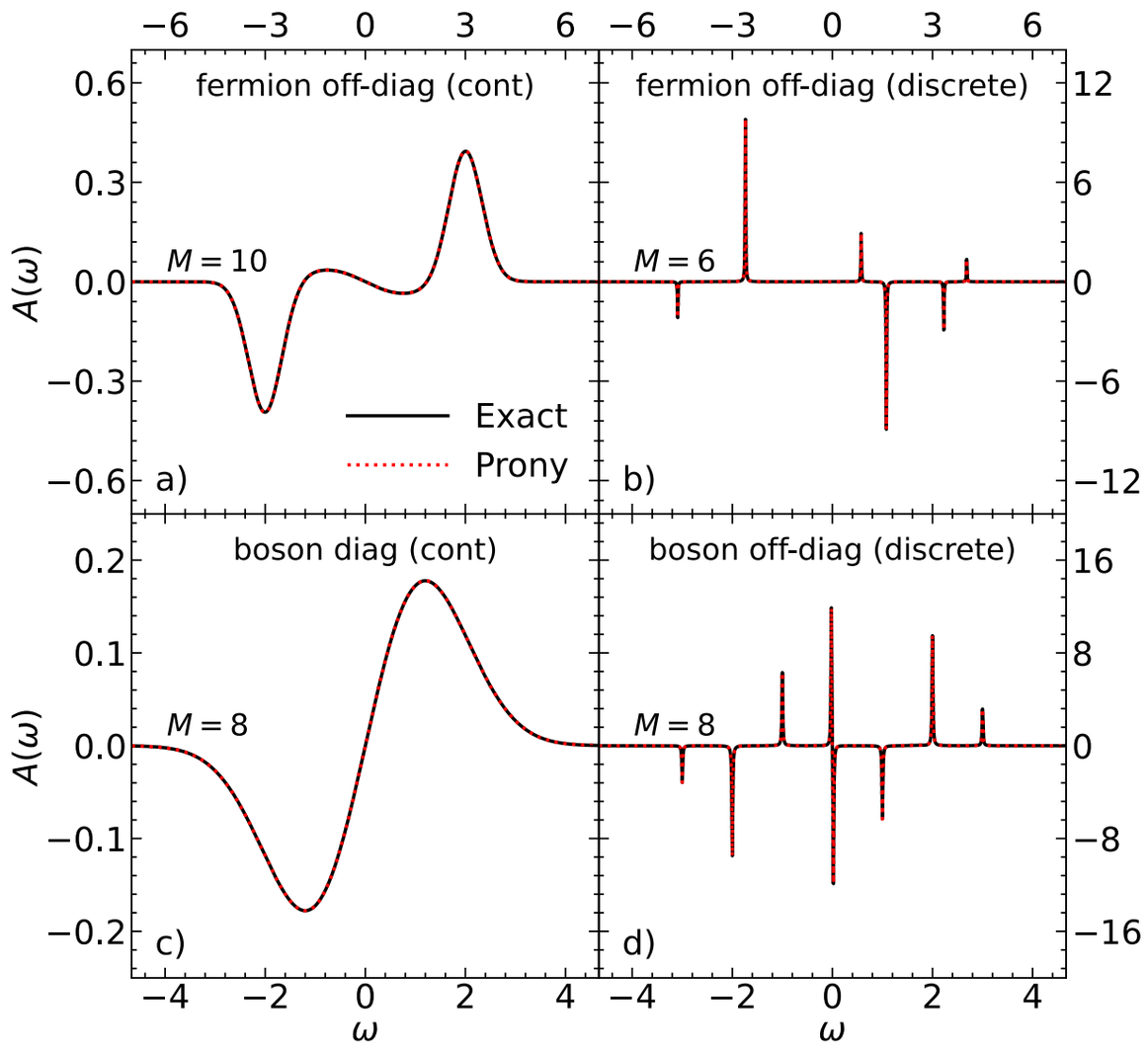
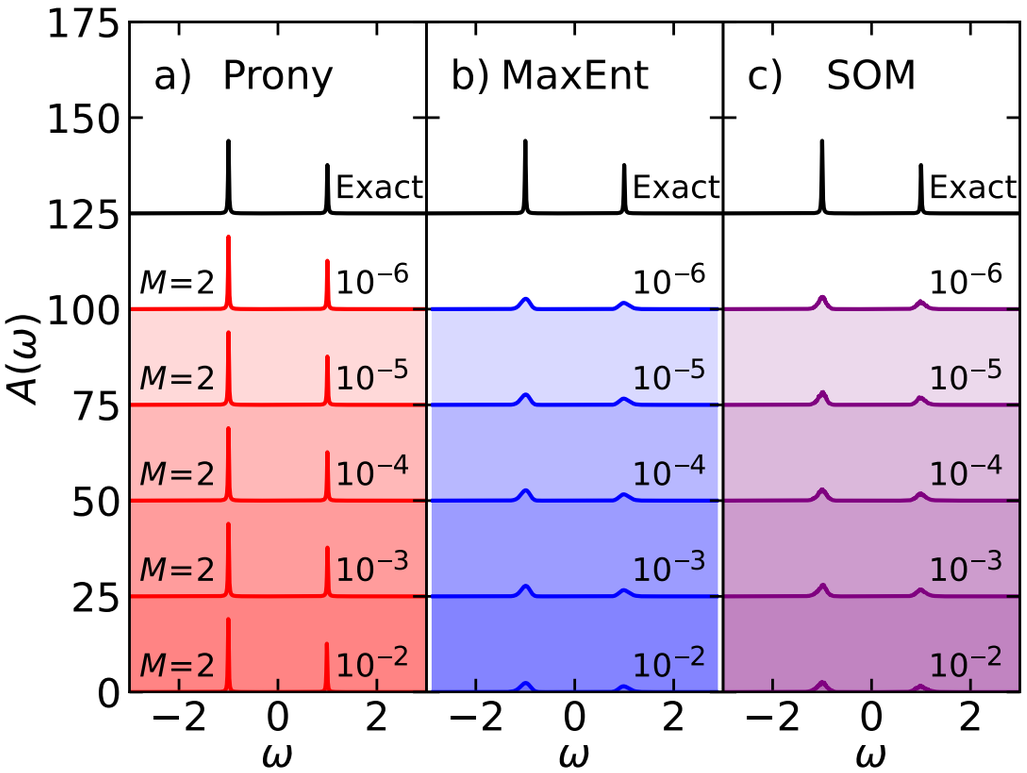
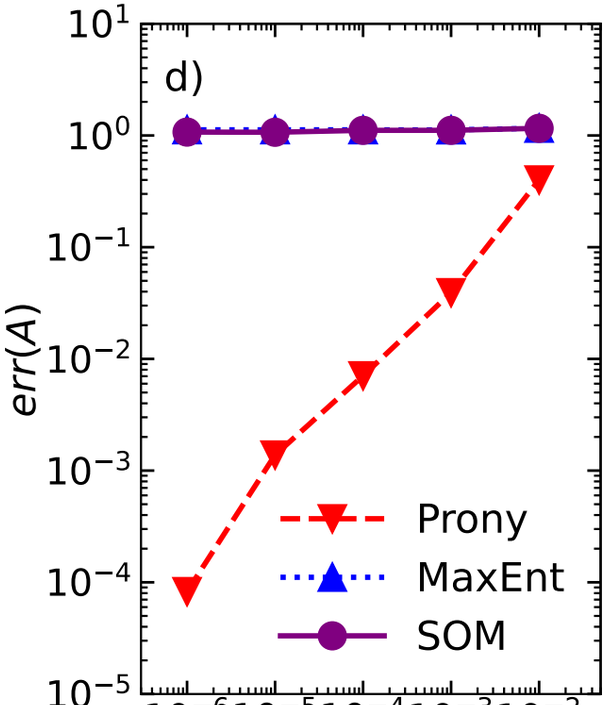


FIG. 4. Analytic continuation of non-positive spectral functions. Black: Exact input. Red: Continuation. Panel (a/b): off-diagonal continuous (a) and discrete (b) fermion case. (c) diagonal boson case. (d) discrete off-diagonal boson case.

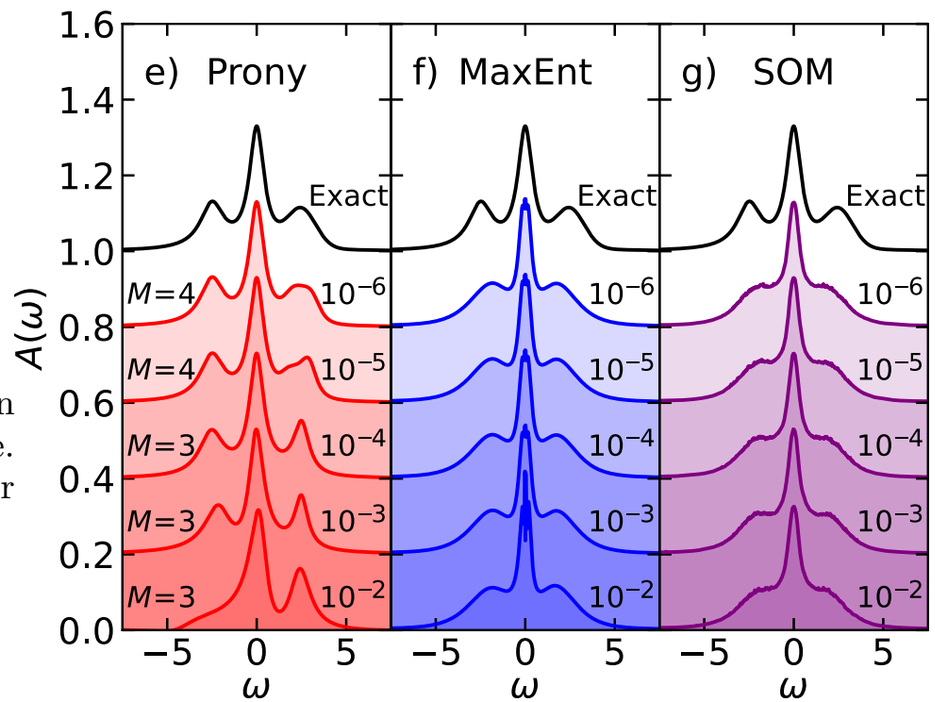
arXiv:2312.10576

Prony and noise





$$G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l},$$



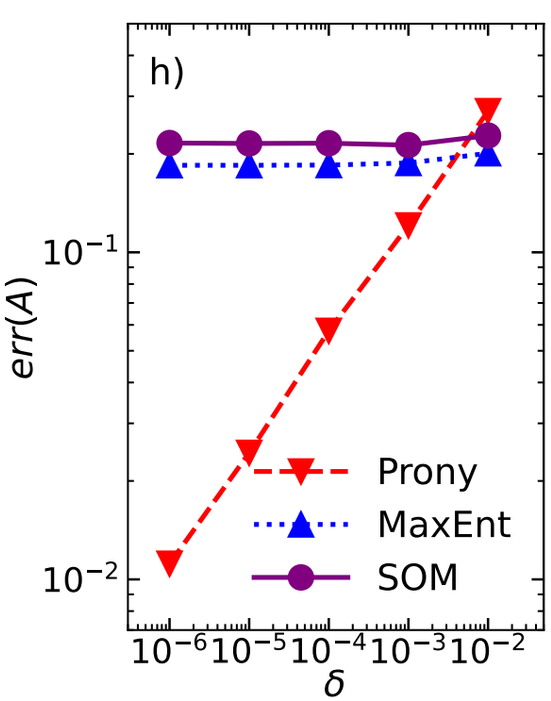


FIG. 5. Spectral functions for different levels of Gaussian noise δ on the imaginary axis. Upper panel: discrete case. Lower panel: continuous case. Also indicated is the number of poles M.

arXiv:2312.10576