

# Nevanlinna Analytical Continuation

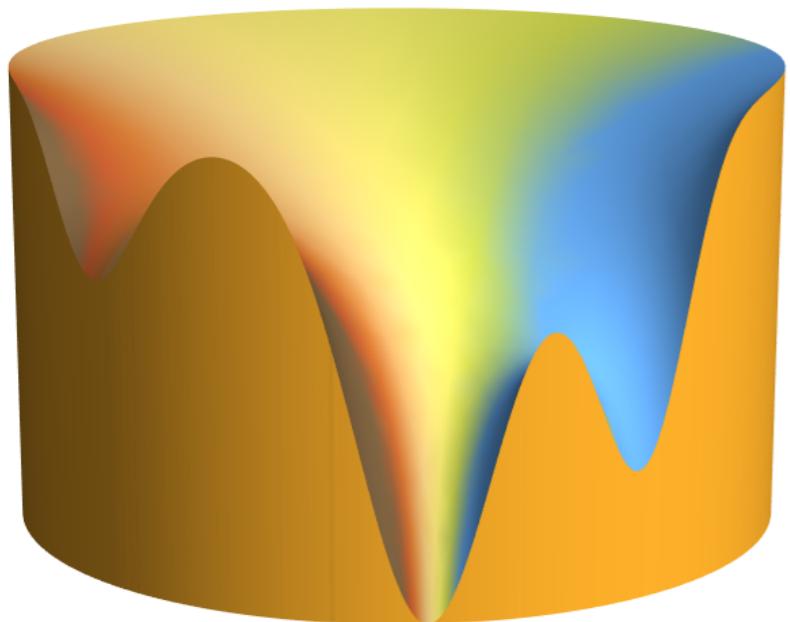
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# Collaborators



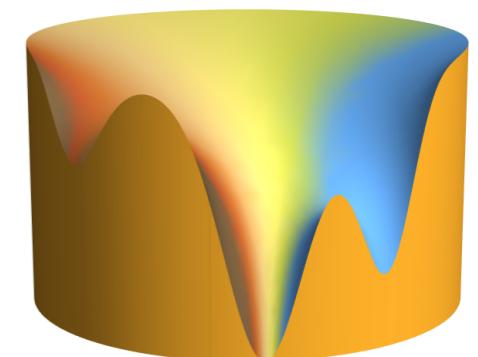
Jiani Fei



Chia-Nan  
Yeh

# This talk

- Introduction to Analytic Continuation
  - Existing methods, common challenges
  - Nevanlinna Theory and connection to Analytic Continuation
  - Pick matrices
  - Hamburger Moments
  - Carathéodory Generalizations
  - Results for model systems
  - Results for GW calculations
  - Outlook and future prospects
- Not in this talk
- Physics
  - Real-world applications



# Analytic Continuation

Finite-temperature simulations

$$Z = \text{Tr} e^{-\beta H}$$

$$G(\tau) = -\frac{1}{Z} \text{Tr}[e^{-(\beta-\tau)H} c e^{-\tau H} c^\dagger]$$

$$G(i\omega_n) = \int_0^\beta d\tau e^{-i\omega_n \tau} G(\tau)$$

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

Spectral function

Analytic continuation

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

$$G(\tau) = -\frac{1}{\pi} \int \frac{\text{Im}G(\omega)e^{-\tau\omega}d\omega}{1 + e^{-\beta\omega}}$$

Operational problem: inversion of the kernel K,

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

↓

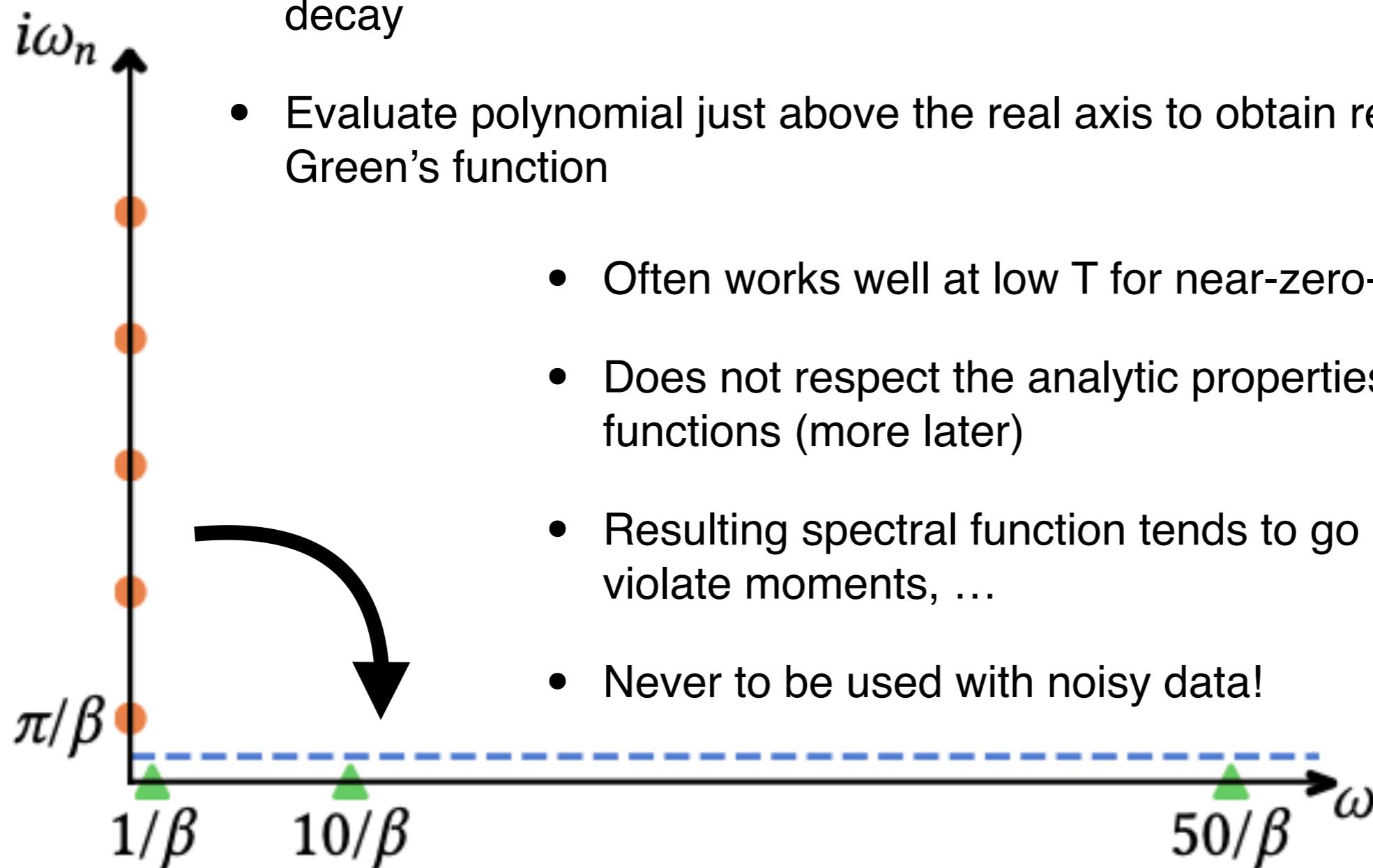
$$G(\omega) = [K(i\omega_n, \omega)]^{-1}G(\omega)$$

...is ill conditioned. Small changes on the imaginary axis cause large changes on the real axis.

Phys. Rev. Lett. 126, 056402 (2021)/arXiv:2107.0078

# Algorithm I – Rational Function Interpolation

- Given  $2n$  points on the Matsubara axis
- Find a rational polynomial interpolant with degree  $n+1$  in denominator, degree  $n$  in numerator, and  $\sim 1/i\omega_n$  high frequency decay
- Evaluate polynomial just above the real axis to obtain retarded Green's function
  - Often works well at low  $T$  for near-zero-frequency properties
  - Does not respect the analytic properties of the Green's functions (more later)
  - Resulting spectral function tends to go negative, oscillate, violate moments, ...
  - Never to be used with noisy data!



# Algorithm II – Maximum Entropy Method

- Define a functional  $Q$  that, for a given spectral function  $A$ , balances the effect of deviations from a default model with the desire to fit imaginary time data as accurately as possible.

$$Q = \alpha S - \frac{1}{2} \chi^2$$

Deviation from a default model       $S[A] = - \int d\omega \left[ A(\omega) \log \frac{A(\omega)}{m(\omega)} \right]$

Deviation from the input data

$$\chi^2 = \sum_{ij}^L (G(i\omega_n) - \bar{G}(i\omega_n))_i (C^{-1})_{ij} (G(i\omega_n) - \bar{G}(i\omega_n))_j$$

Minimize  $Q$ . First term will keep spectral functions smooth, second term will fit imaginary time data as well as possible.

# How do analytic continuations fail?

- In Padé: Rational polynomial approximation will put zeros and poles somewhere on the complex plane. If poles are in the upper half plane, spectral function will be unphysical. The more poles are added (the more data points are fitted), the less likely it is to succeed.
- Maxent: Arbitrary assumptions (minimization of entropy, free parameter  $a$ , default model dependence)
  - Minimization relies on optimization of highly non-linear functional
  - May (will) get stuck in local minima, problems with flat directions, etc.
  - Intrinsic systematics of Matsubara formalism: input data points are spaced at  $(2n+1)\pi T$ , any signal will be *linear* in  $T$  due to systematics
  - Restricted to positive spectral functions. Bosonic continuations rely on

$$\chi(i\Omega_n) = \frac{-1}{\pi} \int d\Omega \frac{\Omega}{i\Omega_n - \Omega} \frac{\text{Im}\chi(\Omega)}{\Omega} \quad \chi(i0) = \frac{-1}{\pi} \int d\Omega \frac{\text{Im}\chi(\Omega)}{\Omega}$$

i.e. to extract chi, continue chi/Omega and multiply by Omega.

# How do analytic continuations fail?

- All of this is a sign of the ill-conditioned continuation matrix and an intrinsic problem of the finite-temperature Green's function formalism
- The higher the frequency, the less trustworthy your data
- Trust integrals over wide areas
- Trust the first gap / peak but nothing behind it. Trust evolutions of features (emergence of gap/peak etc with control parameters)
- You can always trade a bit of a shoulder for a bit of peak height
- Careful with bosonic functions: continuations are even less reliable due to multiplication with Omega.
- If you find that your results depend on the type of continuation method used, the type of default model used, the choice of alpha, the precise noise statistics, etc, they are probably not reliable
- Best practice: only interpret when you can see a clear signature on the imaginary axis



# Our motivation for revisiting AC

- Lots of experience with AC in QMC / DCA / DMFT

- New data coming in

- Is very precise (

- Spans ridiculous range of energy scales

- MaxEnt loses most information if otherwise minimized

- What do other people do?

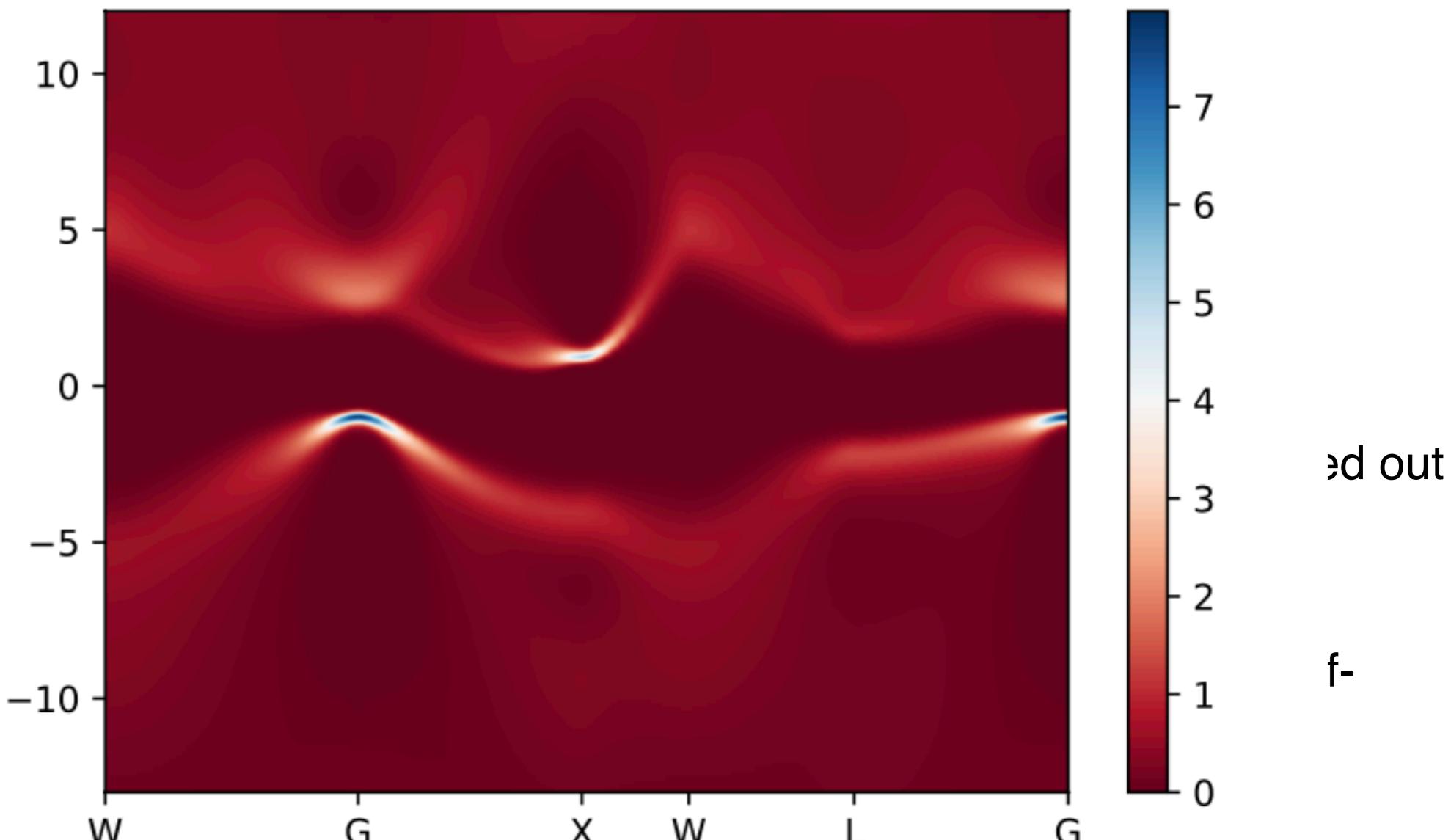
- Take band structure at specific energy

- Downfold to a narrow band

- Generally a brutal approximation

- Missing capabilities: Off-diagonal entries of self-energies & GF

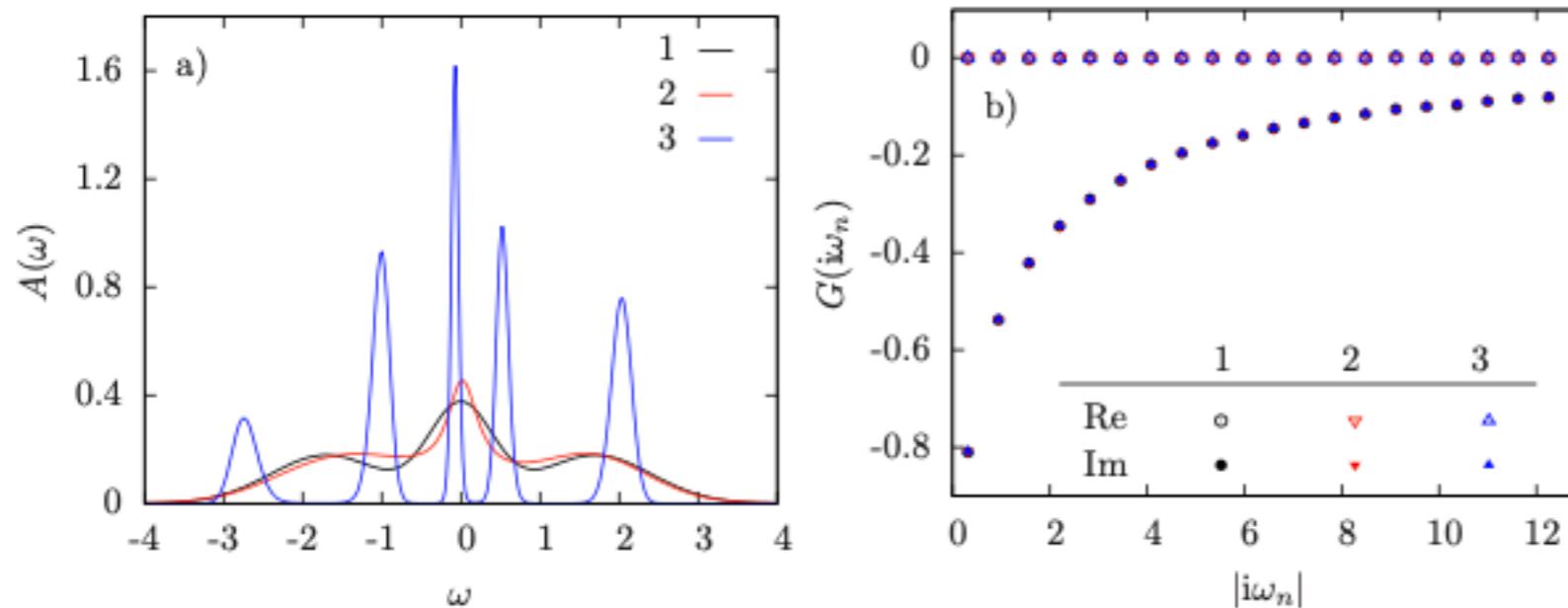
- Real-frequency Dyson equation



Maxent, orbital- and k-resolved

# How do do better?

- Sign of the ill-conditioned continuation matrix and an intrinsic problem of the finite-temperature Green's function formalism
- We can only hope to do better by using additional knowledge of the system to constrain the space of solutions.



S. Fuchs, PhD thesis,  
Göttingen, 2010

- Focus here on interpolation problems (i.e. precise data, not Monte Carlo)
- Realization in 2020: We know that causal functions do not have poles in the upper half plane. Can we use this property to improve the quality of continuations?

# Green's functions are Nevanlinna

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

$$z = x + iy$$

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

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

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

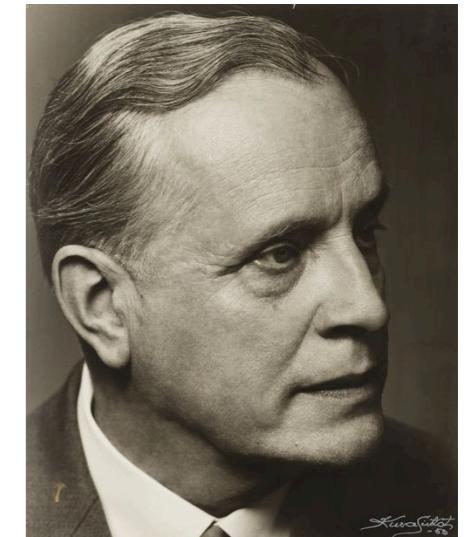
$$\text{Im } G_\gamma(z) \leq 0 \quad \text{for } z \in \mathbb{C}^+$$

Any interpolation algorithm should respect this property. Enforcing it will constrain solutions and give better interpolants.

# Nevanlinna functions

Nevanlinna functions are functions with a positive imaginary part on the upper half of the complex plane. Enforcing a positive imaginary part will enforce positive spectral functions on the real axis.

$$\mathcal{N}G = -G \quad \text{Is Nevanlinna}$$



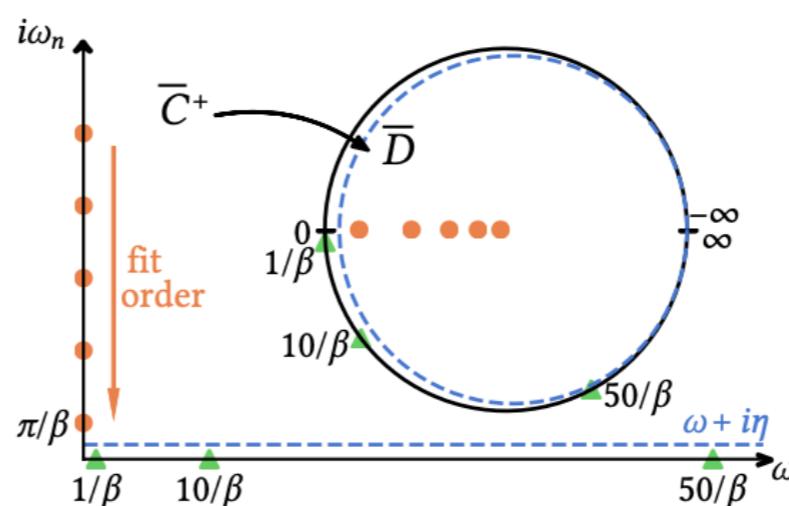
Schur studied a class of functions that map the open unit disk  $D$  to the closed unit disk  $\bar{D}$ , and showed that every Schur function has a continued fraction expansion that can be recursively defined.

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

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

$$\begin{array}{ccc} \mathcal{C}^+ & \xrightarrow{f} & \overline{\mathcal{C}}^+ \\ h_1 \downarrow & \searrow \theta & \downarrow h \\ \mathcal{D} & \xrightarrow[g]{} & \overline{\mathcal{D}} \end{array}$$

$f$  : Nevanlinna function  $\in \mathbb{N}$   
 $g$  : Schur function  $\in \mathbb{S}$   
 $\theta$  : Contractive function  $\in \mathbb{B}$   
 $h/h_1$  : Conformal mapping (e.g. Möbius transform)



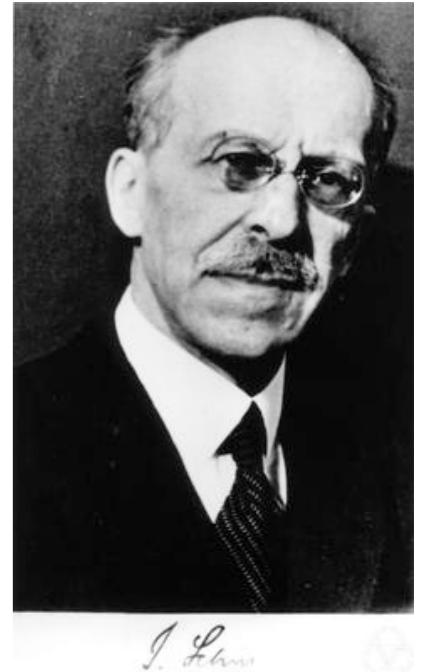
$$\mathcal{D} = \{z : |z| < 1\};$$

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

Rolf Nevanlinna

Thus combine the Möbius transform with Schur's continued fraction algorithm to obtain an intrinsically positive expansion

# The Schur algorithm



Input data

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

Contractive  
interpolant.

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

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  $\lambda_1$ :

We want

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

Issai Schur

Functional form

$$\theta(z) = \frac{\phi(z) + \lambda_1}{\lambda_1^* \phi(z) + 1}$$

Where

$$\phi(z) = \frac{z - Y_1}{z - Y_1^*} \theta_1(z)$$

Such that

$$\phi \in \mathbb{B} \text{ and } \phi(Y_1) = 0$$

Note that  $\theta_1(z)$  is now an arbitrary contractive function. Express it as a sum of a function that is  $\lambda_2$  at  $Y_2$  and an arbitrary contractive function. Express that one as the sum of a function that is  $\lambda_3$  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 contractive function. Note that rather than a single function, we obtain the class of all possible Nevanlinna functions.

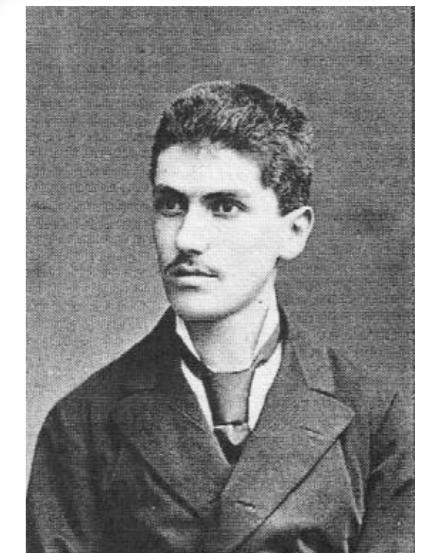
# The Pick criterion: existence of interpolants

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

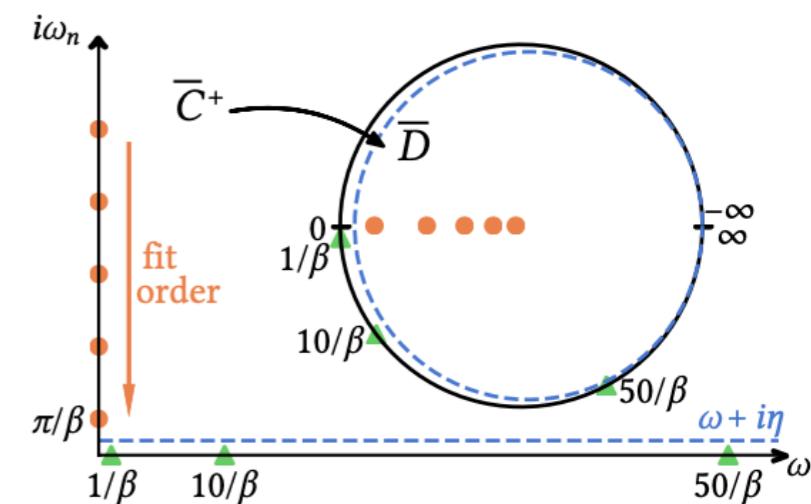
Then a Schur interpolant to  $g$  can be found if and only if the Pick matrix is positive semi-definite. It has a unique solution if furthermore the Pick matrix is singular.

$$P_{ij} = \begin{bmatrix} 1 - y_i y_j^* \\ 1 - x_i x_j^* \end{bmatrix}$$

This provides a straightforward check on any Matsubara 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.



Georg A. Pick



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.

# Results for synthetic systems

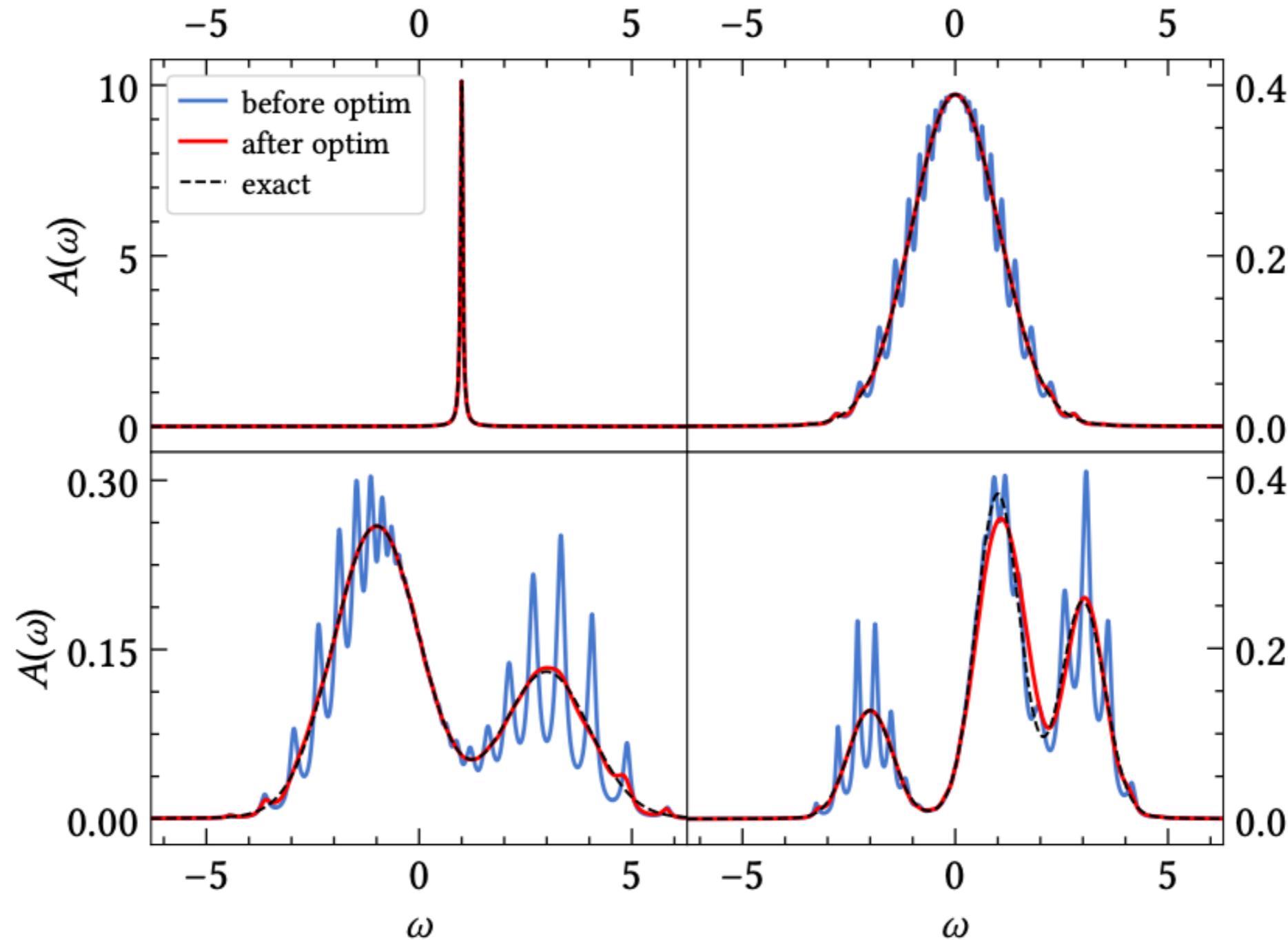


Figure 1.4: Continuation with and without Hardy function optimization. Off-centered  $\delta$  peak (top left), Gaussian (top right), two-peak scenario (bottom left), and a three-peak scenario (bottom right).  $\beta = 100$ , IR grid [13, 14] with 36 Matsubara positive frequency points.

# Comparison to Maximum Entropy

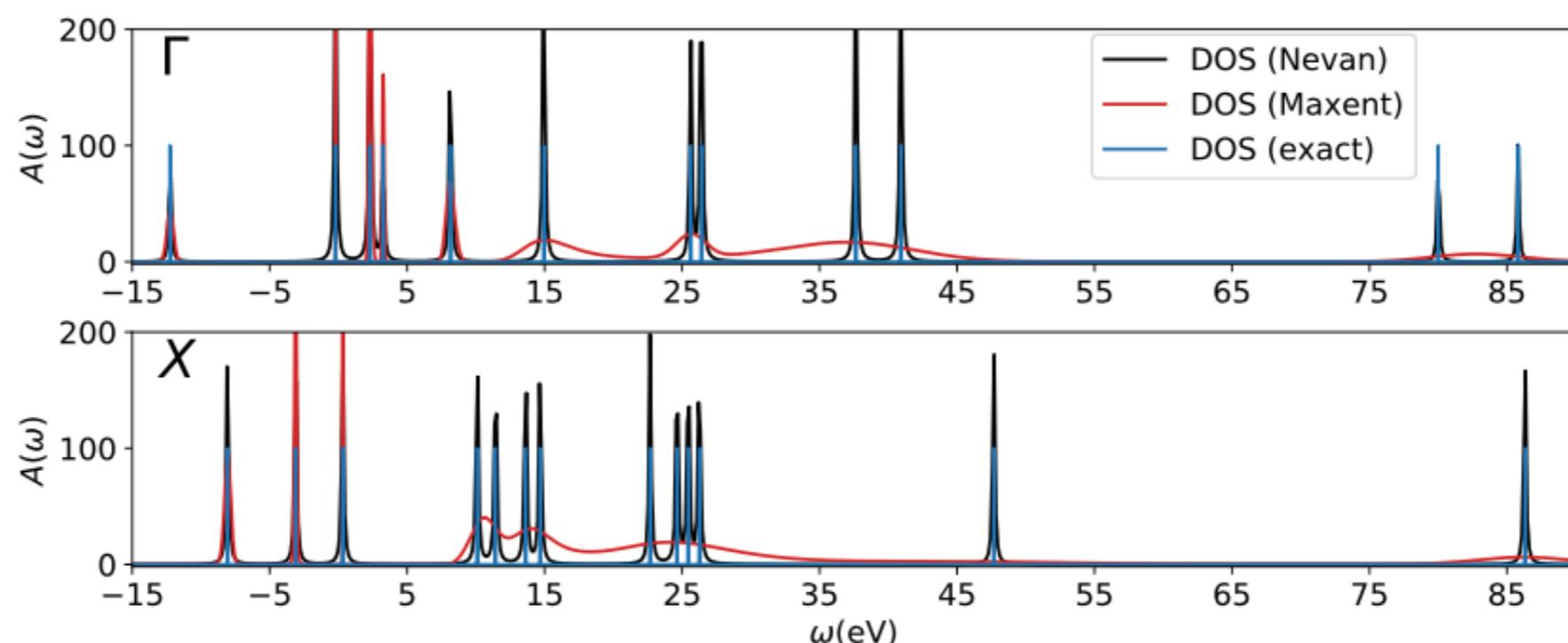
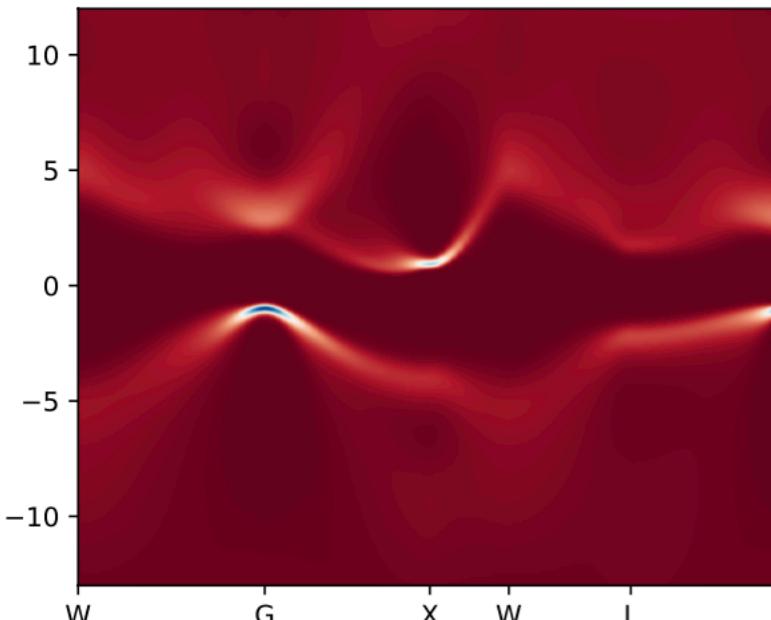


Figure 1.6: LDA band structure (Kohn Sham eigenvalues, DOS) of solid Si (green) at the  $\Gamma$  and the  $X$  point, as well as Nevanlinna (blue) and MaxEnt (orange) continuations of the corresponding Green's functions. T=316 K, 52 non-uniform [14] IR Basis [13] Matsubara positive frequency points.

# Comparison to Maximum Entropy



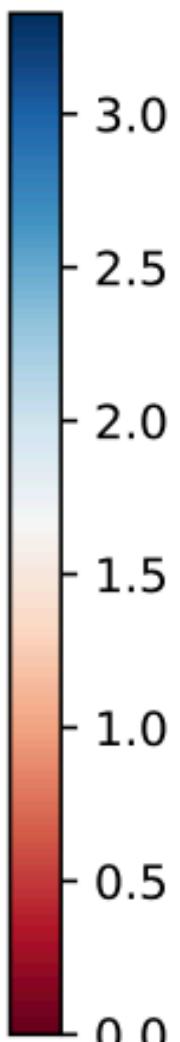
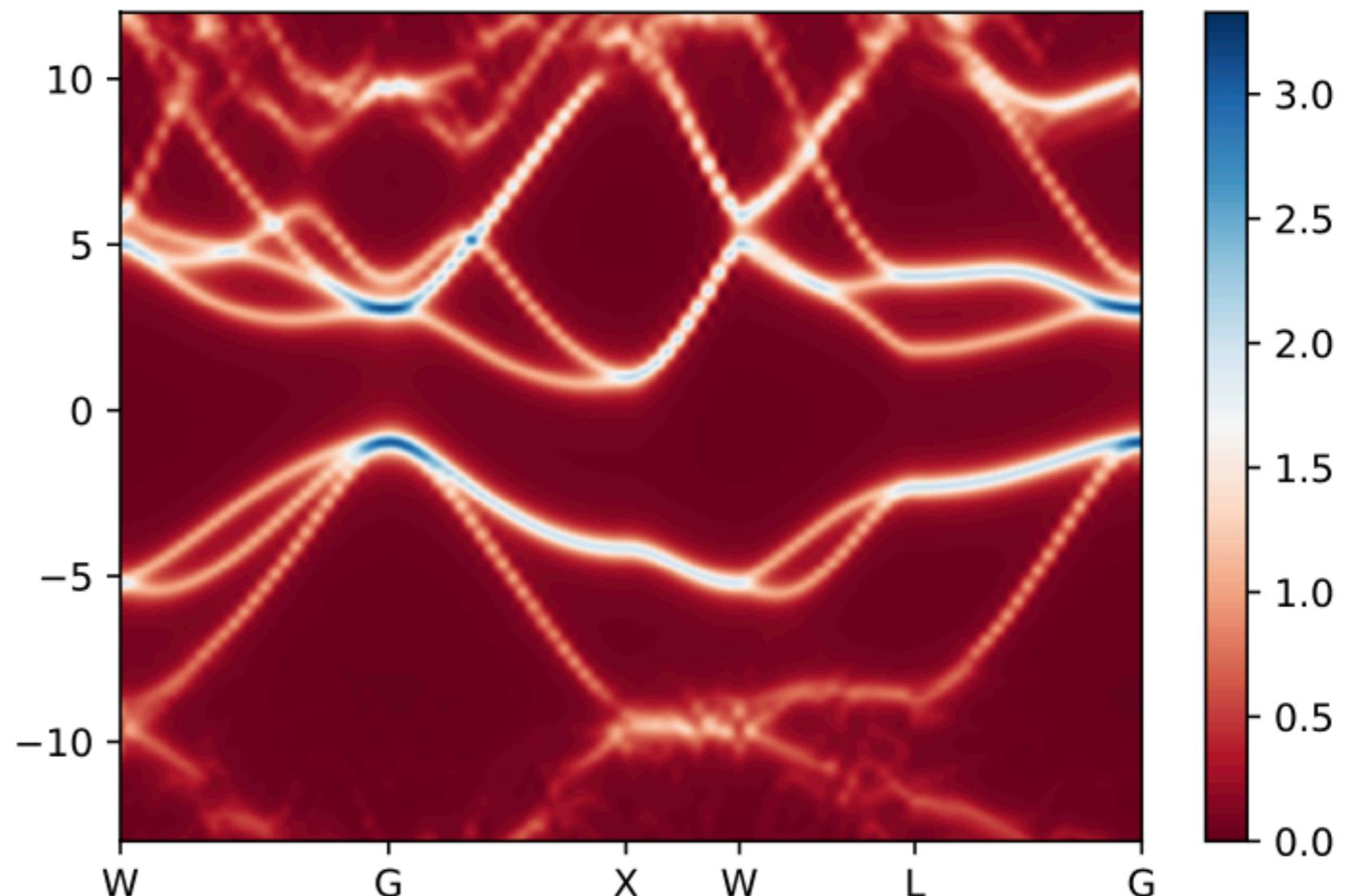
Maxent, orbital- and k-resolved

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



Band structure is visible, individual bands can be separated

Both continuations operating on same input data!



Nevanlinna, orbital- and k-resolved

# Matrix-valued Carathéodory generalization

The Carathéodory class of matrix-valued analytic functions in the unit disk (for us: upper half plane) is defined as

$$C = \{M(z) : M(z) + M^\dagger(z) \geq 0 \quad \forall |z| < 1\}$$

Note that

$$M(z) + M^\dagger(z) \geq 0 \iff \operatorname{Re}\{x^\dagger M(z)x \geq 0\}$$

i.e. the real part of  $M$  is positive semidefinite.

$-iG^<(\omega)$  is Carathéodory:



Κωνσταντίνος  
Καραθεοδωρή

$$G_{ij}^<(\omega) = 2\pi i \sum_{mn} \frac{e^{-\beta E_n}}{Z} \langle n | c_j^\dagger | m \rangle \langle m | c_i | n \rangle \delta(\omega - E_n + E_m)$$

Insert  $x$ , do the Math:

$$\langle x | -iG^<(\omega) | x \rangle = 2\pi \sum_{mn} \frac{e^{-\beta E_n}}{Z} |\langle m | \sum_i c_i x_i^* | n \rangle|^2 \delta(\omega - E_n + E_m)$$

# Carathéodory in many-body

$-iG^<(\omega)$  is Carathéodory / has positive semidefinite real part on upper half plane

$iG^>(\omega)$  is Carathéodory / has positive semidefinite real part on upper half plane

$iG(i\omega_n)$  is Carathéodory / has positive semidefinite real part on upper half plane

Without proof here: if we split the Self-energy into a Hartree term and a dynamical term, and the non-interacting Hamiltonian is quadratic, then

$i\Sigma(i\omega_n)$  is Carathéodory / has positive semidefinite real part on upper half plane

Without proof here: define the cumulant as  $M^{-1}(z) = G^{-1}(z) + F$

(The ‘Green’s function without the Fock matrix’ )

$iM(z)$  is Carathéodory / has positive semidefinite real part on upper half plane

# Carathéodory mapping

The interpolation of Carathéodory functions is a well-known problem. Proceed by Möbius transform to unit disc, Schur algorithm, evaluation on the boundary, and Möbius transform back. Guaranteed to give intrinsically PSD interpolants with full off-diagonal structure!

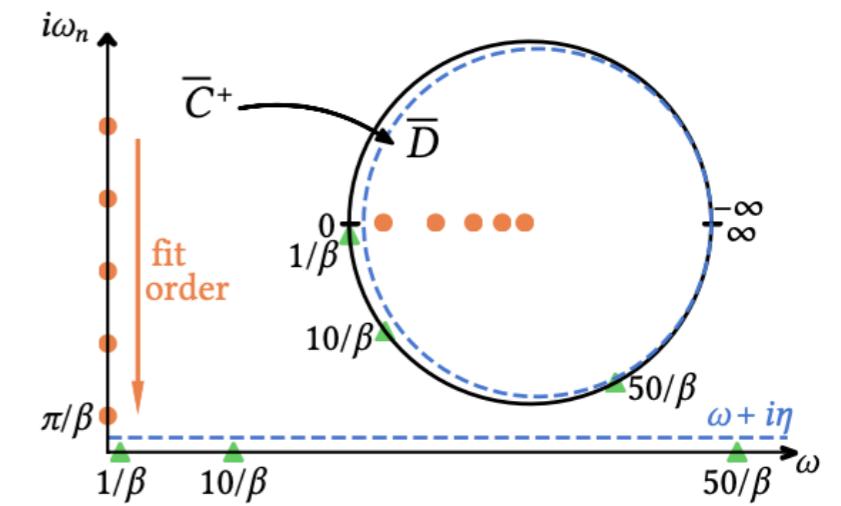
Conformal mapping of Matsubara points:

$$h : \mathcal{C}^+ \rightarrow \mathcal{D}, z \rightarrow \frac{z - i}{z + i}$$

Conformal mapping of function values  
(all quantities are matrices):

$$\Psi(z) = [I - F(z)][I + F(z)]^{-1}$$

...where  $F$  is the PSD function to be interpolated, i.e.



$$\begin{aligned}F(z) &= i\Sigma(z) \\F(z) &= iG(z)\end{aligned}$$

Set  $F(x_i) = Y_i$

$$\Psi(z_i) = [I - Y_i][I + Y_i]^{-1}$$

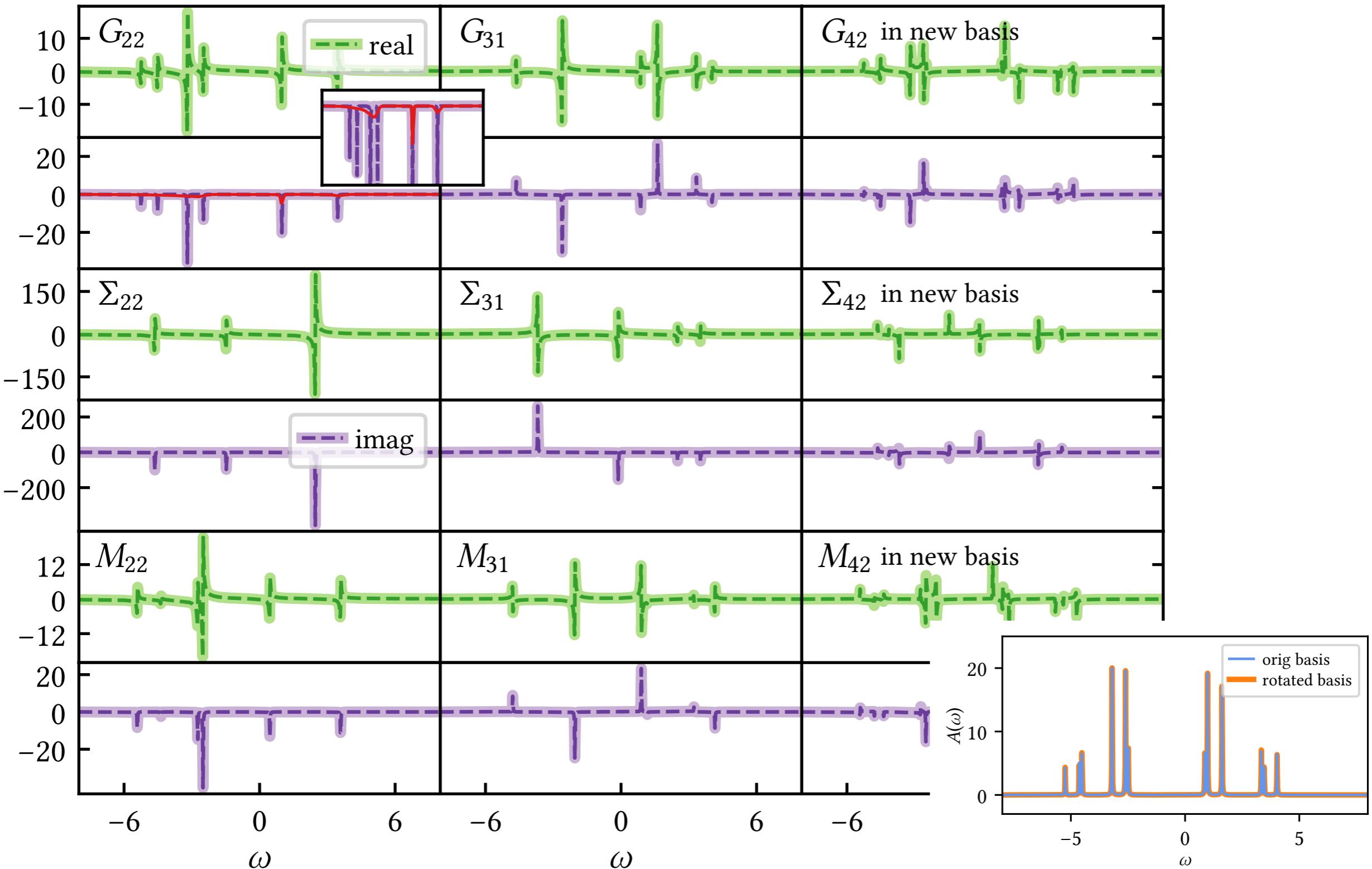
With  $\Psi$  a Schur class function on the unit disc

# The Hubbard Dimer

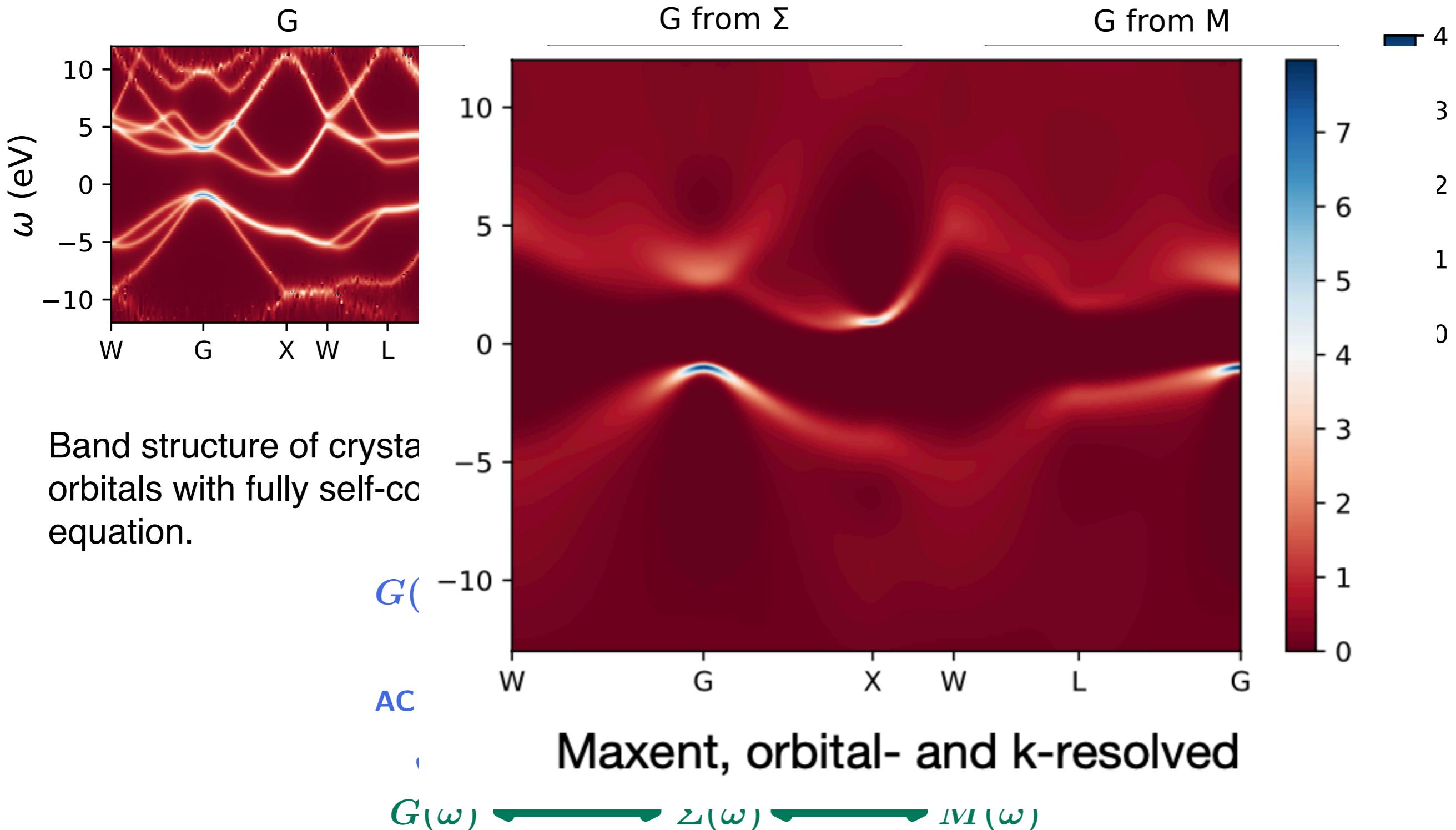
Diagonal

Off-Diagonal

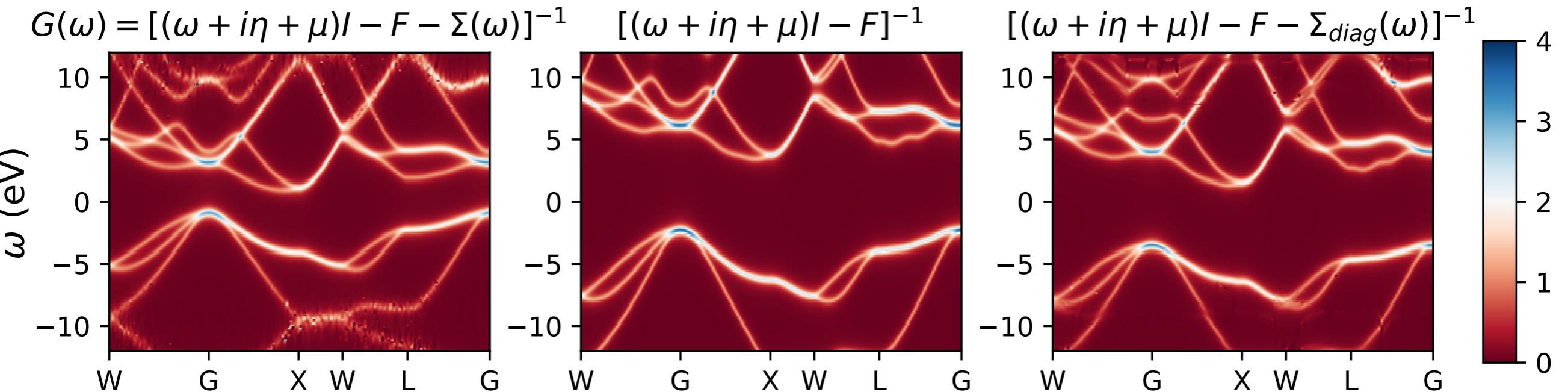
Random rotation



# Dyson commutes with continuation



# Careful with approximations to Sigma!



Truncation of the dynamical part of the self-energy (just the Fock matrix of the fully interacting system); or truncation of the self-energy to just diagonal parts.

‘Diagonal’ approximations to the self-energy have a huge effect on the band structure. Careful, this is what is usually done in LDA+DMFT-type ‘real materials’ calculations.

# Work in progress

- How about noise? Can we do Nevanlinna ‘fits’ or ‘expansions’ rather than interpolations?
  - Use a basis of Schur function space, expand & project
- Can we overcome the limitations of bosonic continuations (such as amplification of error with frequency, etc)?
  - $\omega\chi(\omega)$  is Nevanlinna. Use Hardy functions to enforce normalization of integral via the value at  $\chi(0)$
- Can we use the formalism to overcome some of the limitations of iterative methods (causal projections of intermediate steps, etc)

# Interested in trying it out?

- Write an email to [egull@umich.edu](mailto:egull@umich.edu) and [jianif@umich.edu](mailto:jianif@umich.edu), and we'll help you get started
- ‘Unlicensed’ code (free to use for any purpose with no strings attached) published as supplemental material of our paper:  
<https://journals.aps.org/prl/supplemental/10.1103/PhysRevLett.126.056402>  
(4 pages of C++)
- Have a look at Jiani Fei’s honors thesis  
<http://sites.lsa.umich.edu/gull-lab/wp-content/uploads/sites/480/2021/05/jianif.pdf>

# In conclusion

- Analytic Continuation remains difficult. No way to bring information back that isn't in the data. Careful with 'p-hacking' analytic continuation
- ...but by using the appropriate Math we can obtain much more accurate continuations
  - Build in causality
  - Build in moments
- ...New capabilities: continuation of off-diagonal terms that respect the analytic structure of the Green's function
- ...New capabilities: continuation of moments and self-energies
- Complex Analysis is a very powerful theory. Use it!

# Many Thanks to Jiani & Chia-Nan!



Jiani Fei



Chia-Nan  
Yeh



# Hardy function contribution

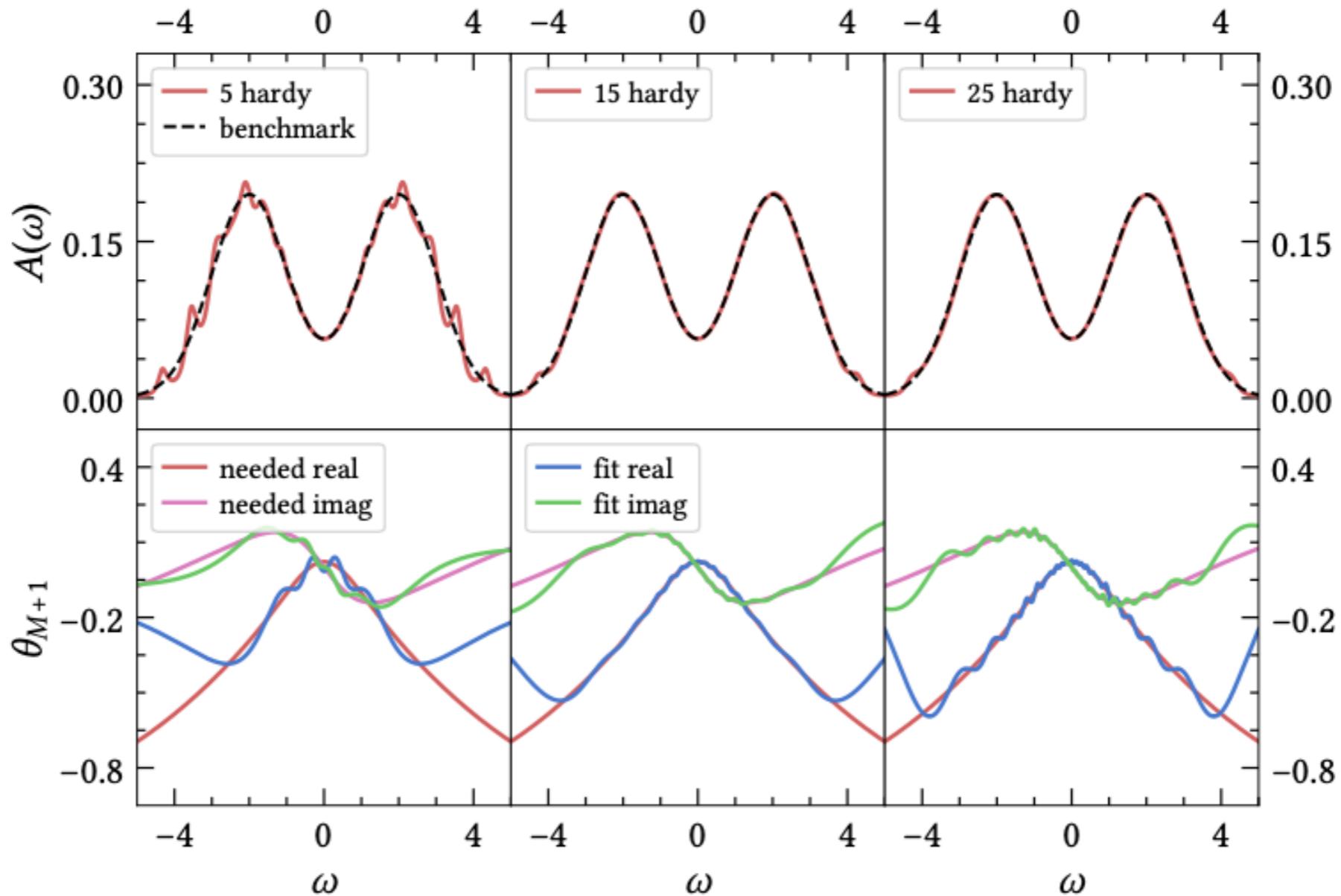


FIG. 1. Optimization with 5, 15 and 25 Hardy basis functions. Top panels: resulting spectral functions  $A(\omega)$ . Bottom panels: real and imaginary part of the exact and fitted parametric functions  $\theta_{M+1}$  ( $\theta_{M+1} : \mathcal{C}^+ \rightarrow \overline{\mathcal{D}}$ ). The needed  $\theta_{M+1}$  is what would restore our synthetic input  $A(\omega)$  when plugged into the final interpolant (Eq. 7 in the manuscript). The fitted  $\theta_{M+1}$  is expanded by the hardy functions with the optimized coefficients  $a_k$ s and  $b_k$ s. Note that 15 hardy functions would give a better result than 25, as the function optimization of the smoothing norm works better.

# Effects of temperature, grid points, noise

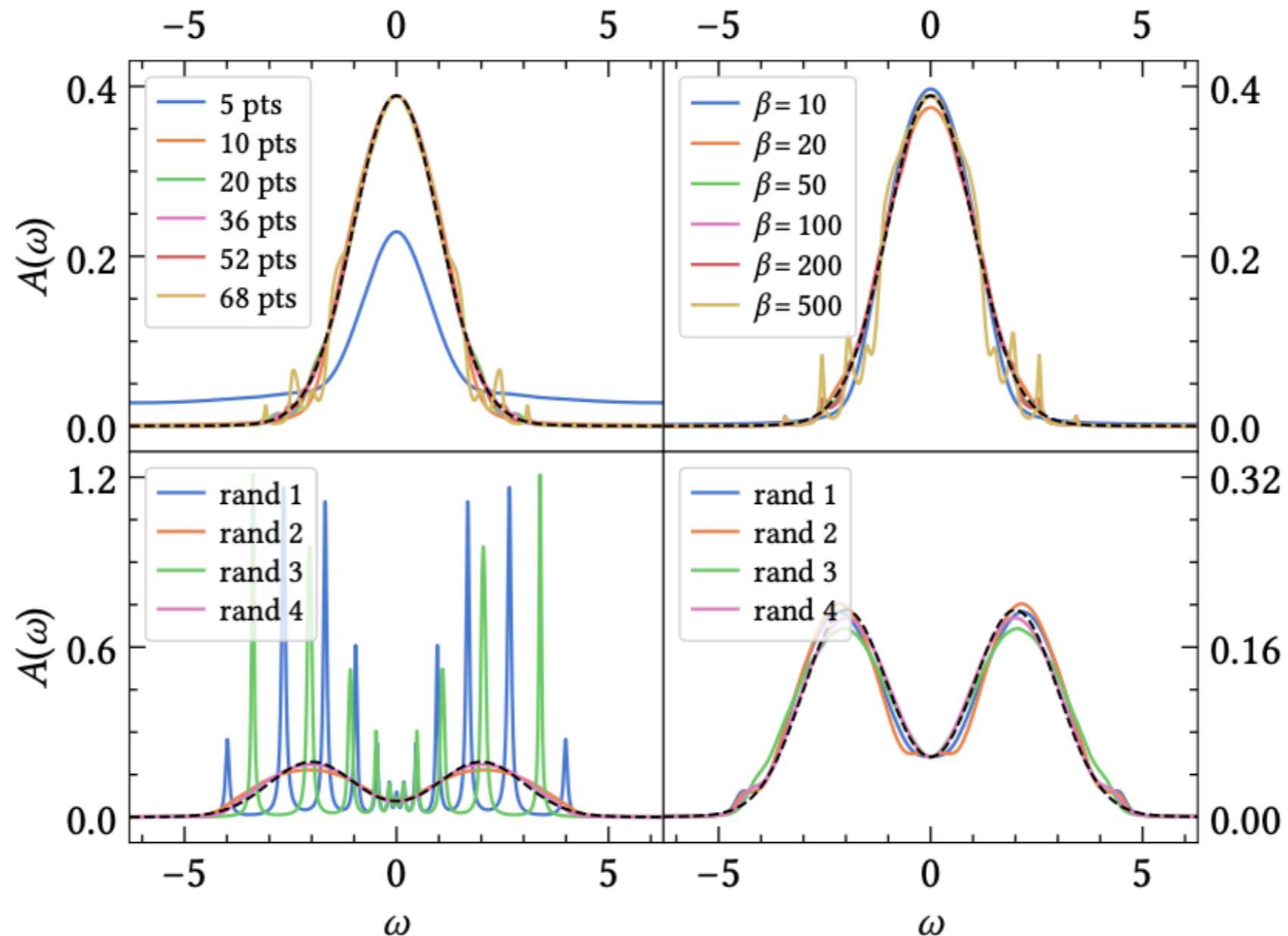


Figure 1.5: Top left: effect of the number of interpolation nodes (IR grid [13, 14]) used. Top right: effect of Matsubara spacing (inverse temperature), uniform grid  $\omega_n = (2n + 1)\pi/\beta$  used. Bottom two panels: effect of independent Gaussian noise with relative standard deviation of  $10^{-4}$  (left) and  $10^{-6}$  (right), four sample curves each.

# Variants – SOM and SpM

- SOM – Stochastic Optimization
- Developed a few times, including in Mishchenko *et al.*, Phys. Rev. B 62, 6317 (2000)
- Optimization problem formulated without default model but as an optimization of the objective function

$$\Delta(m) = \frac{1}{S(m)} \left[ \int_{\xi_{\min}}^{\xi_{\max}} d\epsilon K(\xi_m, \epsilon) A(\epsilon) - O(\xi_m) \right]$$

S characterizes errors, K the kernel, O the input data.

- Failure modes similar to MaxEnt. Much more expensive but error bars!

- SpM – Sparse Modeling
- Yoshimi, ... Shinaoka, CPC 244, 319 (2019)
- Singular value decompose analytic continuation kernel
- Truncate once eigenvalues small, then regularize by enforcing norm & smoothness
- Failure modes similar to MaxEnt but much cheaper and useful byproducts (basis, etc)
- Main use of sparse modeling is in creating precise numerical bases

# The Hamburger moment problem

The (truncated) Hamburger moment problem aims to construct a measure  $\sigma(\omega)$  on the real axis such that

$$h_k = \int \omega^k d\sigma(\omega) \quad b = (h_0, h_1, h_2, \dots)$$



Hans Ludwig  
Hamburger

In our context think of  $d\sigma(\omega) = A(\omega)d\omega$

The Hamburger-Nevanlinna theorem establishes a one-to-one correspondence between solutions to the moment problem and a subset of Nevanlinna functions.

$$\begin{aligned} \mathcal{N}G(i\omega_n) &= -G(i\omega_n) \\ &= - \int_0^\beta d\tau G(\tau) e^{i\omega_n \tau} \\ &= - \sum_{k=0}^{\infty} \frac{(-1)^{k+1} (G^{(k)}(\beta) + G^{(k)}(0))}{(i\omega_n)^{k+1}} \\ &= -\frac{h_0}{i\omega_n} - \frac{h_1}{(i\omega_n)^2} - \frac{h_2}{(i\omega_n)^3} - \dots \end{aligned}$$

It is possible to combine the moment with the interpolation problem to both enforce moments and interpolation values. This further constrains the solution.

The Hamburger moments are routinely computed in a high-frequency tail analysis of the Green's functions, where they typically supplement Green's functions outside of the interval where data is available.

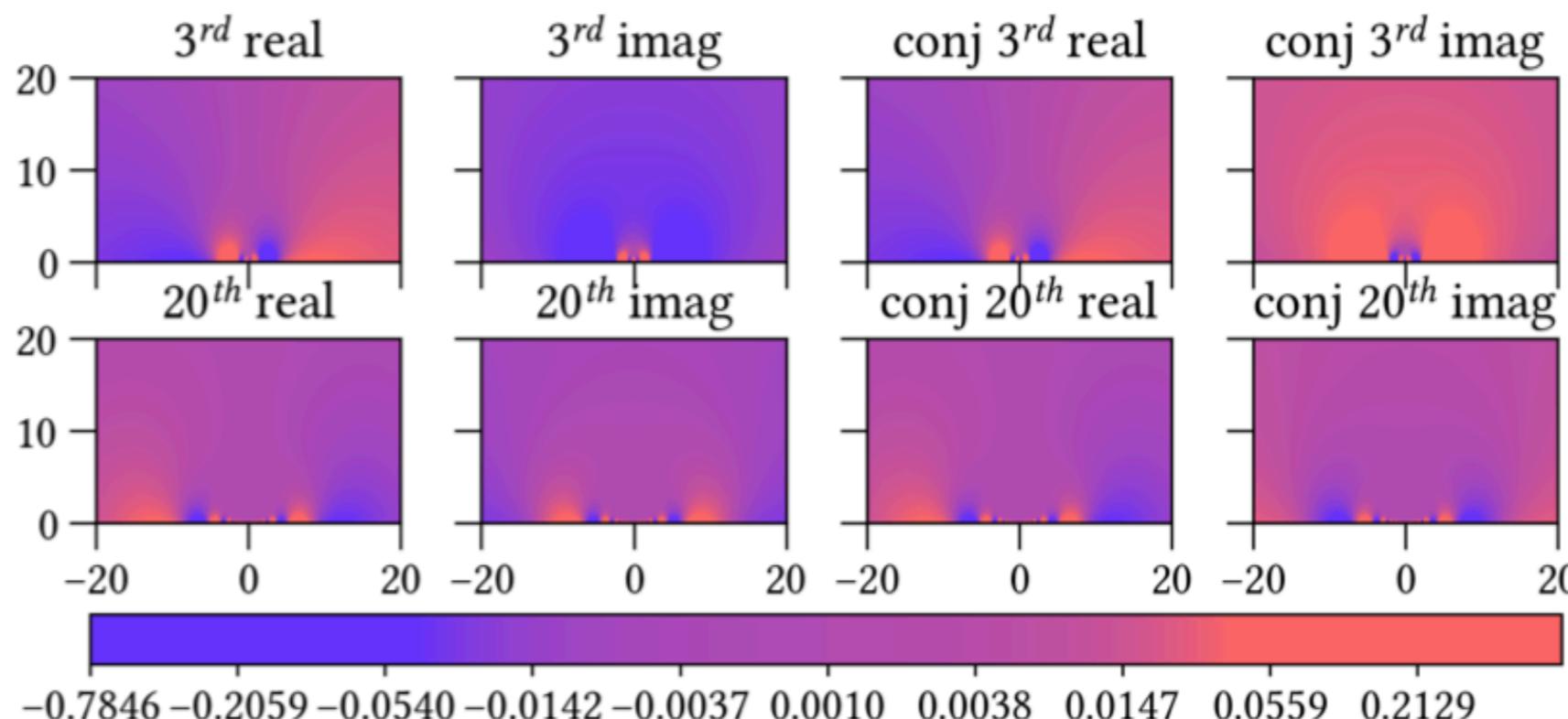
# Hardy function optimization

A non-singular positive definite Pick matrix guarantees an infinite number of solutions. In the Schur algorithm this appears as an arbitrary Nevanlinna function that can be added to the solution. For any Nevanlinna function, the resulting interpolant will still be Nevanlinna and interpolate all possible solutions.

The freedom of choosing an additional function can be used to impose additional properties of the interpolant, e.g. impose smoothness on the real axis.

We chose Hardy functions – other choices are possible

$$B^k(z) = \left\{ \frac{1}{\sqrt{\pi}(z+i)} \left( \frac{z-i}{z+i} \right)^k \right\}_{k \in \mathbb{N}}$$



Minimize F, optimize smoothness  
while respecting norm

$$F[A_{\theta_M}(\omega)] = \left| 1 - \int A_{\theta_M}(\omega) d\omega \right|^2 + \lambda \left\| \frac{d^2 A_{\theta_M}(\omega)}{d\omega^2} \right\|^2$$