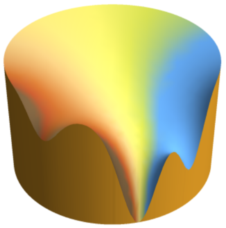


Nevanlinna Analytic Continuation

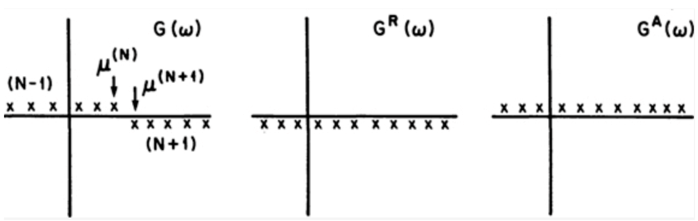
At Gull's group meeting

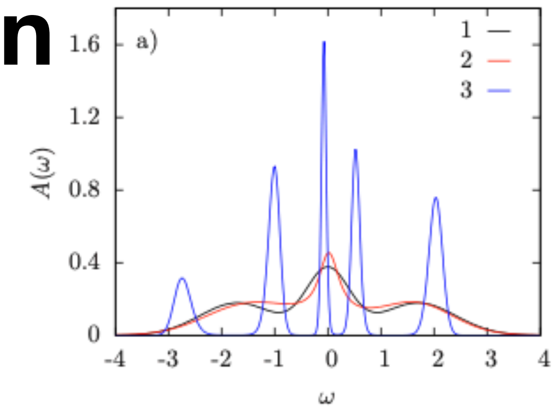
Jiani Fei 06/28/2022

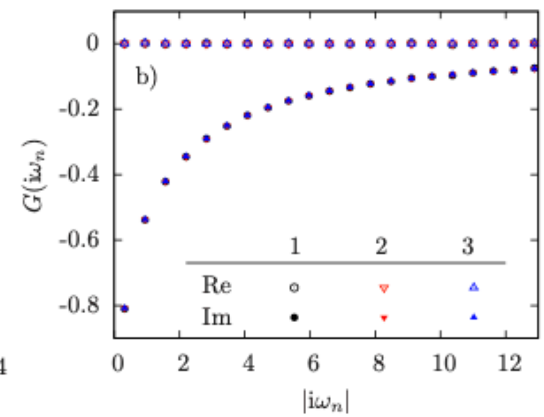
Phys. Rev. Lett. 126, 056402 (2021)
Phys. Rev. B 104, 165111 (2021)

Analytic Continuation

S. Fuchs, PhD thesis, Göttingen, 2010







Partition function $Z = \mathrm{Tr}e^{-\beta H}$

$\tau = it$

Green's function $G(\tau) = -\frac{1}{Z}\mathrm{Tr}[e^{-(\beta-\tau)H}ce^{-\tau H}c^{\dagger}]$

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

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

Analytic Continuation

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

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

Numerical Analytic Continuation

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

$$\downarrow$$

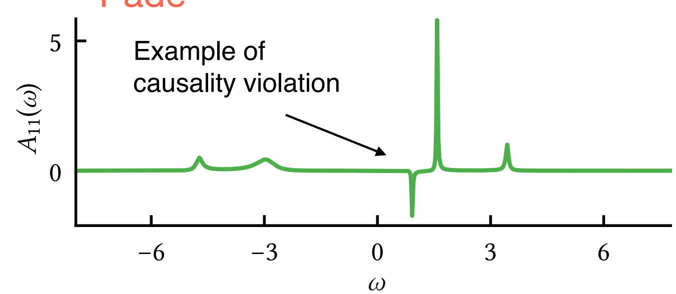
$$G(\omega) = [K(i\omega_n,\omega)]^{-1}G(i\omega_n)$$

$\xrightarrow{\text{Easy}} K$

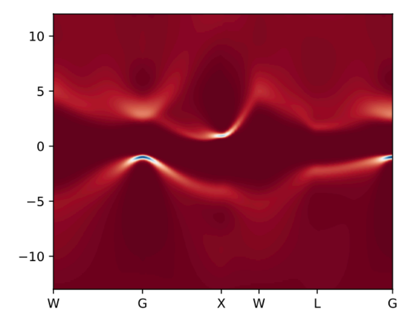
$\xleftarrow{\text{Hard}} K^{-1}$

The kernel K is ill conditioned: small changes on the Matsubara axis cause large changes on the real axis.

Padé



MaxEnt



$NG = -G$ is a Nevanlinna function ($\mathcal{C}^+ \to \overline{\mathcal{C}^+}$)

Proof. Green's function restricted to $\mathcal{C}^+$ can be formulated by Lehmann representation as,

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

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

Let $z = x + yi$ where $y > 0$, i.e. $z \in \mathcal{C}^+$. Then each summand can be represented as,

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

$$Im\{S\} = -\frac{Ay}{(x+E_n-E_m)^2+y^2} \leqslant 0$$

summing all summands gives $Im\{\mathcal{G}(\gamma,z)\} \leqslant 0$ and thus $Im\{\mathcal{NG}(\gamma,z)\} \geqslant 0$ for $z \in \mathcal{C}^+$.

Rolf Nevanlinna

Issai Schur

Every Nevanlinna function N admits a representation

$$N(z) = C + Dz + \int_{\mathbb{R}}\left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right)\mathrm{d}\,\mu(\lambda), \quad z \in \mathcal{H},$$

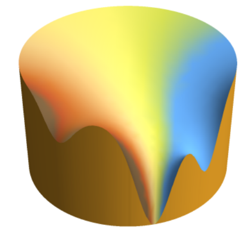
where C is a real constant, D is a non-negative constant, $\mathcal{H}$ is the upper half-plane

$\longleftrightarrow$

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

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

Interpolation Algorithm



$NG = -G$ is a Nevanlinna function ($C^+ \rightarrow \overline{C^+}$)

$$\begin{tikzcd}
\mathcal{C}^+ \arrow[r, "f"] \arrow[d, "h_1"'] \arrow[dr, "\theta"] & \overline{\mathcal{C}^+} \arrow[d, "h"] \\
\mathcal{D} \arrow[r, "g"'] & \overline{\mathcal{D}}
\end{tikzcd}$$

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

f : Nevanlinna function $\in \mathtt{N}$
g : Schur function $\in \mathtt{S}$
θ : Contractive function $\in \mathtt{B}$
h/h_1 : Conformal mapping (e.g. Möbius transform)
$h(z) : z \rightarrow \dfrac{z-i}{z+i}$

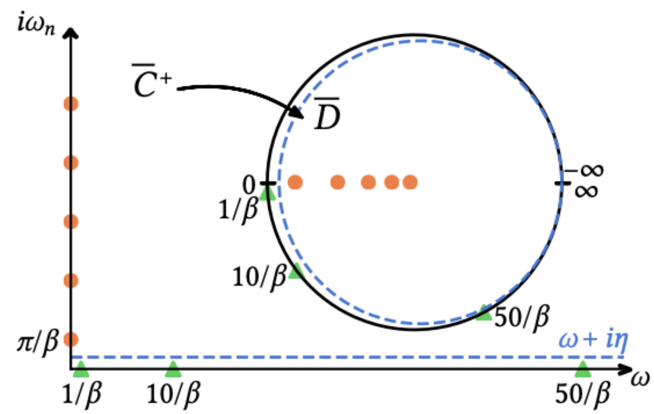
Schur's algorithm

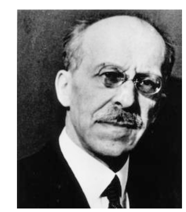
$$\theta(Y_k) = \gamma_k, k = 1 \ldots\ M$$

$$\theta(z) = \frac{\frac{z-Y_1}{z-Y_1^*}\tilde{\theta}(z) + \gamma_1}{\gamma_1^* \frac{z-Y_1}{z-Y_1^*}\tilde{\theta}(z) + 1}$$

$$\theta(z)[z; \theta_{M+1}(z)] = \frac{a(z)\theta_{M+1}(z) + b(z)}{c(z)\theta_{M+1}(z) + d(z)}$$

$$\begin{pmatrix} a(z) & b(z) \\ c(z) & d(z) \end{pmatrix} = \prod_{j=1}^{M} \begin{pmatrix} \frac{z-Y_j}{z-Y_j^*} & \phi_j \\ \phi_j^* \frac{z-Y_j}{z-Y_j^*} & 1 \end{pmatrix} \quad \text{where} \quad \theta_j(Y_j) = \phi_j\ .$$

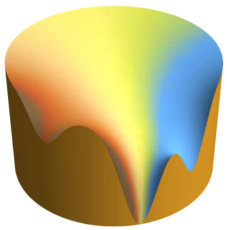




Issai Schur

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

Choose a solution: optimization

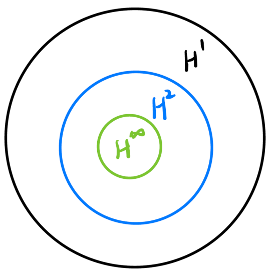


$NG = -G$ is a Nevanlinna function ($C^+ \to \overline{C^+}$)

$$\theta(z)[z;\theta_{M+1}(z)] = \frac{a(z)\theta_{M+1}(z)+b(z)}{c(z)\theta_{M+1}(z)+d(z)}$$

$$\begin{tikzcd}
\mathcal{C}^+ \arrow[r, "f"] \arrow[d, "h_1"'] \arrow[dr, "\theta"] & \overline{\mathcal{C}^+} \arrow[d, "h"] \\
\mathcal{D} \arrow[r, "g"'] & \overline{\mathcal{D}}
\end{tikzcd}$$

f : Nevanlinna function $\in \mathtt{N}$
g : Schur function $\in \mathtt{S}$
θ : Contractive function $\in \mathtt{B}$
h/h_1 : Conformal mapping (e.g. Möbius transform)
$h(z) : z \to \dfrac{z-i}{z+i}$

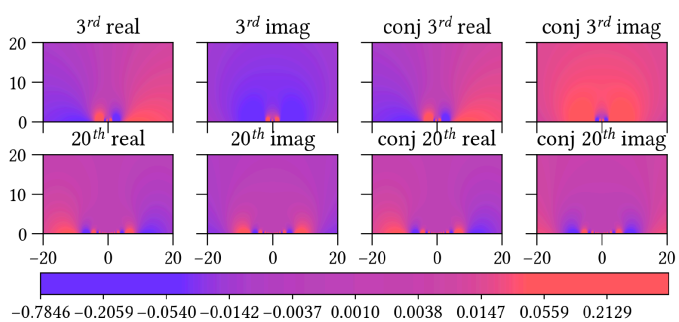


Hardy function optimization

$$f^k(z) = \frac{1}{\sqrt{\pi}(z+i)}\left(\frac{z-i}{z+i}\right)^k$$

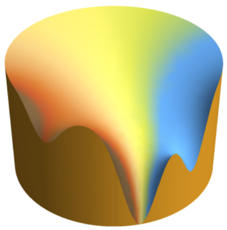
$$\theta_{M+1} = \sum_{k=0}^{H} a_k f^k(z) + b_k(f^k(z))^*$$

$$F[A_{\theta_{M+1}}(\omega)] = |1 - \int A_{\theta_{M+1}}(\omega)|^2 + \lambda \int A''_{\theta_{M+1}}(\omega)^2$$



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

Choose a solution: optimization



Synthetic benchmark system

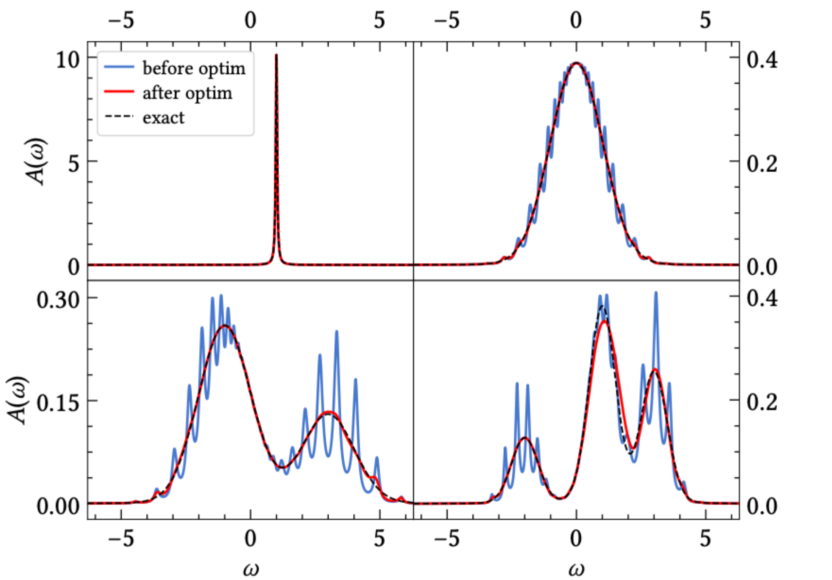


Figure 1.4: Continuation with and without Hardy function optimization. Off-centered δ peak (top left), Gaussian (top right), two-peak scenario (bottom left), and a three-peak scenario (bottom right). $\beta = 100$, IR grid [13, 14] with 36 Matsubara positive frequency points.

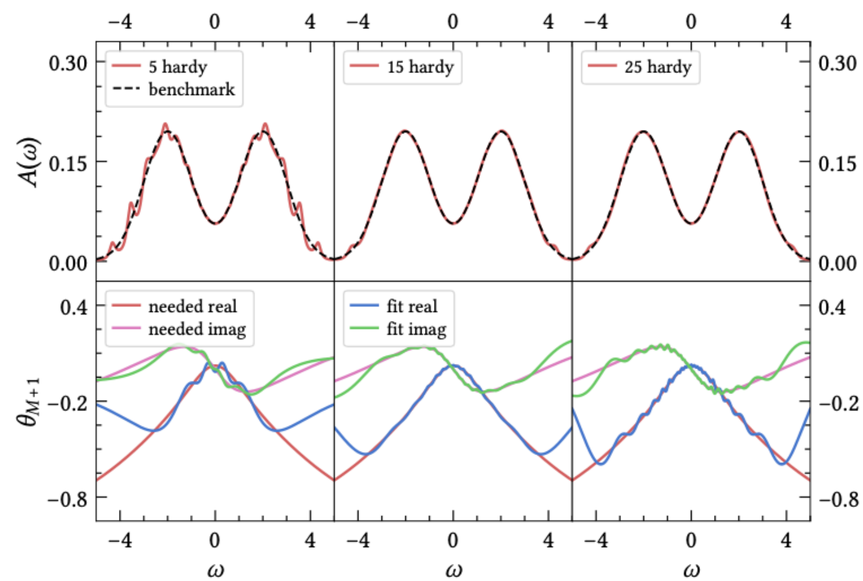
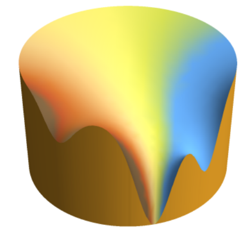


FIG. 1. Optimization with 5, 15 and 25 Hardy basis functions. Top panels: resulting spectral functions $A(\omega)$. Bottom panels: real and imaginary part of the exact and fitted parametric functions θ_{M+1} ($\theta_{M+1} : \mathcal{C}^+ \to \overline{\mathcal{D}}$). The needed θ_{M+1} is what would restore our synthetic input

Existence and Uniqueness

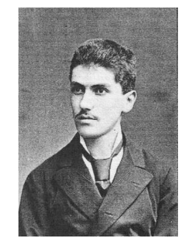


$NG = -G$ is a Nevanlinna function ($C^+ \to \overline{C^+}$)

$$\theta(z)[z;\theta_{M+1}(z)] = \frac{a(z)\theta_{M+1}(z) + b(z)}{c(z)\theta_{M+1}(z) + d(z)}$$

$$\begin{tikzcd} \mathcal{C}^+ \arrow[r, "f"] \arrow[d, "h_1"'] \arrow[dr, "\theta"] & \overline{\mathcal{C}^+} \arrow[d, "h"] \\ \mathcal{D} \arrow[r, "g"'] & \overline{\mathcal{D}} \end{tikzcd}$$

f : Nevanlinna function $\in \mathtt{N}$
g : Schur function $\in \mathtt{S}$
θ : Contractive function $\in \mathtt{B}$
h/h_1 : Conformal mapping (e.g. Möbius transform)
$h(z) : z \to \dfrac{z-i}{z+i}$



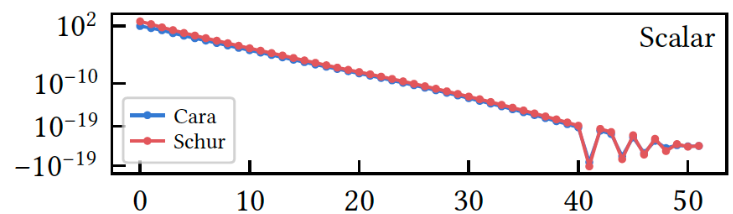
Georg Pick

The Pick criterion: Nevanlinna / Schur interpolants'

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

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

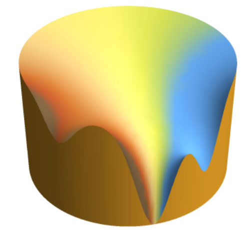
Existence ($P \geq 0$) and Uniqueness (P furthermore singular)



e.g. noise SD 1e-3, smallest eigenvalue ~ -1e-3

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

Noisy data

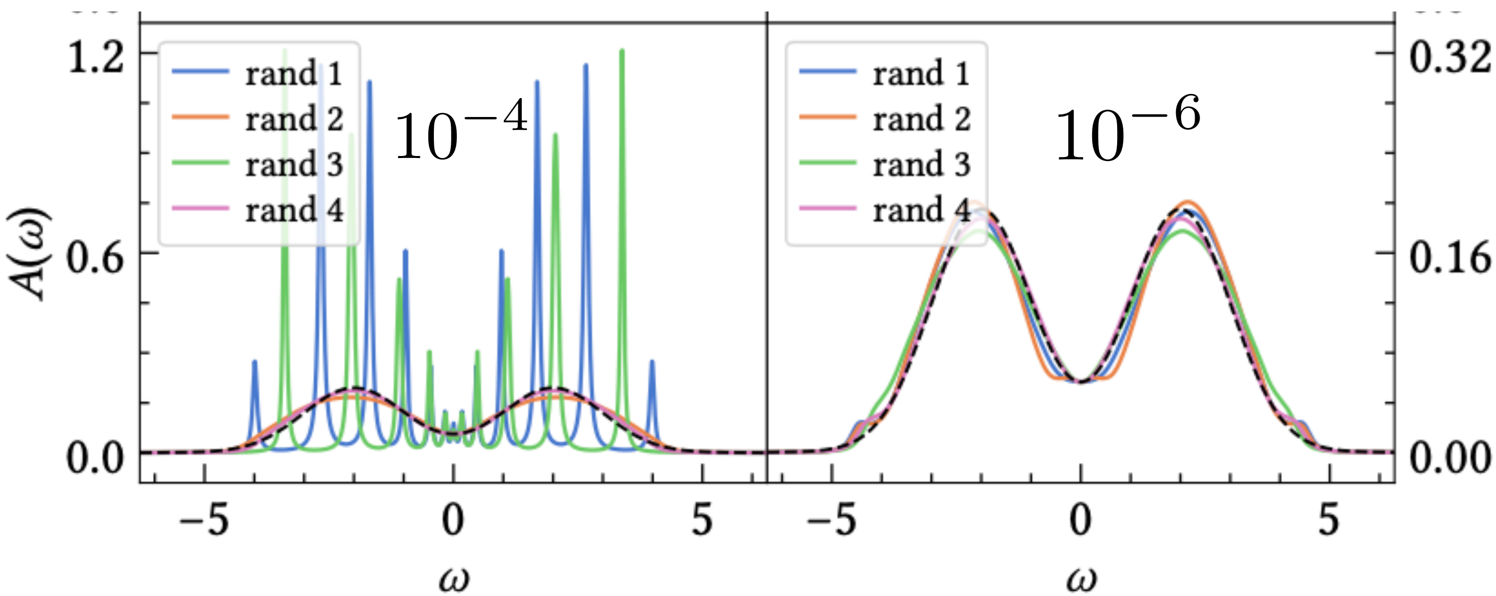


Continuous fraction interpolation is very sensitive to noise.

If input data does not satisfy Pick criterion, output may or may not be causal.

In practice poles are often close to real axis, evaluation just above the real axis will skip them.

Behavior with noise similar to Padé continued fractions. This is not a method for noisy data.



The Hamburger Moment Problem

Hans Ludwig Hamburger

$NG = -G$ is a Nevanlinna function ($C^+ \rightarrow \overline{C^+}$)

$$\theta(z)[z;\theta_{M+1}(z)] = \frac{a(z)\theta_{M+1}(z)+b(z)}{c(z)\theta_{M+1}(z)+d(z)}$$

$$\begin{tikzcd}
\mathcal{C}^+ \arrow[r, "f"] \arrow[d, "h_1"'] \arrow[dr, "\theta"] & \overline{\mathcal{C}^+} \arrow[d, "h"] \\
\mathcal{D} \arrow[r, "g"'] & \overline{\mathcal{D}}
\end{tikzcd}$$

f : Nevanlinna function $\in \mathtt{N}$
g : Schur function $\in \mathtt{S}$
θ : Contractive function $\in \mathtt{B}$
h/h_1 : Conformal mapping (e.g. Möbius transform)
$h(z) : z \rightarrow \dfrac{z-i}{z+i}$

Hamburger moment problem

Given $b = (h_0, h_1, h_2, \ldots)$, construct $\sigma(\omega)$ s.t.

$h_k = \int \omega^k d\sigma(\omega)$ In our case, $d\sigma(\omega) = A(\omega)d\omega$

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

Hamburger-Nevanlinna theorem

$$f(z) = \int_{-\infty}^{\infty}\frac{d\sigma(\omega)}{\omega - z} \quad z \in \mathcal{C}^+$$

$$f(z) = -\frac{h_0}{z} - \frac{h_1}{z^2} - \frac{h_2}{z^3} - \cdots - \frac{h_{2N-2}}{z^{2N-1}} - o\left(\frac{1}{z^{2N-1}}\right)$$

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

Matrix-valued Carathéodory generalization

The Carathéodory class of matrix-valued analytic functions in D (or: C^+) is defined as

$$C = \{M(z) : M(z) + M^\dagger(z) \geq 0 \ \ \forall\, |z| < 1\} \ \ \Leftrightarrow \ \ \mathrm{Re}\{x^\dagger M x\} \geq 0$$

$-iG^<(\omega), iG^>(\omega)$ are PSD; $iG(z), i\Sigma(z), iM(z)$ (cumulant: defined as $M^{-1}(z) = G^{-1}(z) + F$) are Carathéodory.

Proof.

$$\langle x|-iG^<(\omega)|x\rangle = 2\pi \sum_{mn} \frac{e^{-\beta E_n}}{Z} \langle m|\sum_i c_i x_i^* |n\rangle^2 \delta(\omega - E_n + E_m) \geq 0$$

$$\langle x|iG^>(\omega)|x\rangle = 2\pi i \sum_{mn} \frac{e^{-\beta E_n}}{Z} \langle n|\sum_i c_i x_i^* |m\rangle^2 \delta(\omega + E_n - E_m) \geq 0$$

$$\langle x|i\mathcal{G}(z) + (i\mathcal{G}(z))^\dagger|x\rangle = \frac{1}{Z}\sum_{mn} \frac{2\mathrm{Im}\{z\}\ (e^{-\beta E_m} + e^{-\beta E_n})}{\mathrm{Im}\{z\}^2 + (\mathrm{Re}\{z\} + E_n - E_m)^2} \langle n|\sum_i c_i x_i^* |m\rangle^2 \geq 0$$

$$\begin{aligned} -iG^{-1}(z) + i(G^{-1}(z))^\dagger &= -iM^{-1}(z) + iF + i(M^{-1}(z))^\dagger - iF^\dagger \\ &= -iM^{-1}(z) + i(M^{-1}(z))^\dagger \end{aligned}$$

[Gramsch, Potthoff; Phys. Rev. B 92, 235135 (2015)]

$$H(t) = \sum_{ij} [T_{ij}(t) - \mu\delta_{ij}] c_i^\dagger(t) c_j(t) + \frac{1}{2} \sum_{iji'j'} U_{ii'jj'}(t) c_i^\dagger(t) c_{i'}^\dagger(t) c_{j'}(t) c_j(t)$$

$$H_{\mathrm{eff}}(t) = \sum_{xy} h_{xy}(t) c_x^\dagger c_y \ \Rightarrow \ \boxed{\begin{array}{r}\text{physical orbitals denoted } \boldsymbol{i},\ \boldsymbol{j}; \\ \text{all orbitals denoted } \boldsymbol{x},\ \boldsymbol{y}\end{array}}$$

$$\Sigma_{ij}(t,t') = \delta_C(t,t')\Sigma_{ij}^{\mathrm{HF}}(t) + \Sigma_{ij}^C(t,t')$$

$$\Sigma_{ij}^{\mathrm{HF}}(t) \equiv 2\sum_{i'j'} U_{ii'jj'}(t) \langle \mathcal{T}_C\ c_{i'}^\dagger(t) c_{j'}(t)\rangle_{H_{\mathrm{eff}}}$$

$$\Sigma_{ij}^C(t,t') \equiv \sum_s h_{is}(t) g(h_{ss}; t, t') h_{js}^*(t').$$

Fourier transform of $\delta_C(t,t')\Sigma_{ij}^{\mathrm{HF}}(t)$ Hermitian and z-independent

$$\begin{aligned} &\langle x|i\Sigma(z) + (i\Sigma(z))^\dagger|x\rangle \\ =&\langle x|i\Sigma^C(x+yi) - i\Sigma^C(x-yi)|x\rangle \\ =&\sum_s \frac{2y(\sum_i x_i h_{is}(0))^2}{(h_{ss}-x)^2 + y^2} \geqslant 0 \end{aligned}$$

Phys. Rev. B 104, 165111 (2021)

Matrix-valued Carathéodory generalization

Generalized Schur's algorithm

Assuming $\Psi_i(z_i) = W_i$,

$$y_i L_i(z) = [I - W_i W_i^\dagger]^{-1/2}[\Psi_i(z) - W_i] \cdot [I - W_i^\dagger \Psi_i(z)]^{-1}[I - W_i^\dagger W_i]^{1/2}$$

where $y_i = |z_i|(z_i - z)/(z_i(1 - z_i^* z))$. $L_i(z) \in \mathcal{S}$ by the Schwarz lemma [53]. Define $\Psi_{i+1}(z)$ as

$$\Psi_{i+1}(z) = [I - K_i K_i^\dagger]^{-1/2}[L_i(z) - K_i] \cdot [I - K_i^\dagger L_i(z)]^{-1}[I - K_i^\dagger K_i]^{1/2}$$

where K_i is an arbitrary matrix such that $\|K_i\| < 1$.

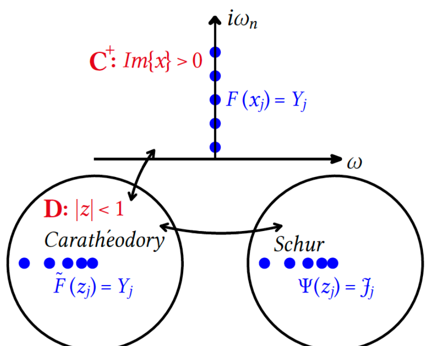
Carathéodory

Generalized Pick criterion

$$\Psi(z_j) = J_j = \Psi\left(\frac{x_j - i}{x_j + i}\right) = [I - Y_j][I + Y_j]^{-1},$$

$$j = 0, 1, \ldots, n-1.$$

$$P_C = \left[\frac{Y_k + Y_l^*}{1 - z_k^* z_l}\right]_{(mn)\times(mn)} \quad \text{or} \quad P_S = \left[\frac{I - J_k^* J_l}{1 - z_k^* z_l}\right]_{(mn)\times(mn)}$$



Existence ($P \geq 0$) and Uniqueness (P furthermore singular)

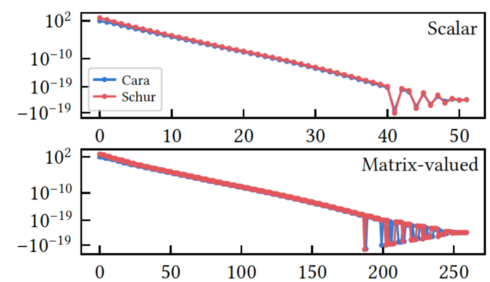


FIG. 6. Eigenvalues of the Pick matrices, Eqs. 3 (blue) and 4 (red). Top panel: scalar (Nevanlinna [41]) continuation of the Green's function of Si. Bottom panel: Eigenvalues of the generalized Pick matrix of the matrix-valued problem.

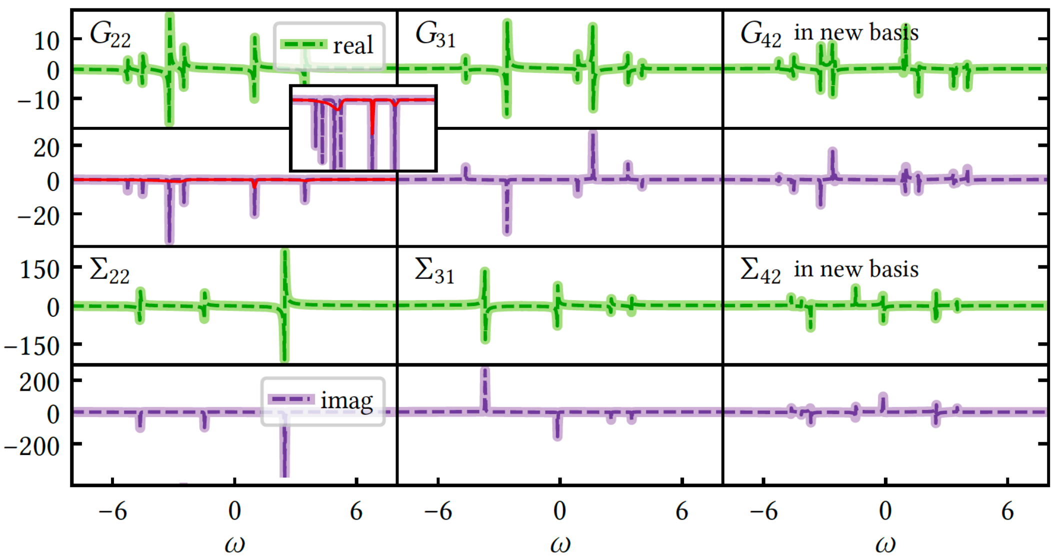
Phys. Rev. B 104, 165111 (2021)

Matrix-valued Carathéodory generalization

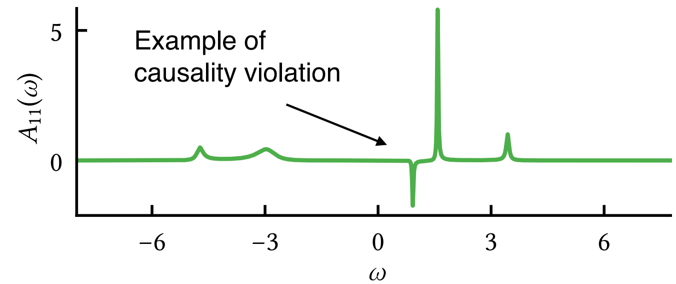
Hubbard dimer (2-site)

$$H_{asym} = H_0 + H_V + H_{\boldsymbol{H}} + H_{\text{breaksym}}$$

Here we use the degeneracy-lifted Hamiltonian $H = H_{asym}$ with parameters $\beta = 10$, $t = 1$, $U = 5$, $\mu = 0.7$, $\boldsymbol{H} = 0.3$, $U_a = 0.5$, $\mu_a = 0.2$, $\boldsymbol{H}_a = 0.03$.



Padé



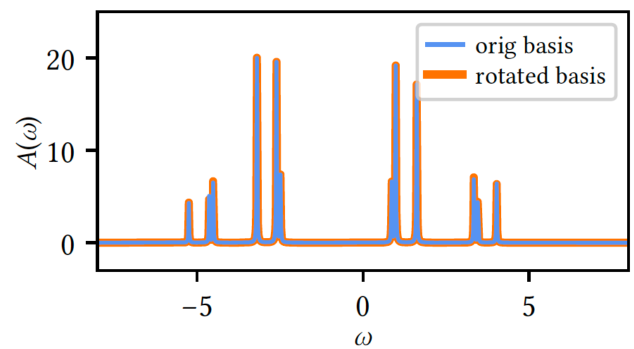
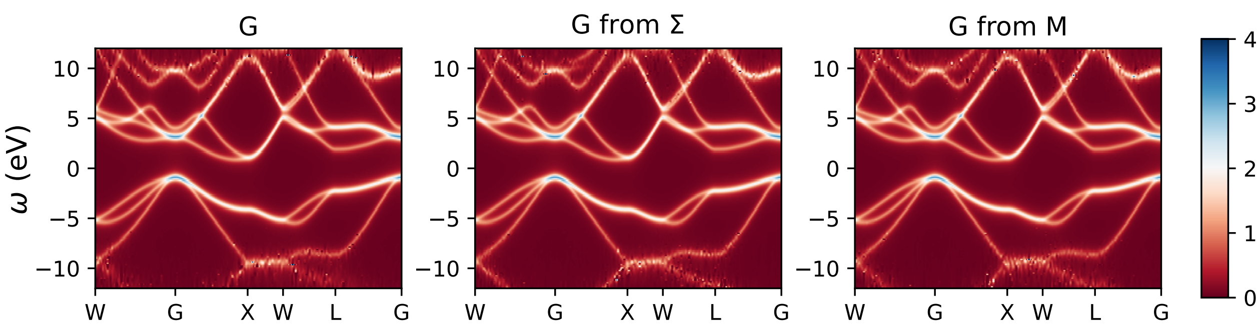


FIG. 3. Total spectral function of the Hubbard dimer, obtained in the site basis and in a randomly rotated basis, illustrating the basis independence of the continuation procedure.

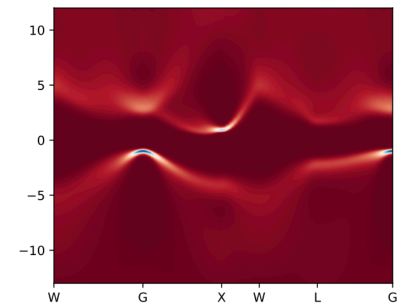
Phys. Rev. B 104, 165111 (2021)

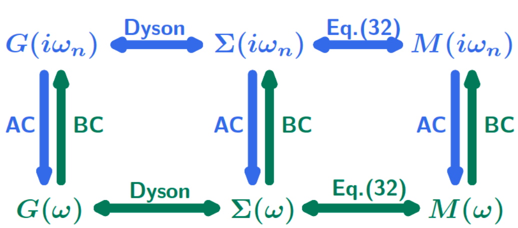
Matrix-valued Carathéodory generalization

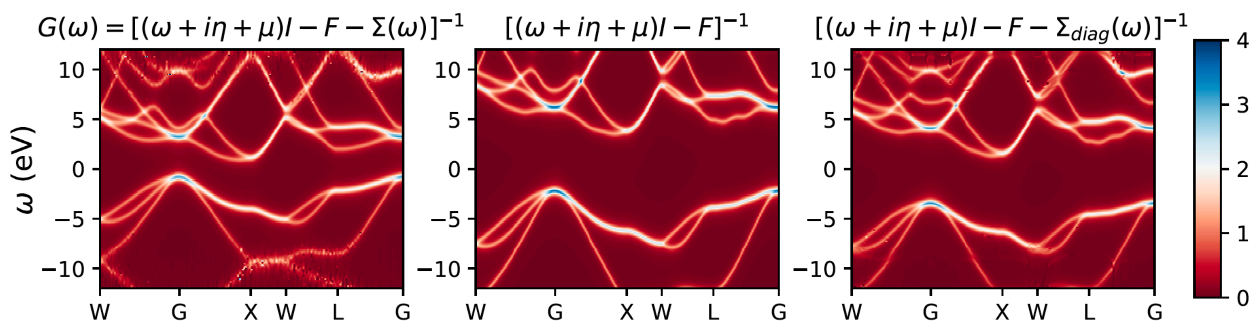
Self-consistent GW silicon



MaxEnt

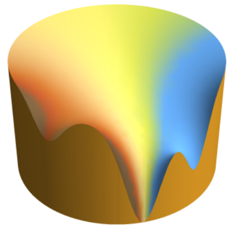






Phys. Rev. B 104, 165111 (2021)

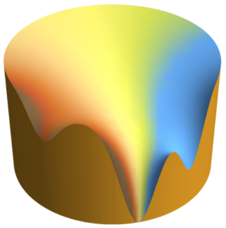
Comments



- This work eliminates the leading problem in analyzing diagrammatic / stat mech / finite temperature calculations with semi-analytic formalisms (GW, FLEX, T-Matrix, fRG, etc)
- Noise case was untouched.
  Ideas from Nevanlinna?
  holographic mapping, hardy space and Fourier coefficients [Ying 22; 2202.09719];
  Project to the causal space then choose a solution
  (1) handling Schur interpolant, systematic way to project / eliminate noise [control theory / operator theory]
  (2) projecting Matsubara data to the Nevanlinna space (may be NP hard and useless: dense causal volume in the high-dimensional Matsubara data space; many causal data are 'close' enough to the given noisy data but give unmovable bad spectra)

Phys. Rev. Lett. 126, 056402 (2021)
Phys. Rev. B 104, 165111 (2021)

How to run Nevanlinna



Dependencies: C++, CMake; Dakota (opt)
Linked libraries: MPFR, GMPXX, GMP; FFTW3 (opt)

1. Compile the program inside "Nevanlinna_Schur". Check line 74 of nevanlinna.h and line 28,29 of sobolev.cpp, making sure N_real_=N and omega_min=omega_max=length. \lambda could be adjusted in line 113 of sobolev.cpp.
2. Run "./Nevanlinna < input.txt", the fourth "coeff" in "input.txt" is the name of the coefficient file that will be used in Hardy optimization.
3. Put the generated "coeff", "Nev_opt.py" and "Nev_opt_result.py" under the same directory used for optimization.
4. Run "Nev_opt.py". ***It*** creates folder "dakota"; writes three files "dakota/dakota_pstudy.in" [optimization method, number of parameters which is 4*basis -> Re/Im of ak and bk, initial values], "dakota/driver" [it runs the driver program "sobolev.cpp" inside the iteration folder "dakota/0", "dakota/1", ...] and "dakota/params.template" [the template for dakota to fill in trial parameters in each iteration]; and runs "jobopt".
5. After optimization, run "Nev_opt_result.py". ***It*** extracts result files and puts them into "opt_result" folder.
6. Run the "job" file created ***by*** "Nev_opt_result.py". This would finally give "Aopt.txt" in the same directory, which is the optimized spectrum.

Phys. Rev. Lett. 126, 056402 (2021)
Phys. Rev. B 104, 165111 (2021)