Controlled analytic continuation of Matsubara correlation functions using minimal pole representation

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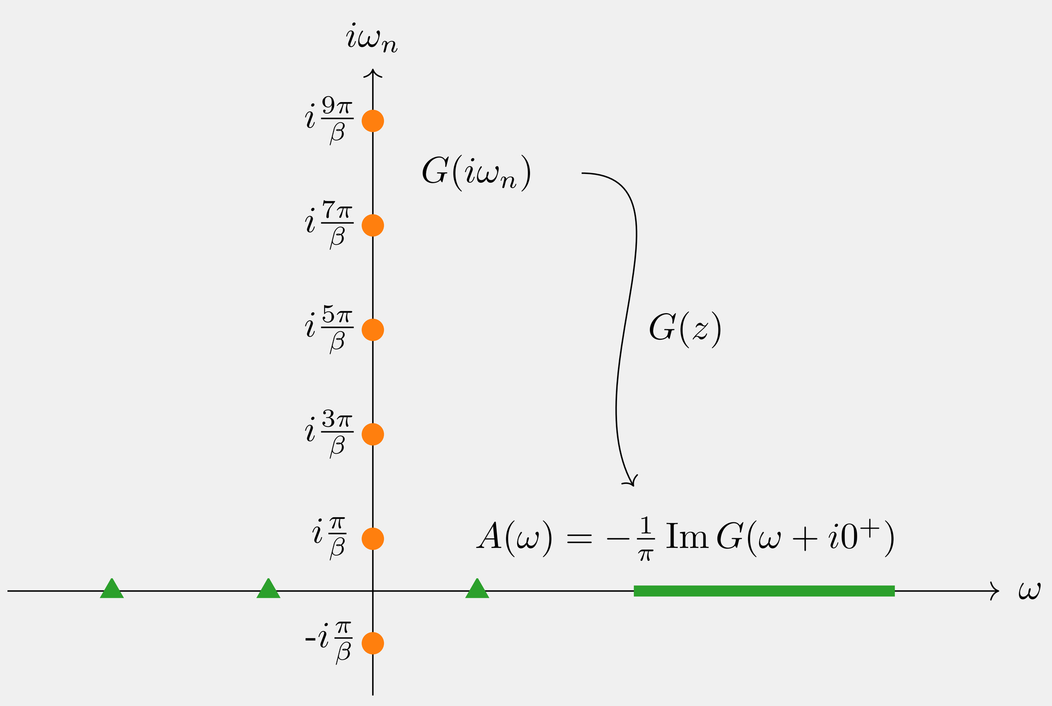
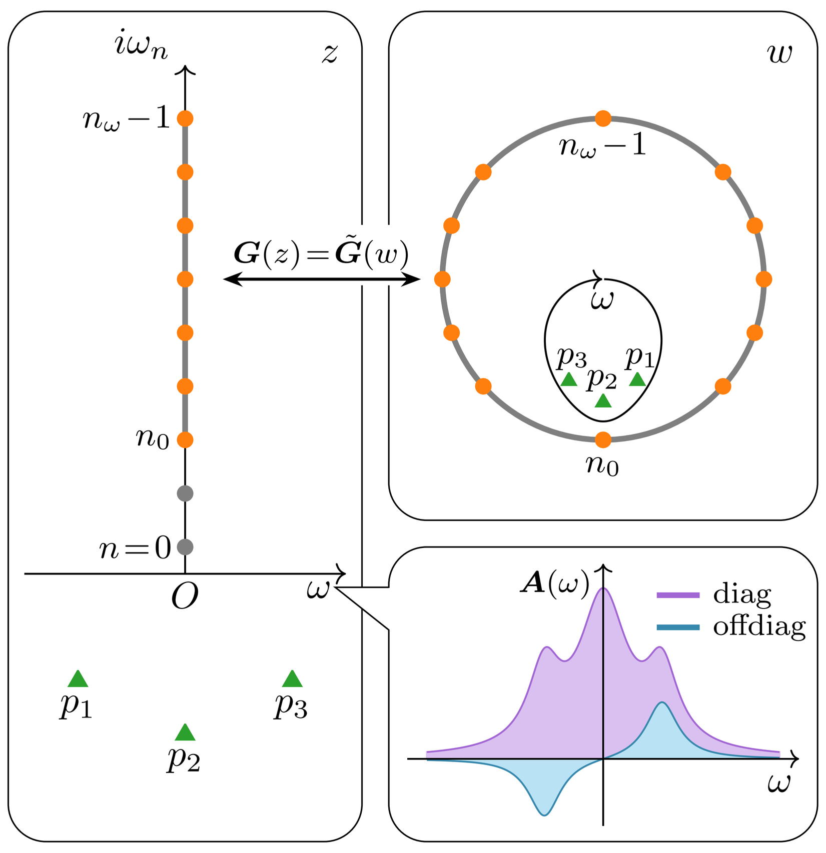
Background

- Simulations are performed on the imaginary axis (orange circles)
- Physical interpretation requires evaluation right above singularities (green)
- Bridging the two requires numerical analytic continuation (NAC)

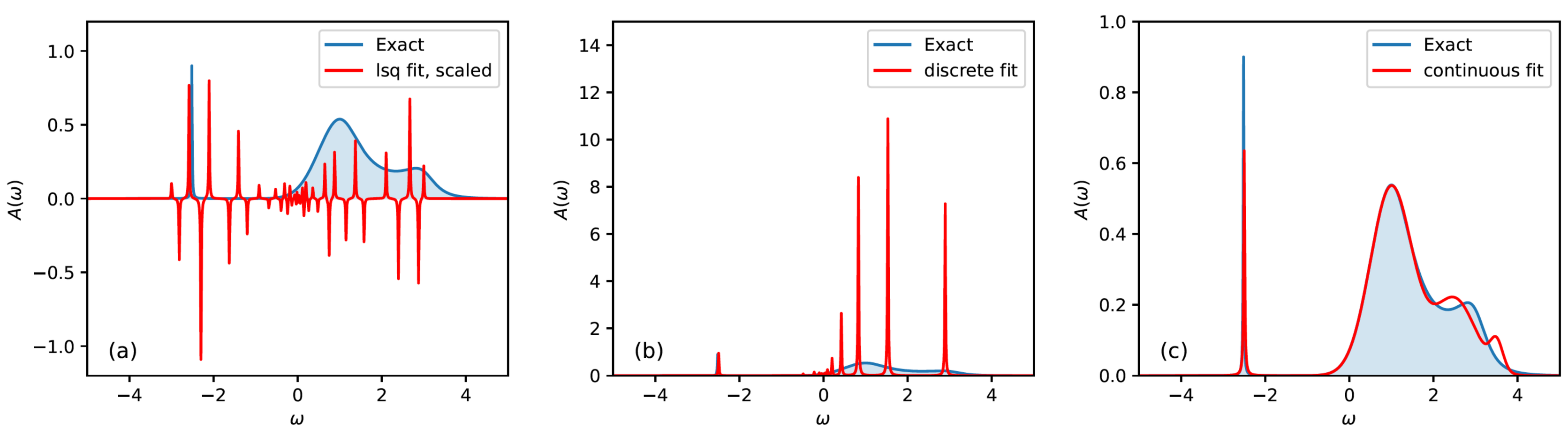


Method



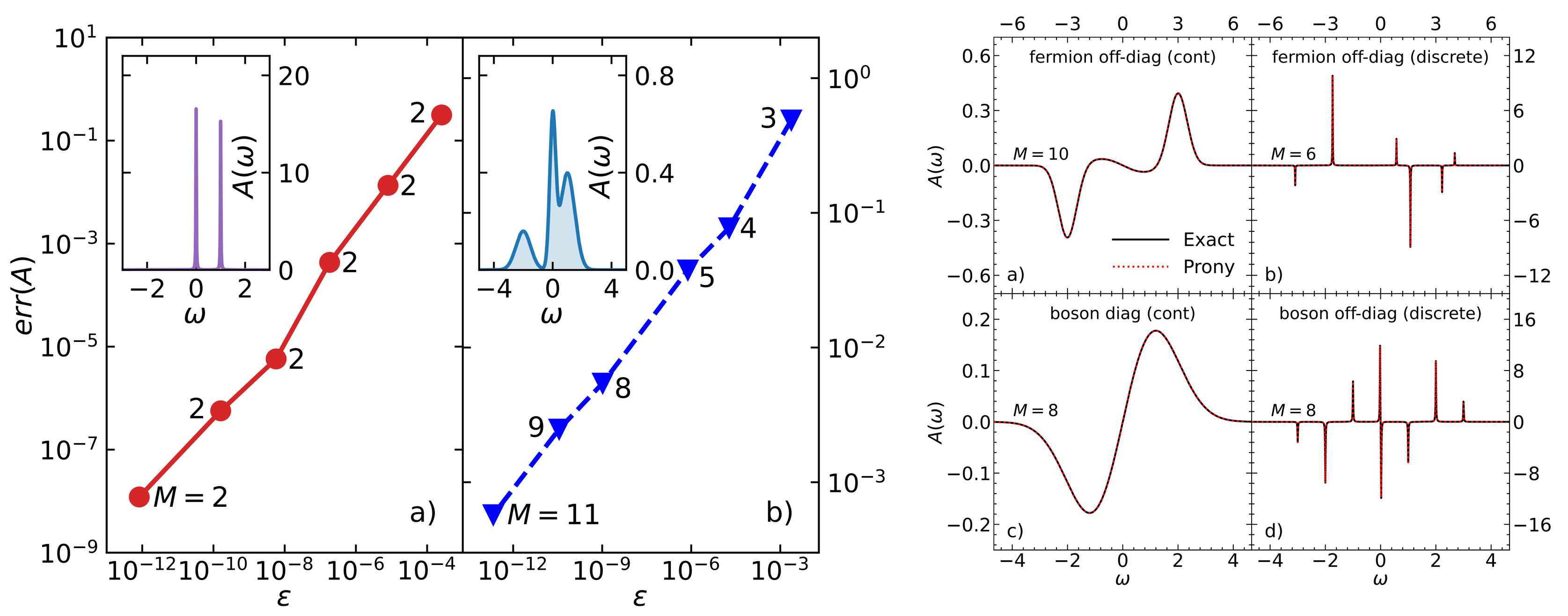
- For $\mathrm{Im}z > 0$: $G(z) = \sum_{l=1}^{M} \frac{A_l}{z - \xi_l}$, $\mathrm{Im}\xi_l \le 0$
- Holomorphic mapping to unit disk
  $$G(z) \to \tilde{G}(w)$$
- Calculation of moments
  $$h_k := \frac{1}{2\pi i}\int_{\partial \bar{D}} \tilde{G}(w) w^k dw$$
- Residue theorem [4, 5]
  $$h_k = \sum_l \tilde{A}_l \tilde{\xi}_l^k, \quad k \ge 0$$
- Transform poles back
  $$\xi_l = g^{-1}(\tilde{\xi}_l), \; A_l = \tilde{A}_l \frac{dz}{dw}\Big|_{\tilde{\xi}_l}$$
- Identify the minimal number M of complex poles that *must* be present

Key problems

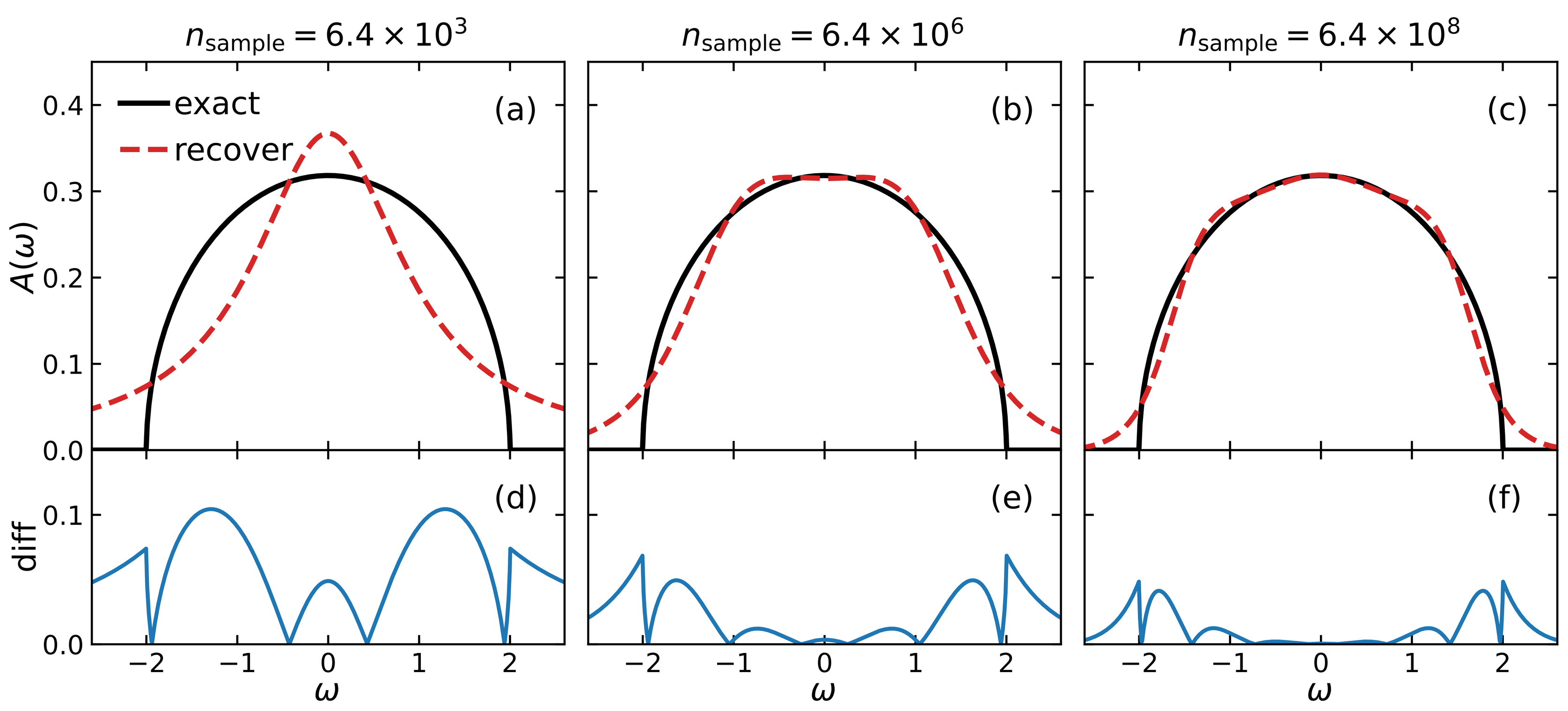


- Infinite solutions $\{A_i\}$ at any finite precision, even after excluding non-causal ones
- Different solutions differ *a lot*: $\sup_{ij}|A_i(\omega) - A_j(\omega)| = +\infty$ for any $\omega \in (-\infty, +\infty)$
- Without prior knowledge, no clear criterion that which solution should be chosen
- Impossible for *any* method to completely eliminate bias in the recovered solution

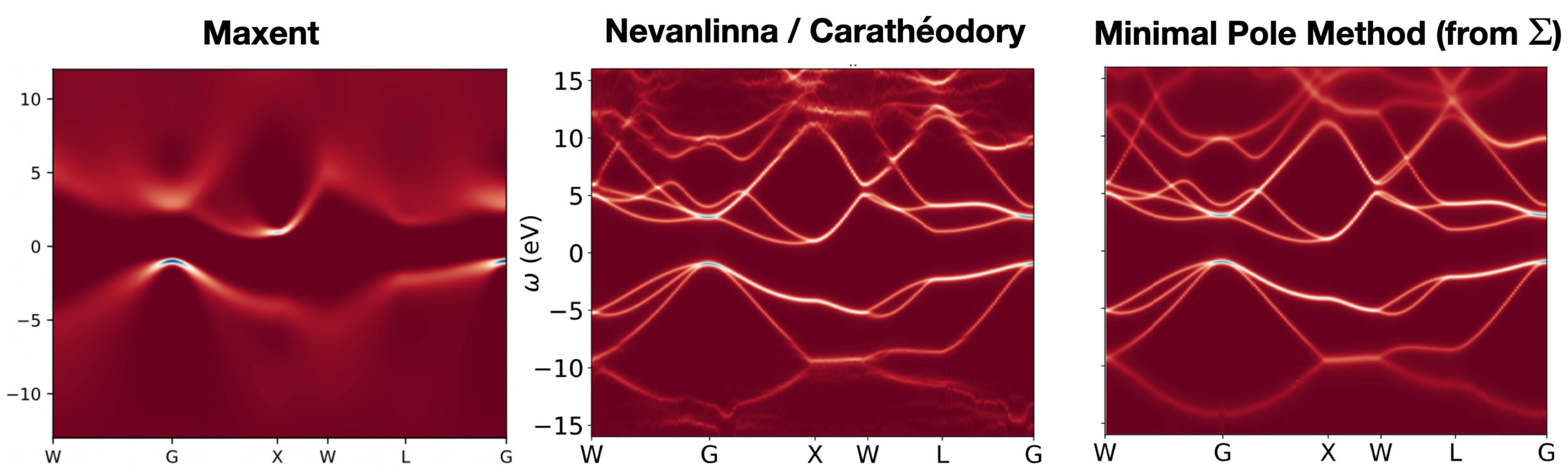
Results



- ε: precision; $err(A) = \int_{\mathbb{R}} d\omega |A - A_{\text{cont}}|$
- Systematically improvable, independent of β and system specifics
- Robust to n_ω: $(n_\omega)_{\min} \gtrsim 2n_{\text{pole}} + 1$
- Noiseless, double precision
- Spectral function can be accurately recovered
- Versatile across different systems



- CT-HYB: the recovered results improve progressively as runtime increases



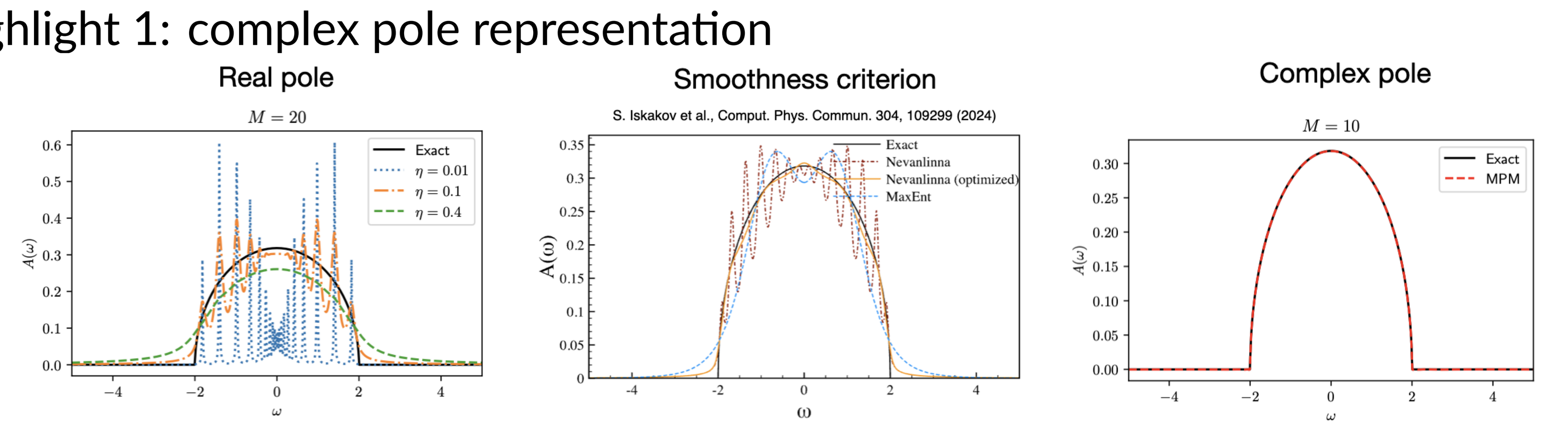
- Self-consistent GW, Si, $6 \times 6 \times 6$ lattice, 200 k-points, 26 orbitals, $\beta = 700\ \mathrm{Ha}^{-1}$
- MaxEnt: unable to resolve distinct bands
- Nevanlinna/Carathéodory: state-of-the-art, uses multiprecision arithmetic, not robust to noise, introduces artificial broadening, requires 800 CPU hrs
- MPM: operates in double precision, robust to noise, no artificial broadening, yields analytic expressions, 80 CPU hrs (MiniPole) and 160 CPU secs (MiniPoleDLR)

Our Contribution

- We demonstrate that bias can always be reduced as data quality improves
- A general-purpose method applicable to all cases: fermionic / bosonic, noisy / noise-free, diagonal / off-diagonal / matrix-valued, discrete / continuous
- Systematically improvable — the spectral function can, in principle, be recovered to arbitrary precision given sufficiently accurate input data

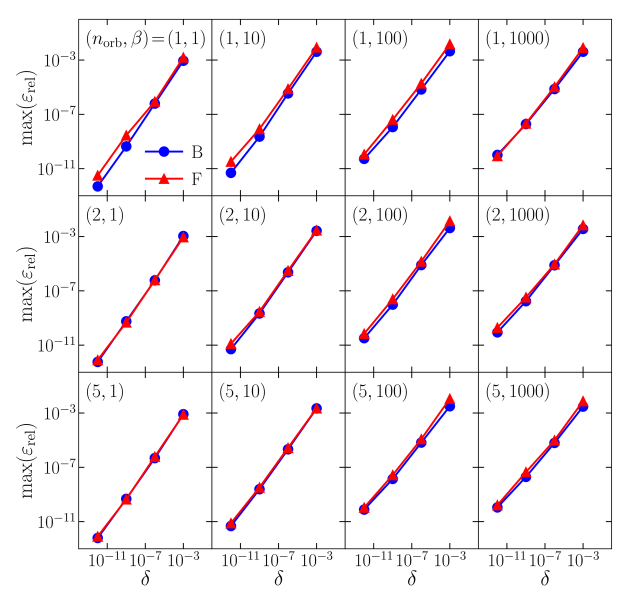
Highlights

Highlight 1: complex pole representation



- Real-axis poles capture discrete features, as in conventional approaches
- Branch cuts are approximated by poles in the lower-half complex plane
- Numerically sufficient to capture all features of the spectrum [3]

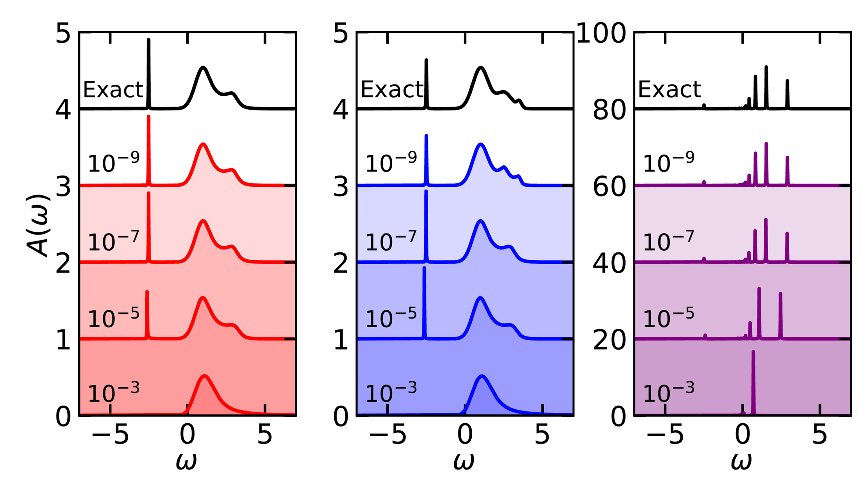
Highlight 2: controlled approximation for $G(iy)$



$$\|G^{(L)}_{\text{approx}}(i\omega_n) - G_{\text{input}}(i\omega_n)\| \le \varepsilon \text{ for } 0 \le n \le n_\omega$$
$$\|G^{(L')}_{\text{approx}}(iy) - G^{(L)}_{\text{approx}}(iy)\| \le \varepsilon \text{ for } n_0 \le n \le n_\omega$$

- Fit $G(i\omega_n)$ with the minimal # of exponentials
- Suppress spurious oscillations in between
- Vary L in ESPRIT to identify oversampling points

Highlight 3: minimal information principle



- Indistinguishable under large noise
- Distinguishable as noise decreases
- No artificial features are recovered
- Symmetry constraints accelerate convergence for discrete systems

- Code available at: `https://github.com/Green-Phys/MiniPole`
- Also available via PyPI (`pip install mini_pole`) and Zenodo

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References

[1] L. Zhang and E. Gull, Phys. Rev. B 110, 035154 (2024).
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[3] L. Zhang, A. Erpenbeck, Y. Yu and E. Gull, arXiv:2504.01163.
[4] L. Ying, J. Comput. Phys. 469, 111549 (2022).
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