Glauber dynamics for quantum systems and its related topics

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Dynamics : time correlation, spectral function

Real time correlation

$$\langle \hat{O}(t)\hat{O}(0)\rangle$$

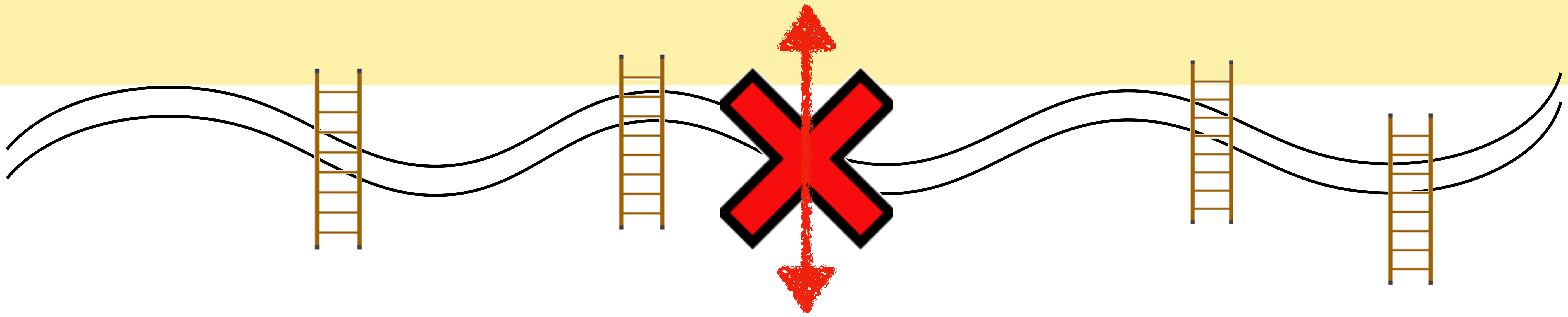
Frequency response

$$\int dt\; e^{itw}\langle \hat{O}(t)\hat{O}(0)\rangle$$

Spectral func.

$$A(w)$$

Experiments



Theory

Huge Hilbelt space $\mathrm{Size}(|\psi\rangle, \rho, H) \sim e^{\alpha V}$

Exponentially growth by a system size, V

It is difficult to calculate a dynamical evolution of a quantum state.

Today's contents

Numerical approaches for calculation of dynamical quantities

Time correlation

- Glauber dynamics of quantum system (2023)
- Extrapolation from complex time evolution by tensor networks (2024)

Spectral function

- Stochastic analytical continuation (2024)

Green function

- Nevanlinna analytical continuation (2021)

Glauber dynamics of classical systems

(Glauber, JMP, 1963)

Ex. magnetic lattice model

State $S = (s_1, s_2, s_3, \cdots)$

Canonical distribution

Probability of a state $P(S) \propto e^{-\beta H(S)}$

β : inverse tenmepature, H : Hamiltonian

Static quantity: $\langle A \rangle = \sum_S A(S)P(S)$

By Markov chain Monte Carlo method,

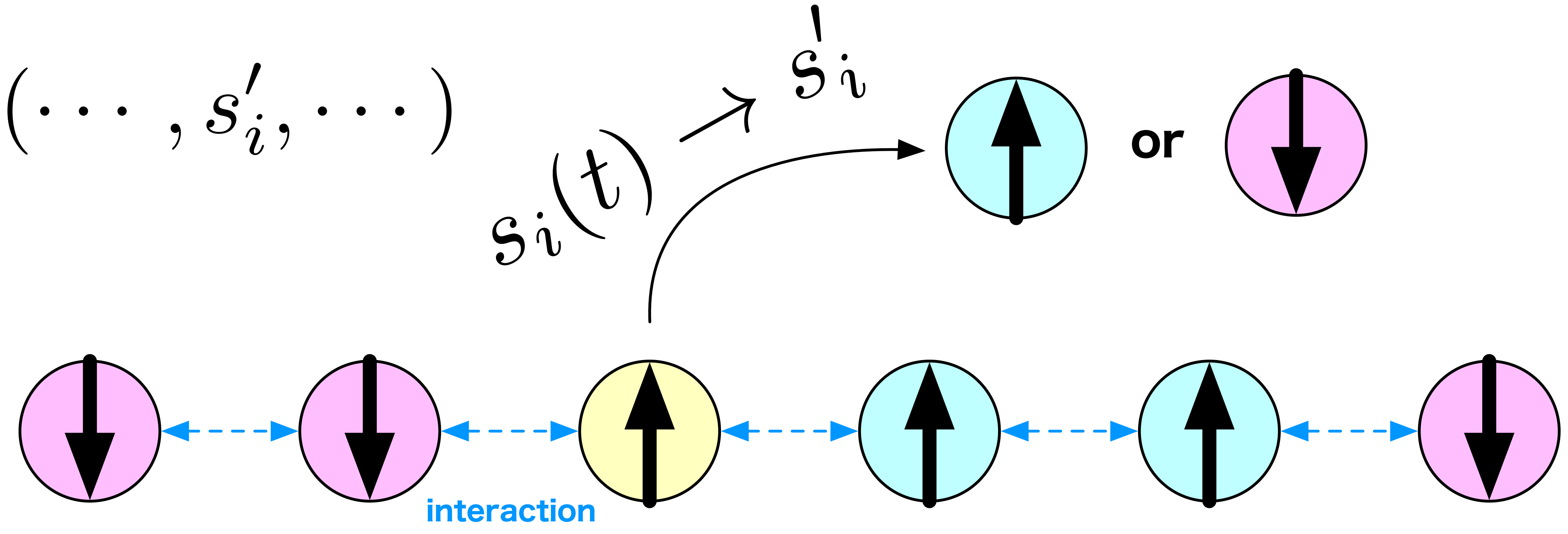
$$\langle A \rangle \approx \frac{1}{M} \sum_{i=1,M} A(S(i)), \quad S(i) \text{ is sampled by } P(S(i))$$

Glauber dynamics is a Markov process in which the stational distribution is canonical.

Glauber dynamics for Ising spin model

State change $S(t) = (\cdots, s_i, \cdots) \to S(t+1) = (\cdots, s'_i, \cdots)$

Glauber update



Conditional prob.

$$\mathrm{Prob}(s_i(t) \to s'_i) = P(s'_i | S_{\neq i}(t)) = P(S(t+1))/P(S_{\neq i}(t))$$

Configuration except $s_i(t)$: $S_{\neq i}(t) = (\cdots, s_{i-1}(t), s_{i+1}(t), \cdots)$

Ex. Ising model

Effective field

$$H(S) = -\left(\sum_j J_{ij} s_j\right) s_i + \cdots$$

inverse temp. β

$$\mathrm{Prob}(s'_i) \propto e^{\beta[\sum_j J_{ij} s_j(t)] s'_i}$$

If the temperature is high, a spin fluctuates, and if it is low, the Ising interaction stochastically determines the next spin state.

Thermal fluctuations

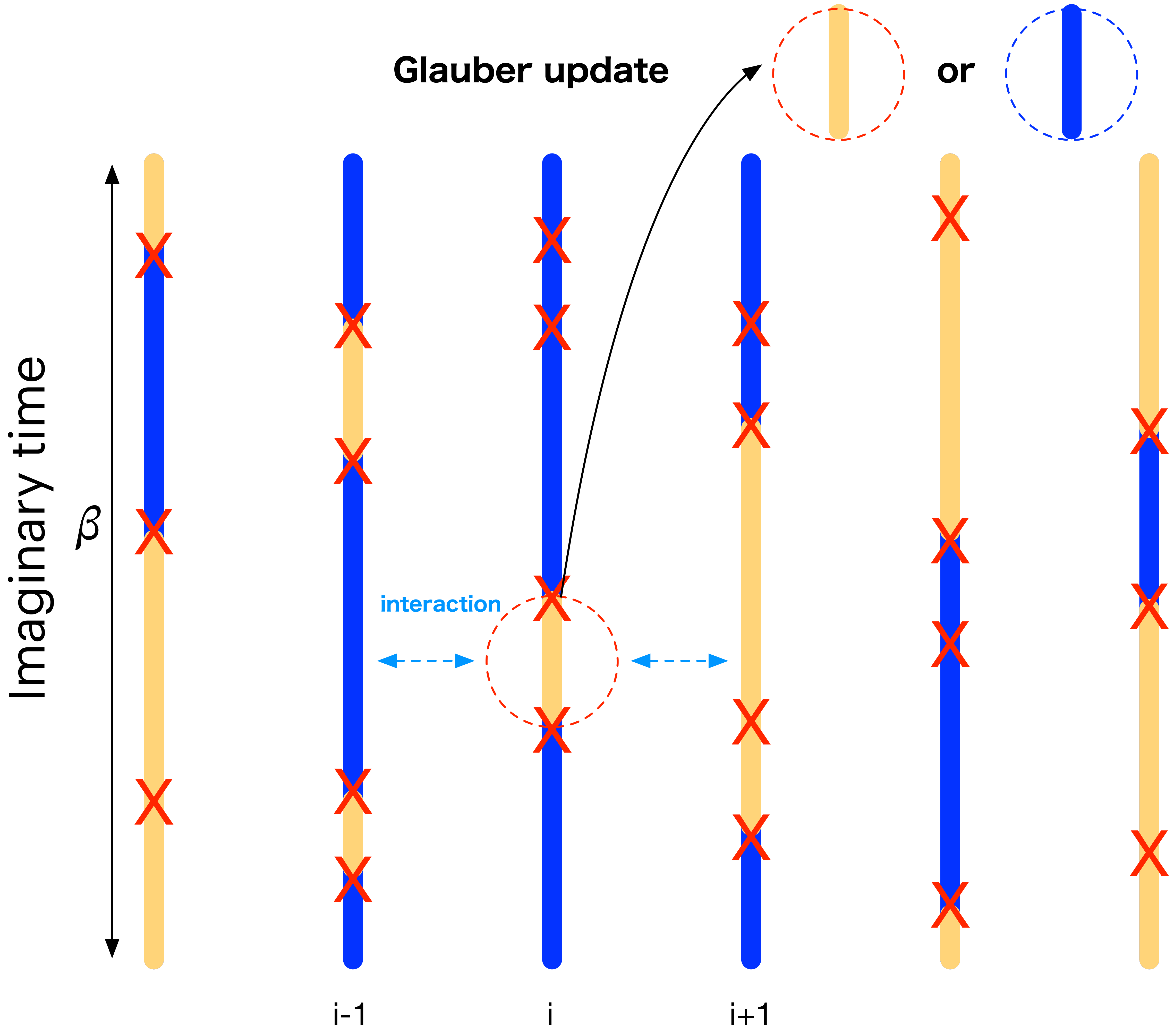
(Glauber, JMP, 1963)

Glauber dynamics of quantum Ising model

$$H = \sum_{(i,j)} -J_{ij}\sigma_i^z\sigma_j^z - \Gamma\sum_i \sigma_i^x$$

$$\langle \mathcal{O} \rangle = \mathrm{Tr}\left[\mathcal{O}e^{-\beta H}\right]/Z$$

MCMC on a path-integral rep.



Glauber dynamics on a path-integral representation

(Nakamura & Ito, JPSJ 2003)

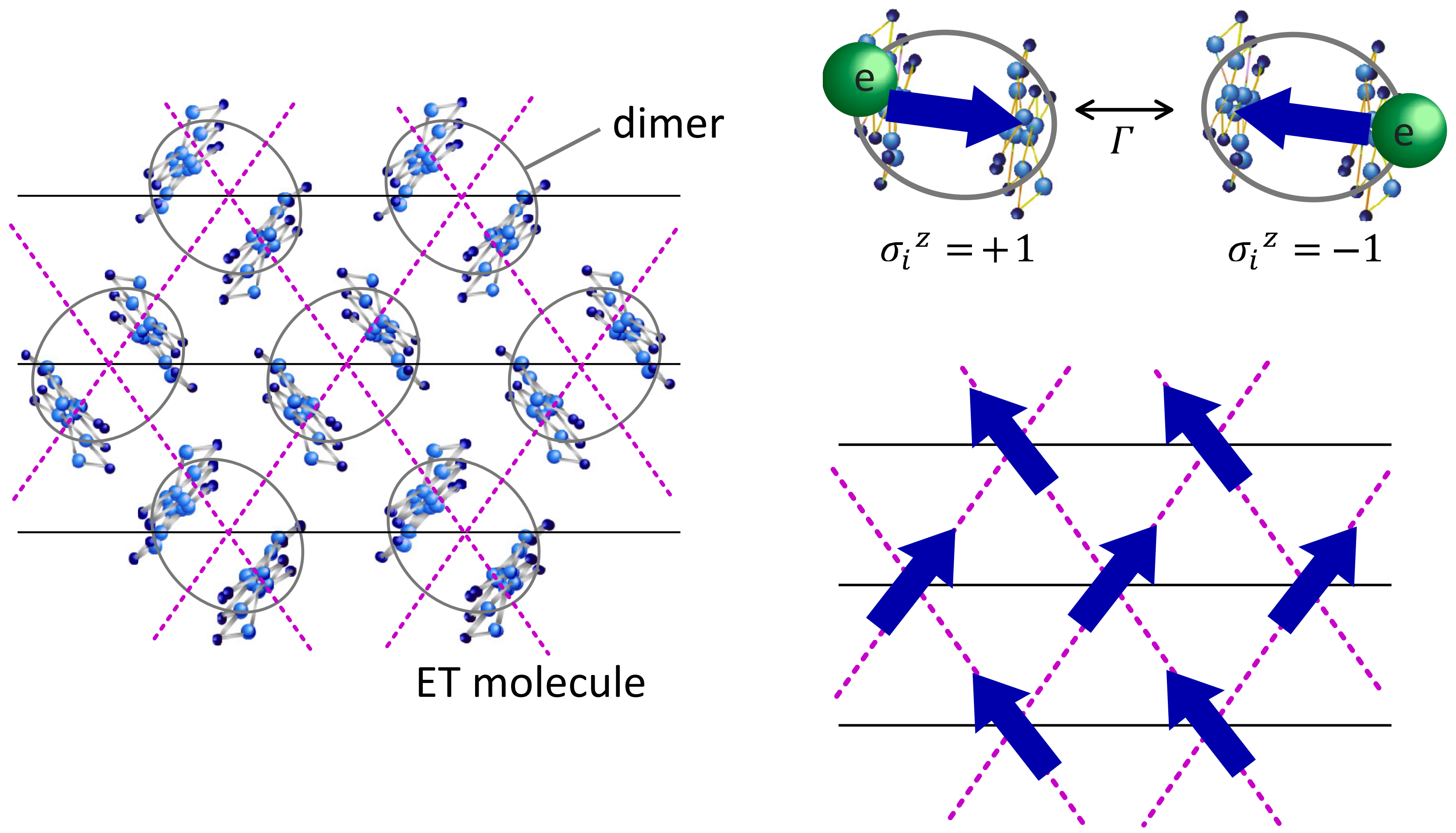
MCMC time evolution
~ real time evolution

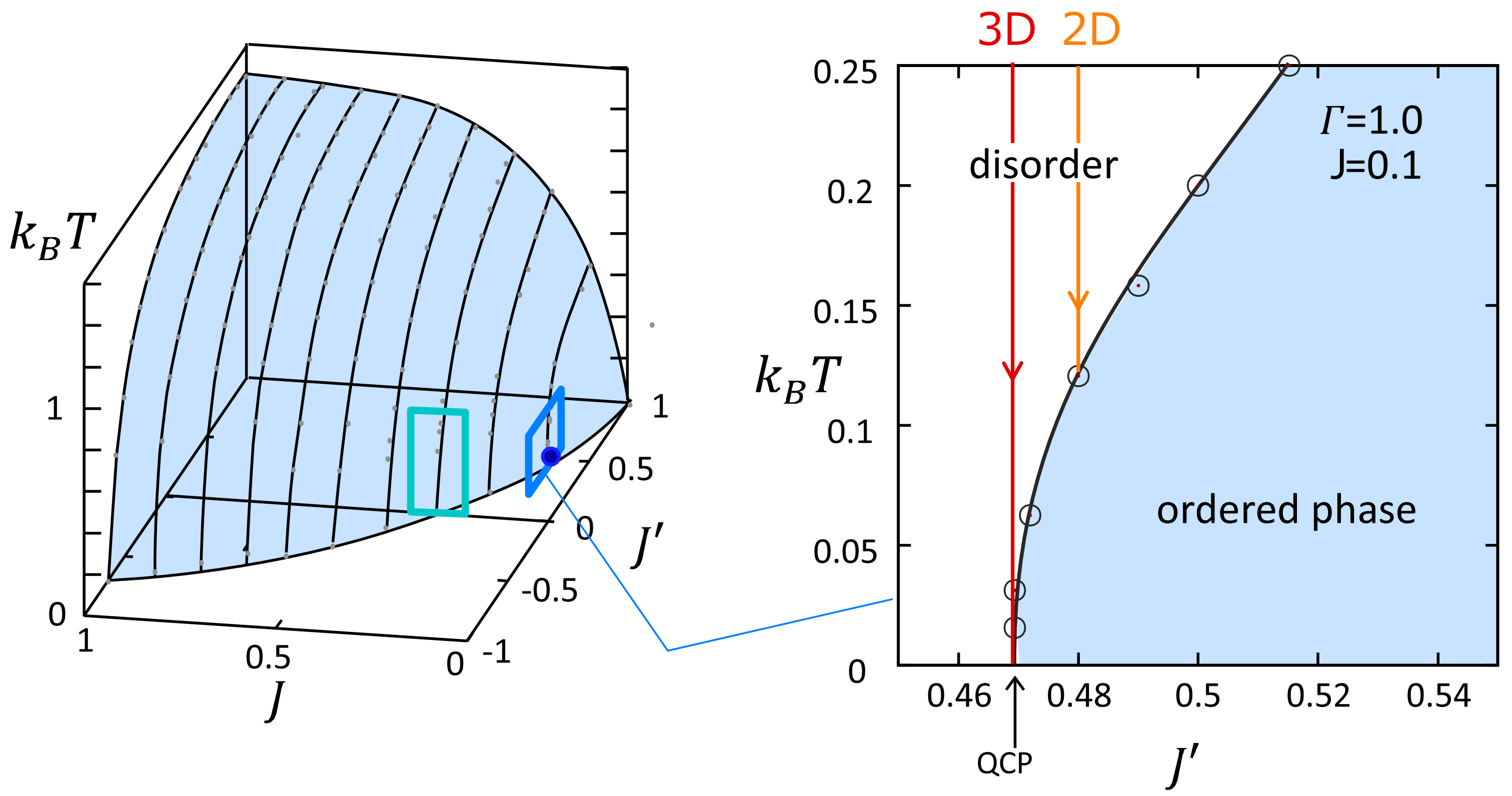
(Hotta, Yoshida, H., PRR 2023)

Quantum critical dynamics in 2D quantum Ising model

(Hotta, Yoshida, H., PRR 2023)

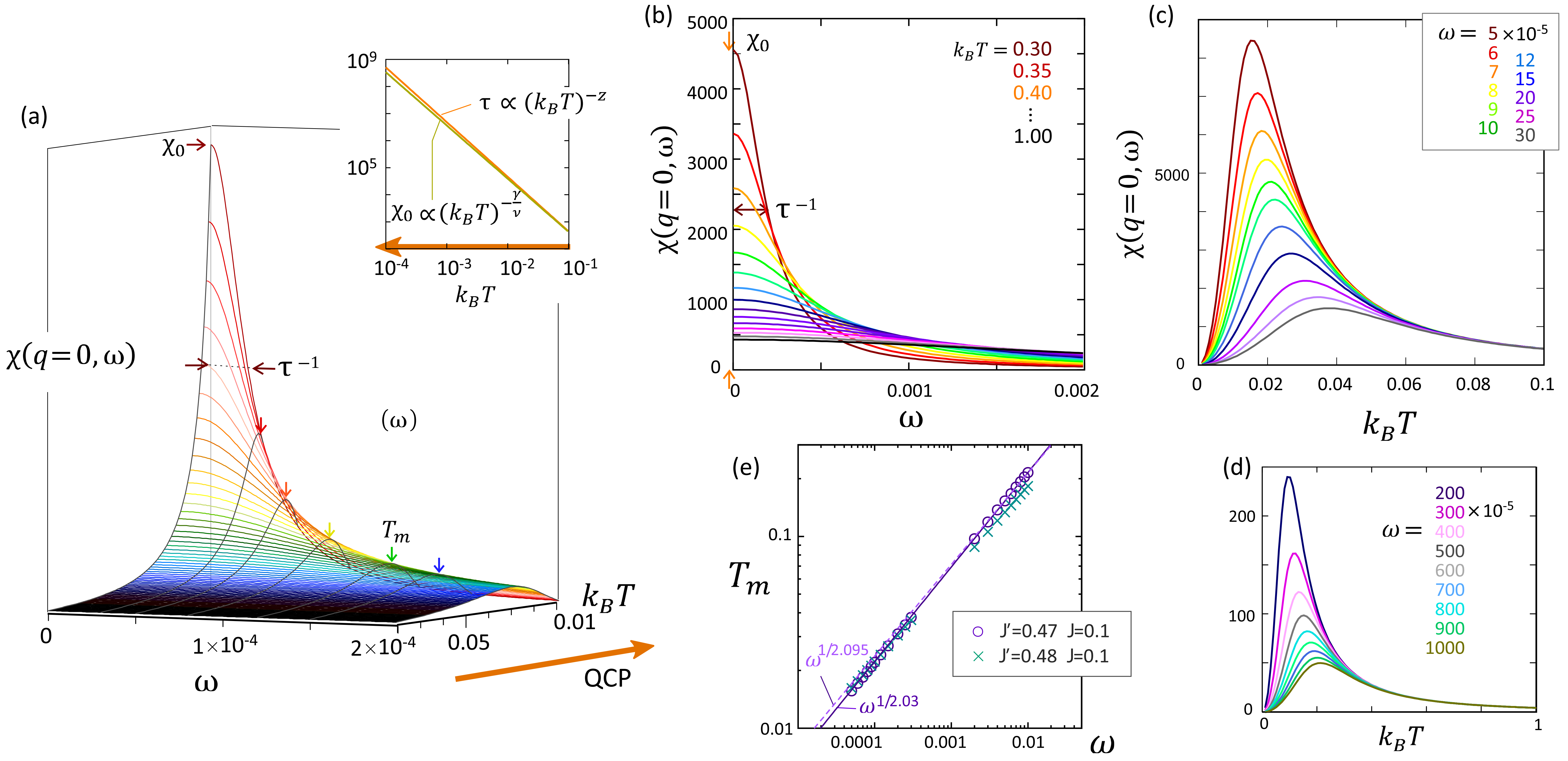
Organic dimer Mott insulator





Very close to QCP?

Dynamic susceptibility by Glauber protocol



Good agreement with the dielectric experiment on κ-ET2Cu2(CN)3

Dynamical correlation function from complex time evolution

(Cao, et al. PRB 2024)

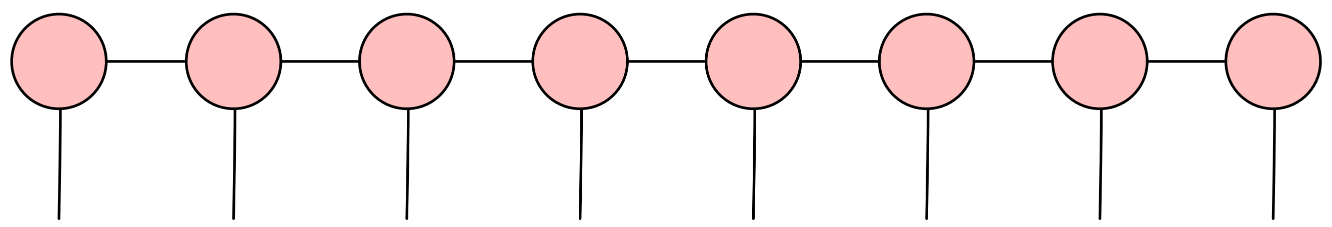
Real time correlation

$$G^{>}_{\hat{O}_1\hat{O}_2}(t) = -i\langle\psi_g|\hat{O}_1(t)\hat{O}_2|\psi_g\rangle$$
$$= -i\langle\psi_g|\hat{O}_1|\psi(t)\rangle$$

However, highly entangled state ⓧ

$$|\psi(t)\rangle \equiv e^{-it\hat{H}}\hat{O}_2|\psi_g\rangle$$

Matrix Product State(MPS)



Large bond dim. Is necessary.

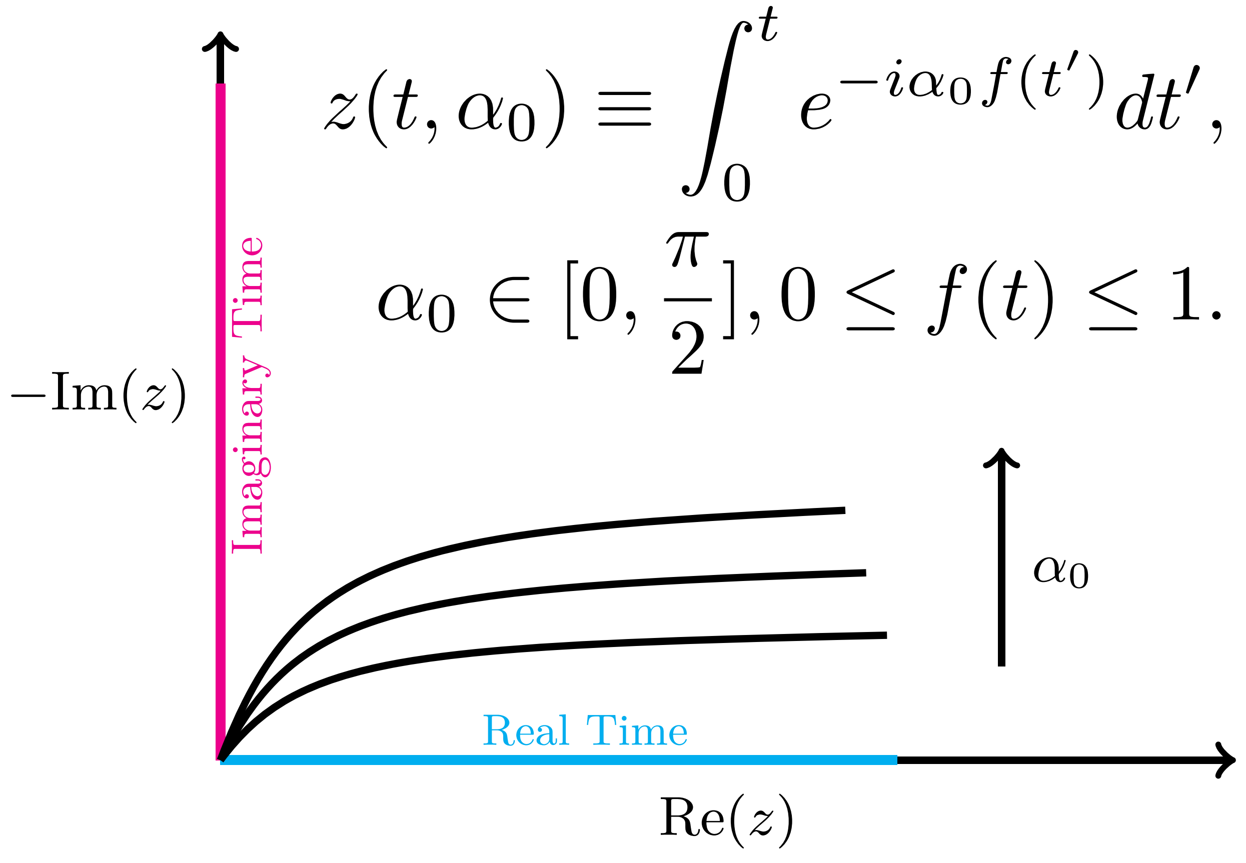
Complex time evolution

$$\hat{O}_1(z) = e^{iz\hat{H}}\hat{O}_1 e^{-iz\hat{H}}$$

$$|\psi(t,\alpha_0)\rangle \equiv e^{-iz(t,\alpha_0)\hat{H}}\hat{O}_2|\psi_g\rangle$$

$$z(t,\alpha_0) \equiv \int_0^t e^{-i\alpha_0 f(t')}dt',$$

$$\alpha_0 \in [0, \frac{\pi}{2}], 0 \le f(t) \le 1.$$



$\alpha_0 = 0 \rightarrow$ real time evolution

$\alpha_0 > 0$ ➡ Low entangled state

Small bond dim. Is enough to represent it.

$$G^{>}_{\hat{O}_1\hat{O}_2}(t,\alpha_0) = -i\langle\psi_g|\hat{O}_1|\psi(t,\alpha_0)\rangle$$

➡ $$G^{>}_{\hat{O}_1\hat{O}_2}(t) = \lim_{\alpha_0\to 0} G^{>}_{\hat{O}_1\hat{O}_2}(t,\alpha_0)$$

Extrapolation

Results for a spectral function of the single impurity Anderson model

(Cao, et al. PRB 2024)

Extrapolation by Taylor expansion

$$G^{>}(t,0) = G^{>}(t,\alpha_0) + \sum_{n\geq 1} \frac{(-\alpha_0)^n}{n!} \frac{d^n G^{>}(t,\alpha_0)}{d\alpha_0^n}$$

<u>Ex. single impurity Anderson model</u>

$$\hat{H} = \hat{H}_{\text{loc}} + \hat{H}_{\text{bath}}$$

$$\hat{H}_{\text{loc}} = \epsilon_d \sum_{\sigma=\uparrow,\downarrow} \hat{n}_{d\sigma} + U \hat{n}_{d\uparrow}\hat{n}_{d\downarrow}$$

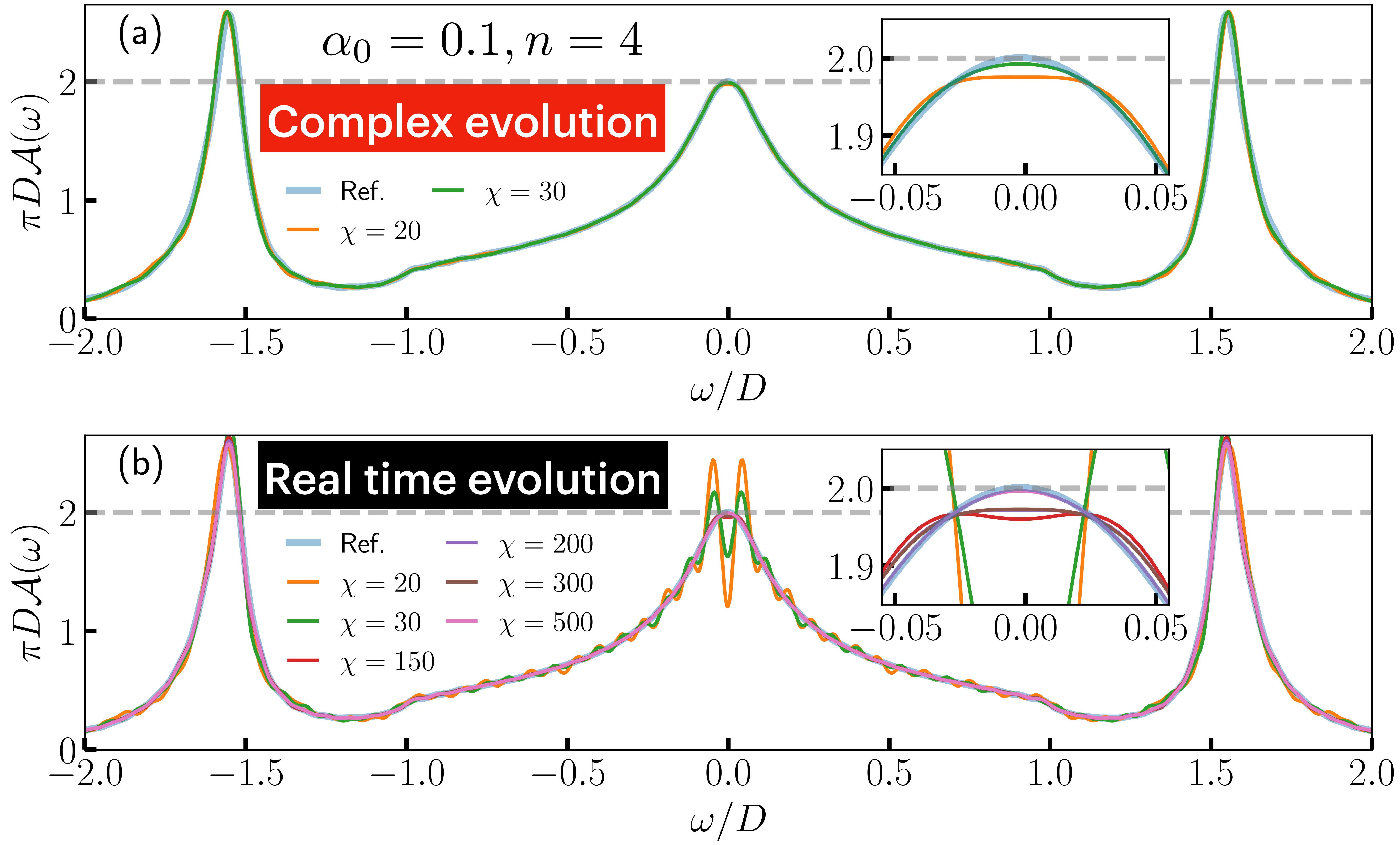
$$\hat{H}_{\text{bath}} = \sum_{\substack{b=0\\ \sigma=\uparrow,\downarrow}}^{N_b-1} \epsilon_b \hat{n}_{b\sigma} + \sum_{\substack{b=0\\ \sigma=\uparrow,\downarrow}}^{N_b-1} (v_b \hat{c}^\dagger_{b\sigma}\hat{d}_\sigma + \text{H.c.})$$

$$N_b = 59, U = 2D, Dt_{\max} = 90$$

The complex time result reproduces the entire spectrum with small bond dimensions.

Spectral function

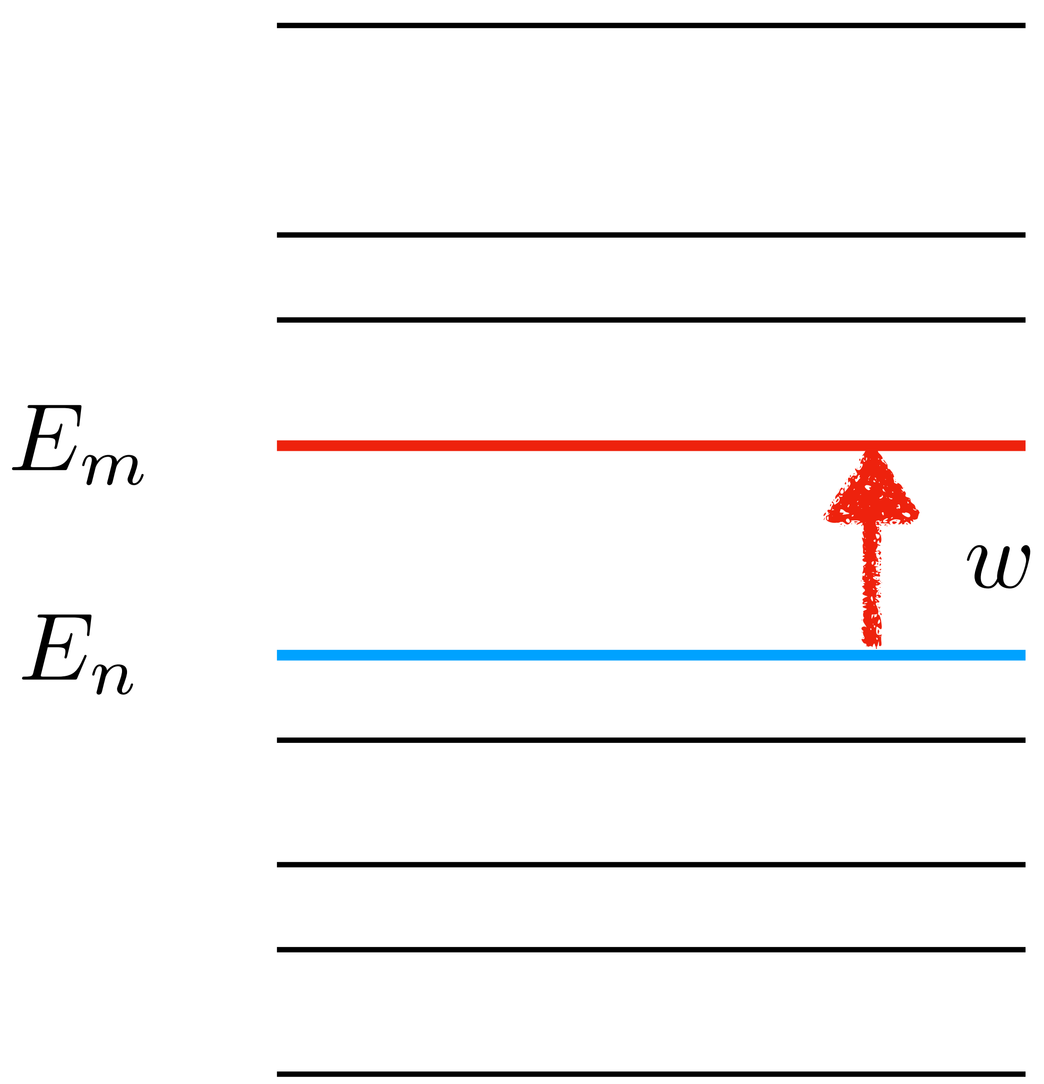
$$A_{\sigma\sigma'}(w) = -\frac{1}{\pi}\text{Im}\int_0^{+\infty} dt\; e^{itw} G^R_{\sigma\sigma'}(t)$$



Spectral function and imaginary time correlation

Spectral function

E_n : energy level, O : observable, inverse temperature $\beta = 1/k_B T$



$$S(w) = \frac{\pi}{Z}\sum_{m,n} e^{-\beta E_n}|\langle m|O|n\rangle|^2\delta(w-[E_m-E_n])$$

Average by canonical ensemble

$$A(w) = \frac{1}{Z}\sum_{m,n}(e^{-\beta E_m}+e^{-\beta E_n})|\langle m|O|n\rangle|^2\delta(w-[E_m-E_n])$$

$$= S(w)(1+e^{-\beta w})/\pi$$

Imaginary time correlation

$$\langle O^\dagger(\tau)O(0)\rangle = \int_0^\infty A(w)\tilde{K}(\tau,w),$$

$$O(\tau) = e^{\tau H}Oe^{-\tau H},\ \tilde{K}(\tau,w) = \frac{e^{-\tau w}+e^{-(\beta-\tau)w}}{1+e^{-\beta w}}$$

We can numerically calculate imaginary time correlation.

However, the inverse transformation is ill-posed.

Maximu entropy method for spectral function

Analytic continuation process by the chi-square

$$A(w) \to G^A(\tau) = \int_0^\infty dw A(w)\tilde{K}(\tau,w) \to \chi^2(\tilde{G}, G^A) = \sum_{ij}(G_i^A - \tilde{G}_i)C_{ij}^{-1}(G_j^A - \tilde{G}_j)$$

QMC data

Covariance matrix of QMC data

Directly assume a function form (Maximum entropy method)

or a stochastic model (Stochastic analytic continuation)

Maximum entropy method (Gubernatis, et al. PRB 1991)

Minus of KL-divergence

$$E(A) = -\int_0^\infty dw A(w) \ln\left(\frac{A(w)}{D(w)}\right) \to \min \arg_A F(A) = \chi^2(A)/2 - \alpha E(A)$$

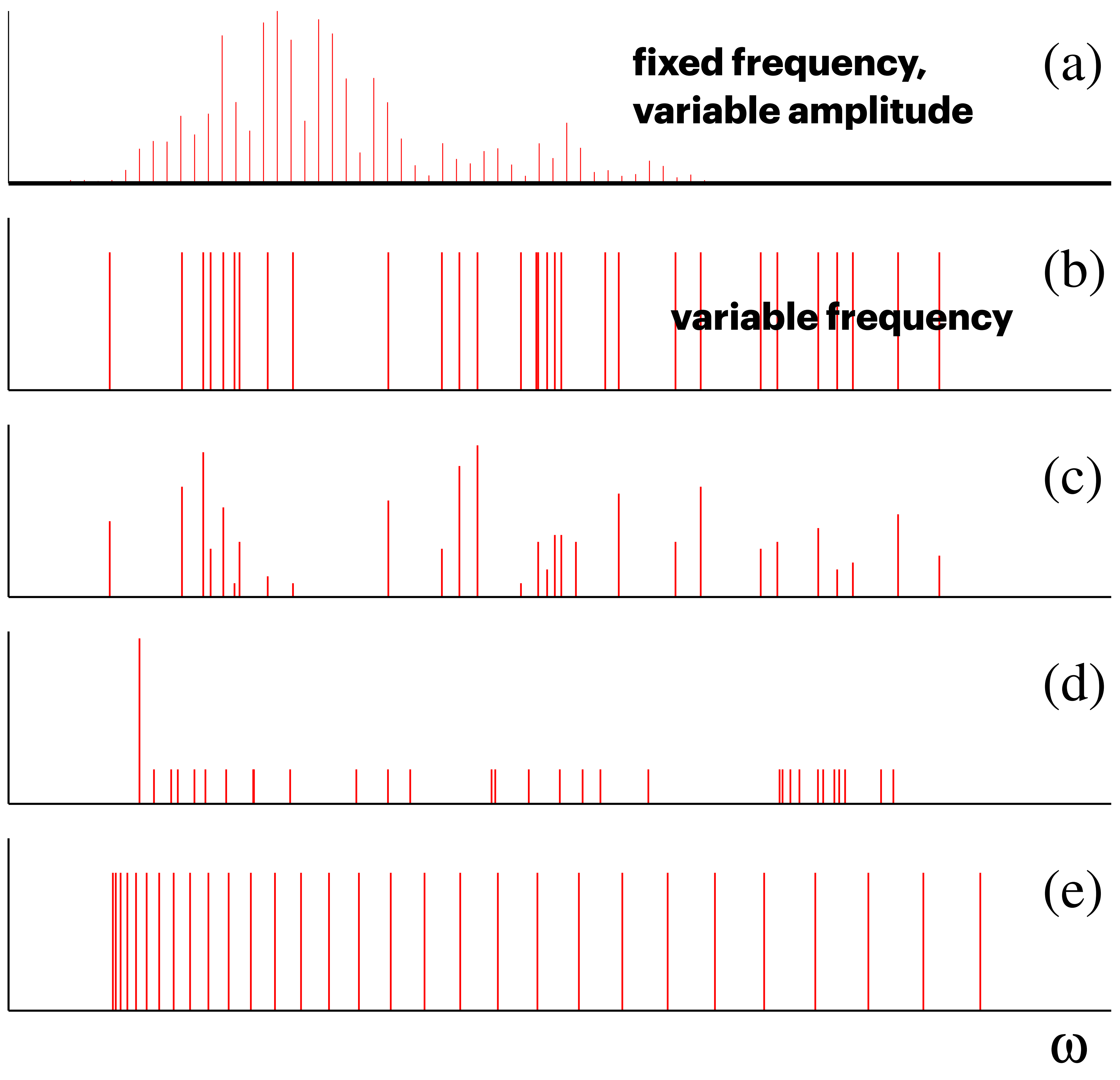
$$A(w) \geq 0, \int_0^\infty A(w)dw = 1$$

The solution is balanced between the chi-square and KL-divergence.

Stochastic analytic continuation

Parameterization of spectra

(White, et al. 1991, ... Review: Shao & Sandvik, Phys. Rep. 2023)



large number of delta functions

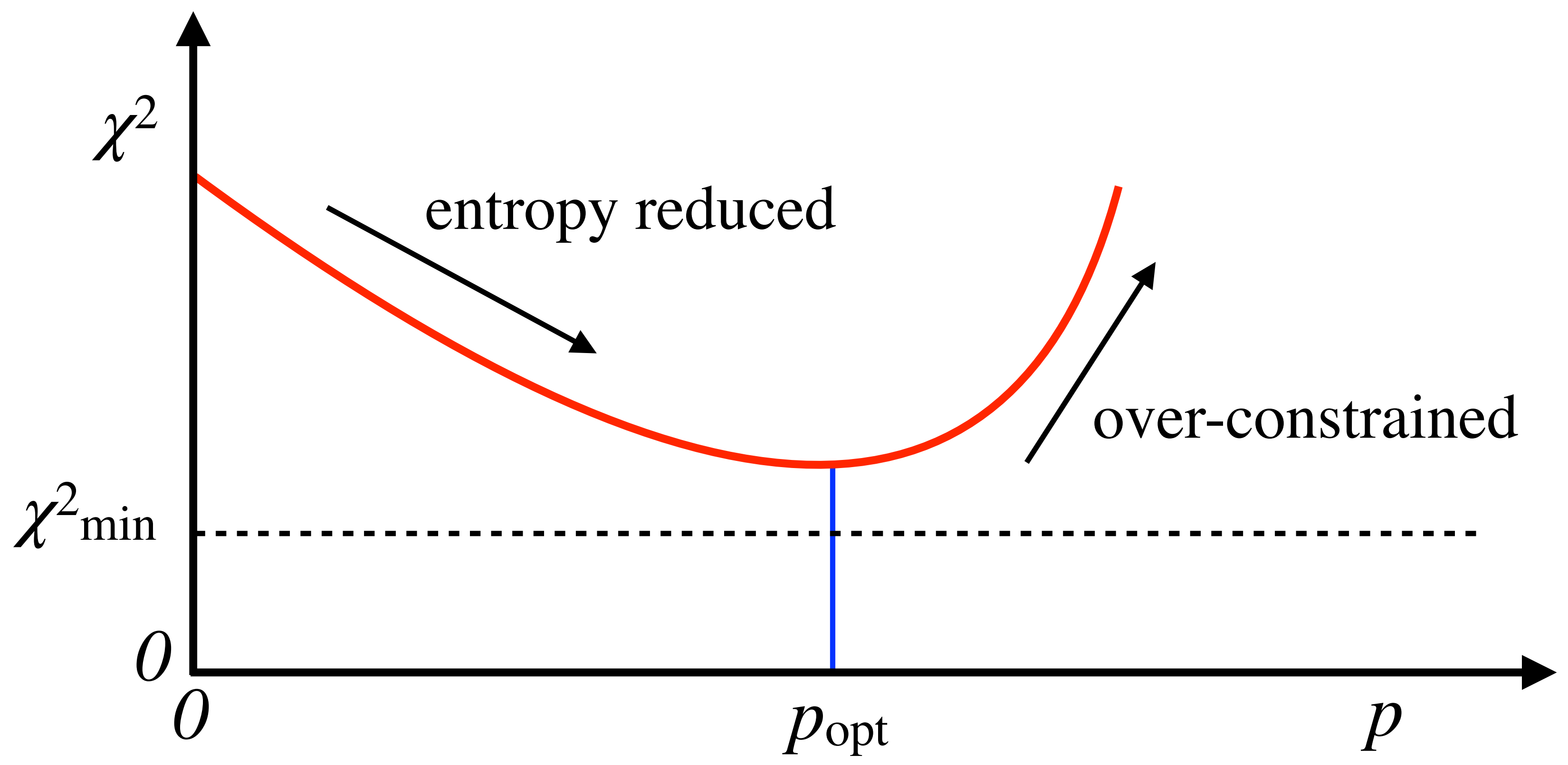
Metropolis MC of parameters at a fictitious temperature Θ

weight $P(A|\tilde{G}) \propto \exp\left(-\frac{\chi^2(A)}{2\Theta}\right)$

spectral function = average of samples

Add constraints

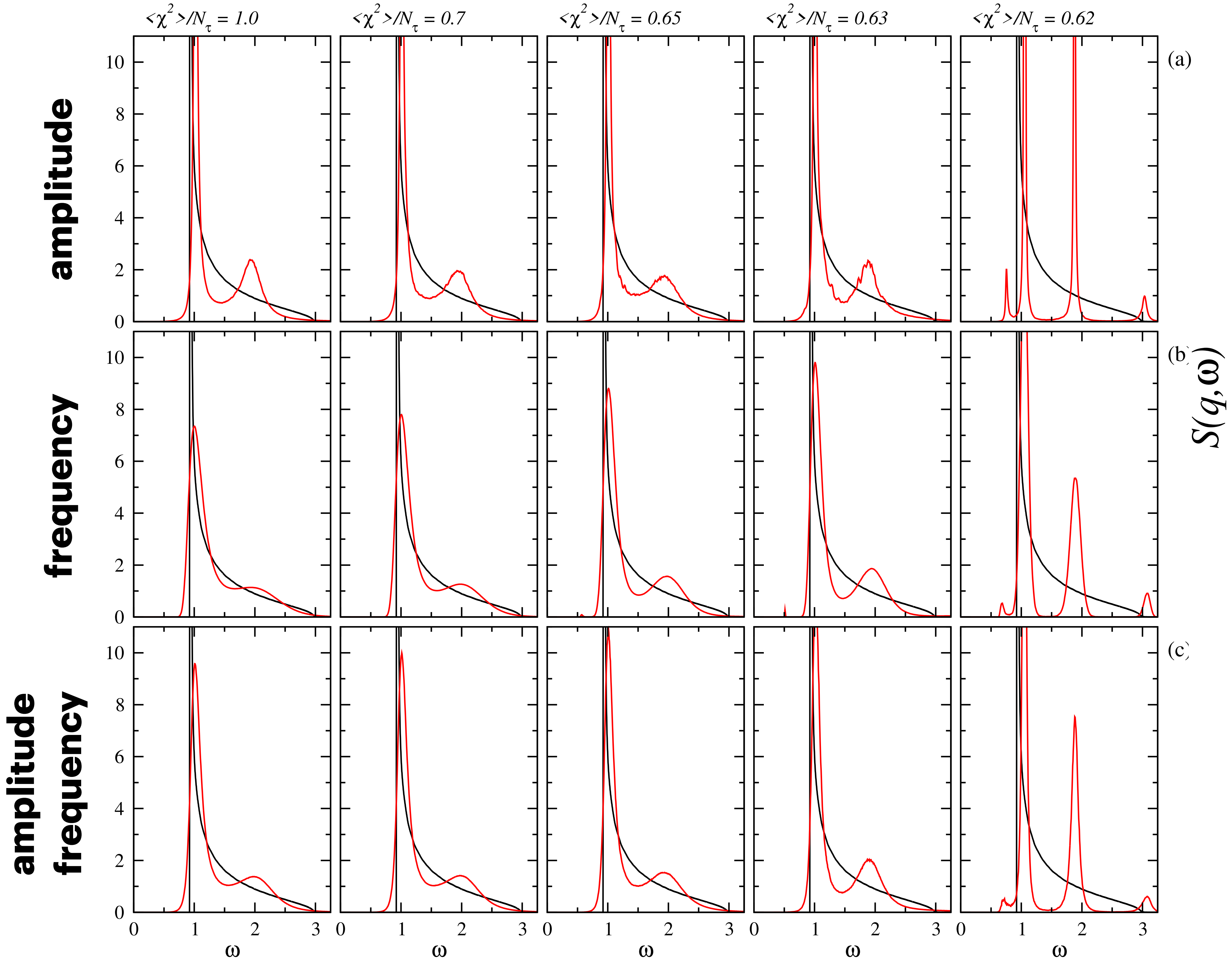
range of frequencies, gap structure, etc.



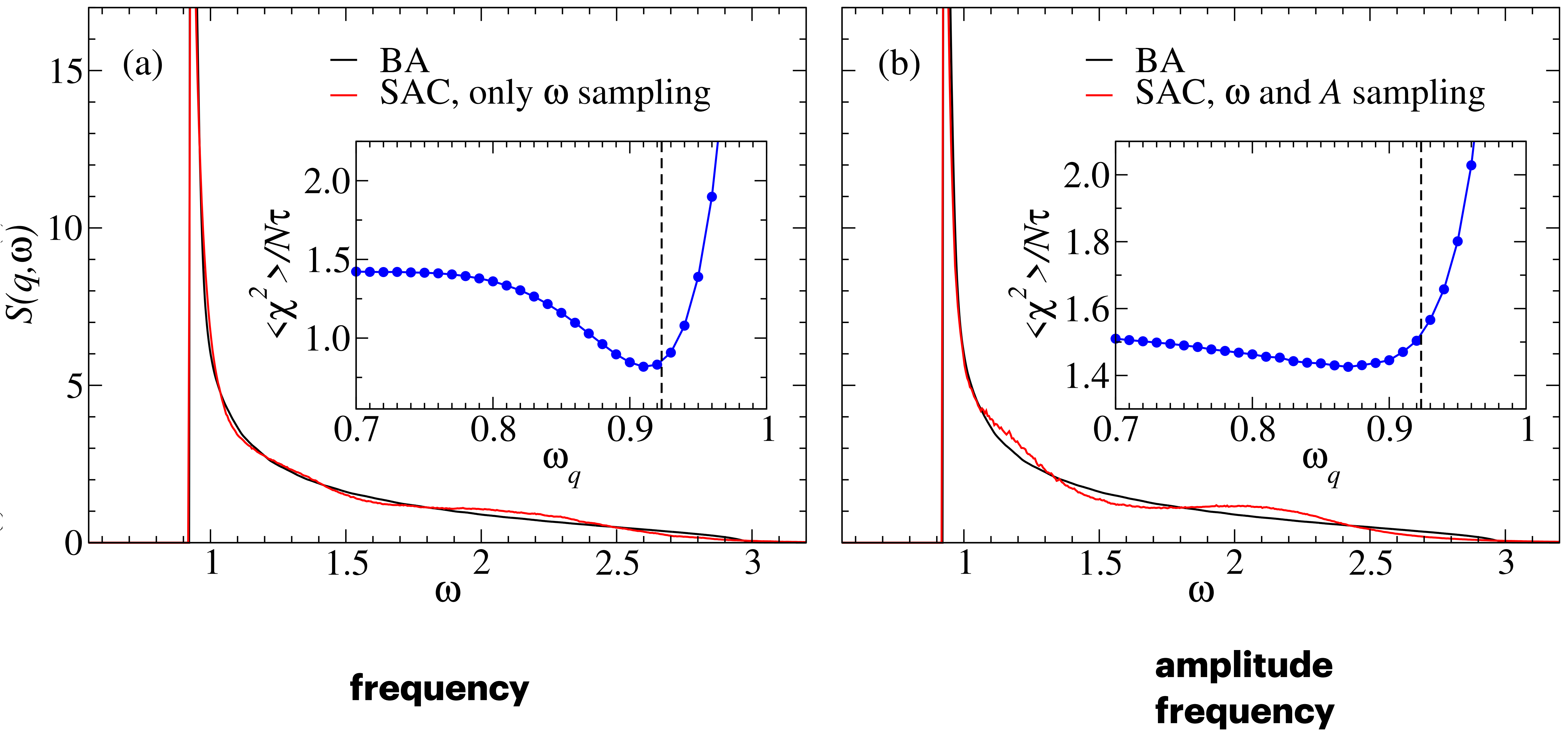
Demonstration of stochastic analytic continuation

HAF chain (L=500, T = J/500) $q = 4\pi/5$

(Shao & Sandvik, Phys. Rep. 2023)



Constraint : lower edge $w_q \approx 0.923$



A constraint is important to improve the quality of a spectral function.

Nevanlinna analytical continuation

(Fei, Yeh & Gull, PRL 2021)

Green function

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

analytic in the open upper half-plane $\mathcal{C}^+$

negative imaginary part into $\overline{\mathcal{C}^+}$

Nevanlinna function: analytic in the open upper half-plane $\mathcal{C}^+$, non-negative imaginary part into $\overline{\mathcal{C}^+}$

The minus of Green function is a Nevanlinna function.

Modified Schur algorithm

expand all contractive functions, which are holomorphic functions mapping from $\mathcal{C}^+ \to \bar{\mathcal{D}} = \{z : |z| < 1\}$

- Map from Nevanlinna functions one-to-one contractive functions

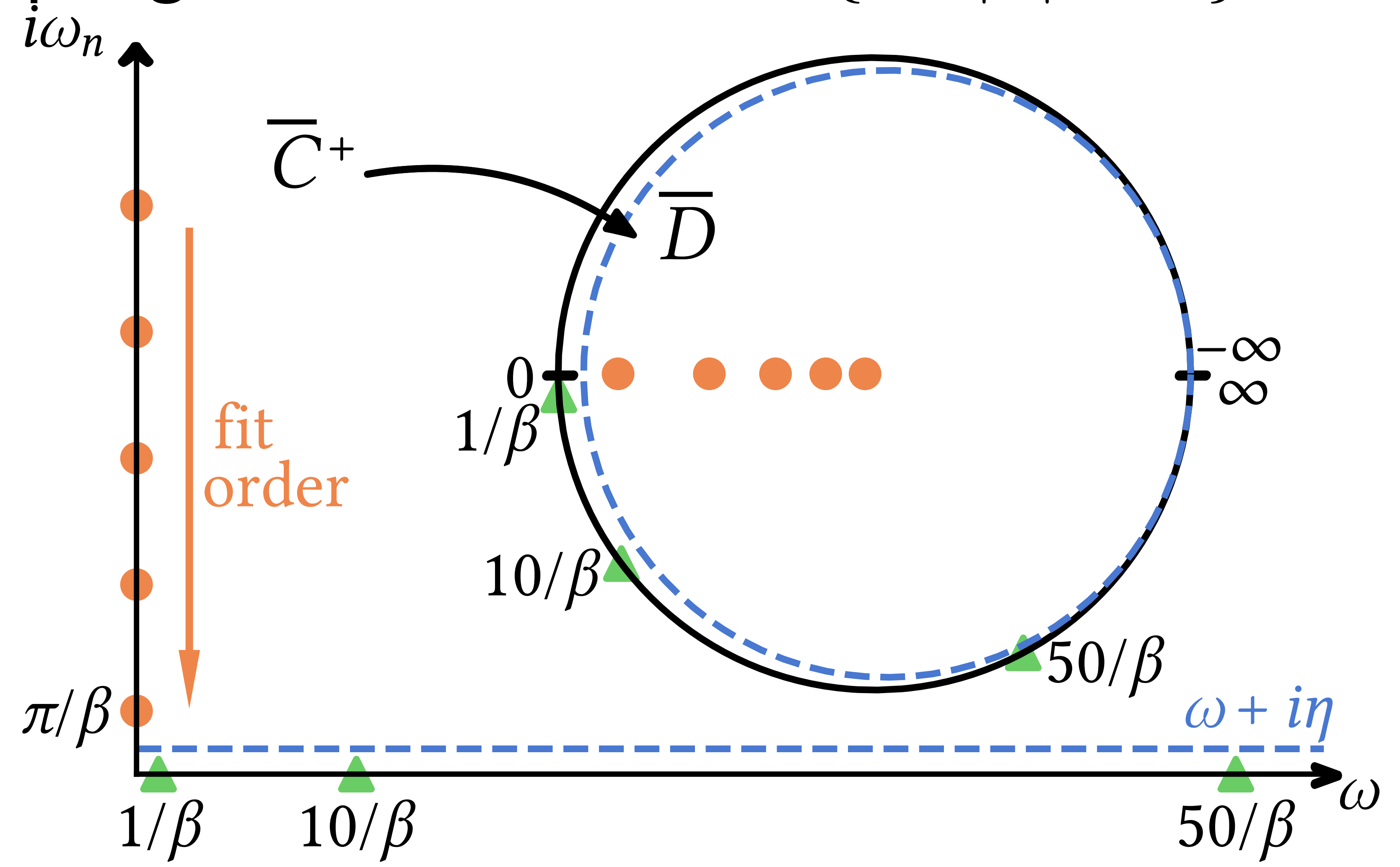
$$\theta(Y_i) = h(-\mathcal{G}(Y_i))$$

invertible Möbius transform
$h : \overline{\mathcal{C}^+} \to \bar{\mathcal{D}}, z \to (z - i)/(z + i)$

- Interpolation problem

Free contractive function

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



Demonstration of Nevanlinna analytical continuation

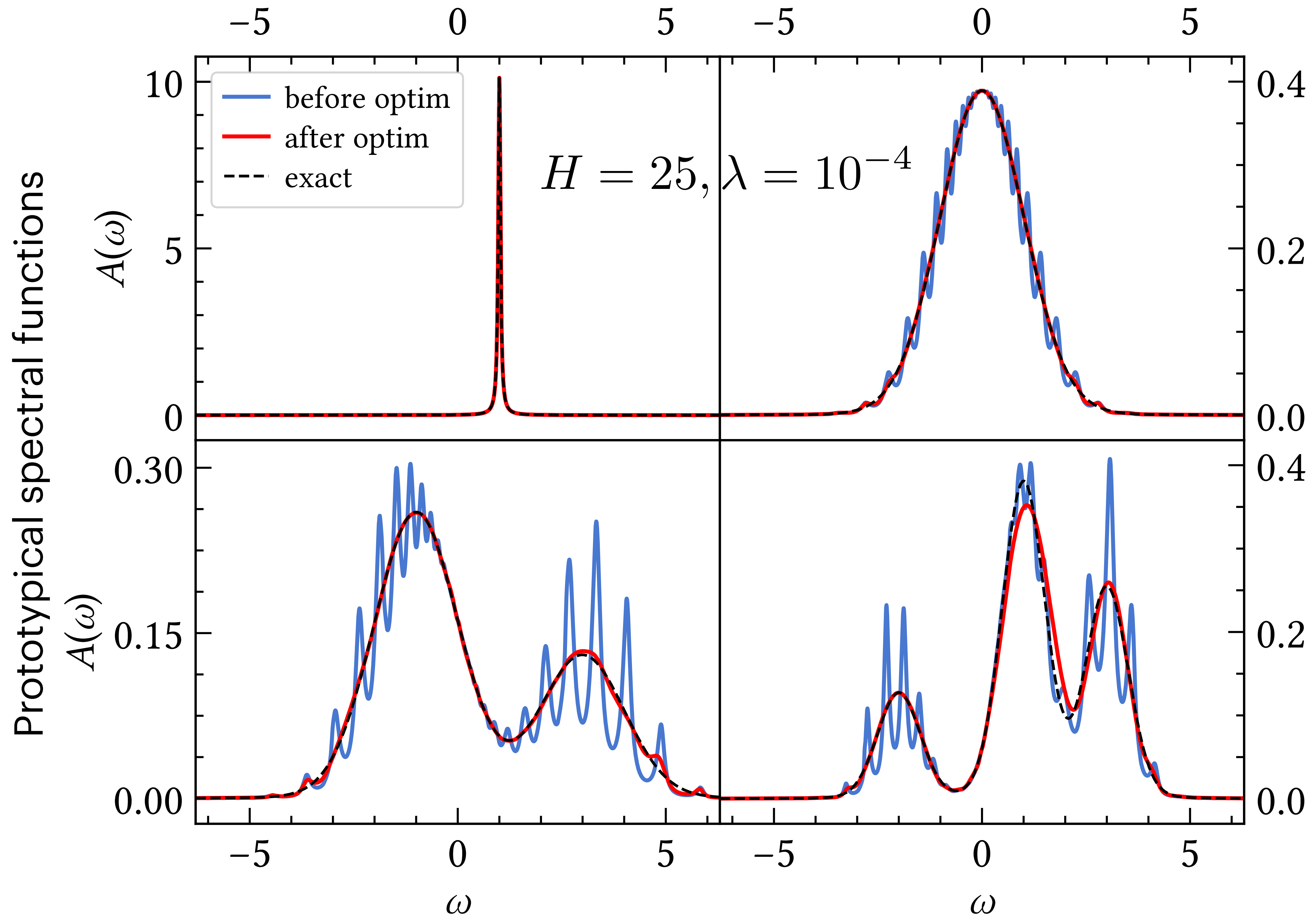
Hardy basis expansion

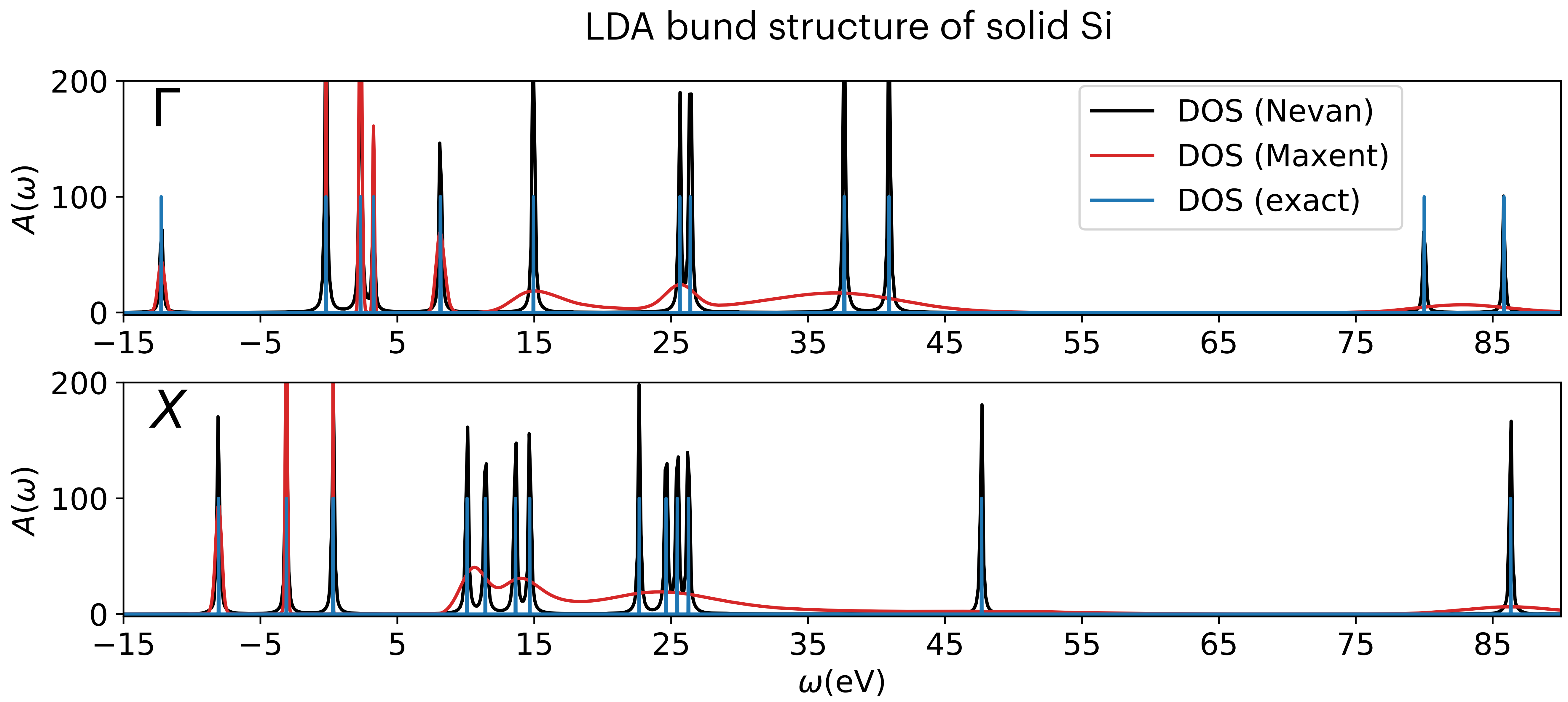
(Fei, Yeh & Gull, PRL 2021)

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

Optimize

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





This method could hold the analytic structure of Green function and resolve both sharp and smooth features.

Summary: numerical approaches for dynamical quantities

Time correlation

- Glauber dynamics of quantum system

  C. Hotta, T. Yoshida, and K. Harada, Phys. Rev. Res. **5** (2023) 013186.

- Extrapolation from complex time evolution by tensor networks

  X. Cao, Y. Lu, E. M. Stoudenmire, and O. Parcollet, Phys. Rev. B **109** (2024) 235110.

Spectral function

- Stochastic analytical continuation

  H. Shao and A. W. Sandvik, Phys. Rep. **1003** (2023) 1.

Green function

- Nevanlinna analytical continuation

  J. Fei, C.-N. Yeh, and E. Gull, Phys. Rev. Lett. **126** (2021) 056402.