Analytic continuation

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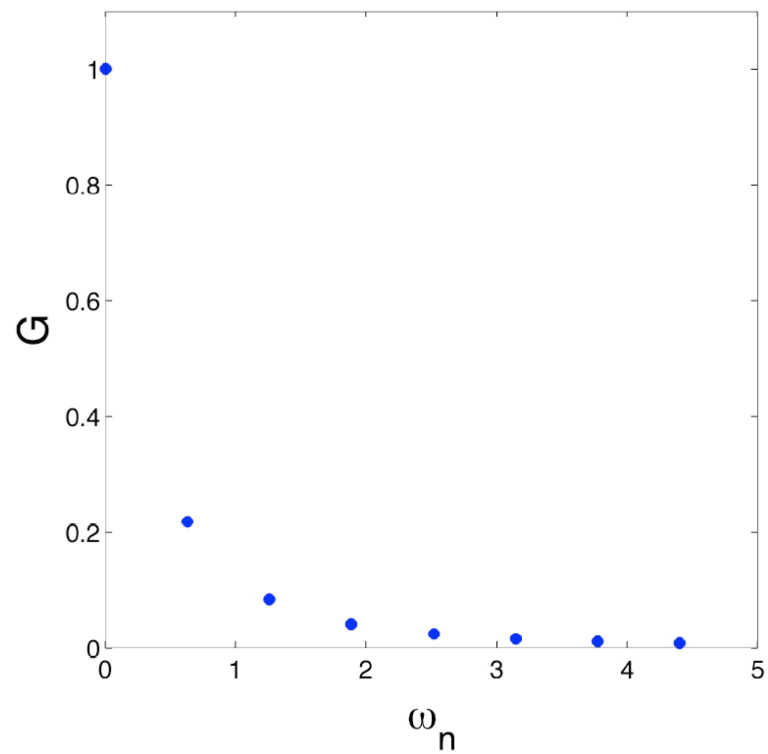
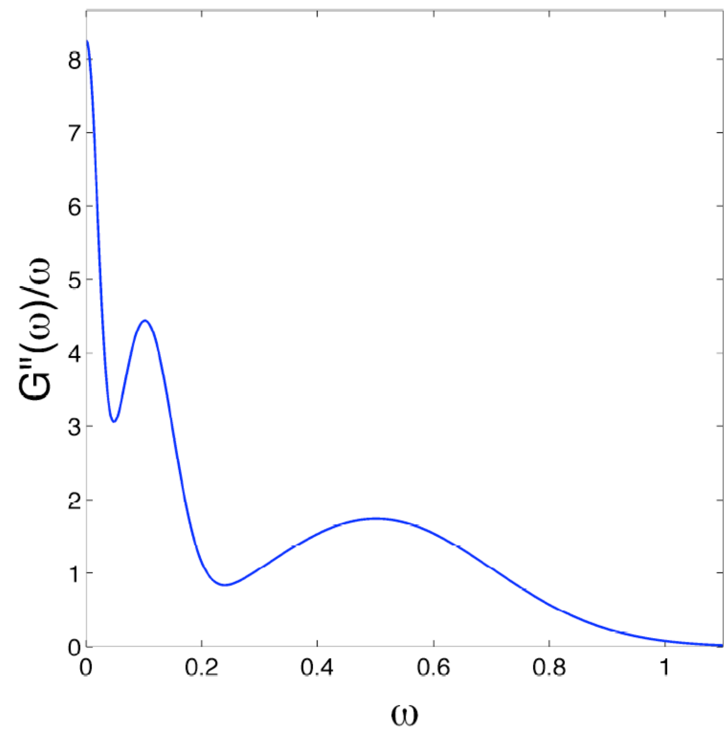
The analytic continuation problem

$$G(i\omega_n) \Rightarrow G(\omega)?$$



$$\Rightarrow$$



Analytically : $i\omega_n \to \omega + i\eta : G^R(\omega)$

Numerically?

Simplest approach : exact fitting

Padé approximant : $P_N(z) = \frac{A_N(z)}{B_N(z)} = \cfrac{a_1}{1 + \cfrac{a_2(z - z_1)}{1 + \cfrac{a_3(z - z_2)}{1 + \cfrac{\cdots}{1 + a_N(z - z_{N-1})}}}}$

$$P_N(i\omega_n) = G(i\omega_n)\,, \qquad n = 1 \ldots N$$

$$\Rightarrow \quad a_n = g_{n,n}\,, \qquad g_{1,n} = G(i\omega_n)\,,$$

$$g_{i,j} = \frac{g_{i-1,i-1} - g_{i-1,j}}{(i\omega_j - i\omega_{i-1})g_{i-1,j}}$$

$$\Rightarrow \quad A_{n+1}(z) = A_n(z) + a_{n+1}(z - z_n)A_{n-1}(z)$$

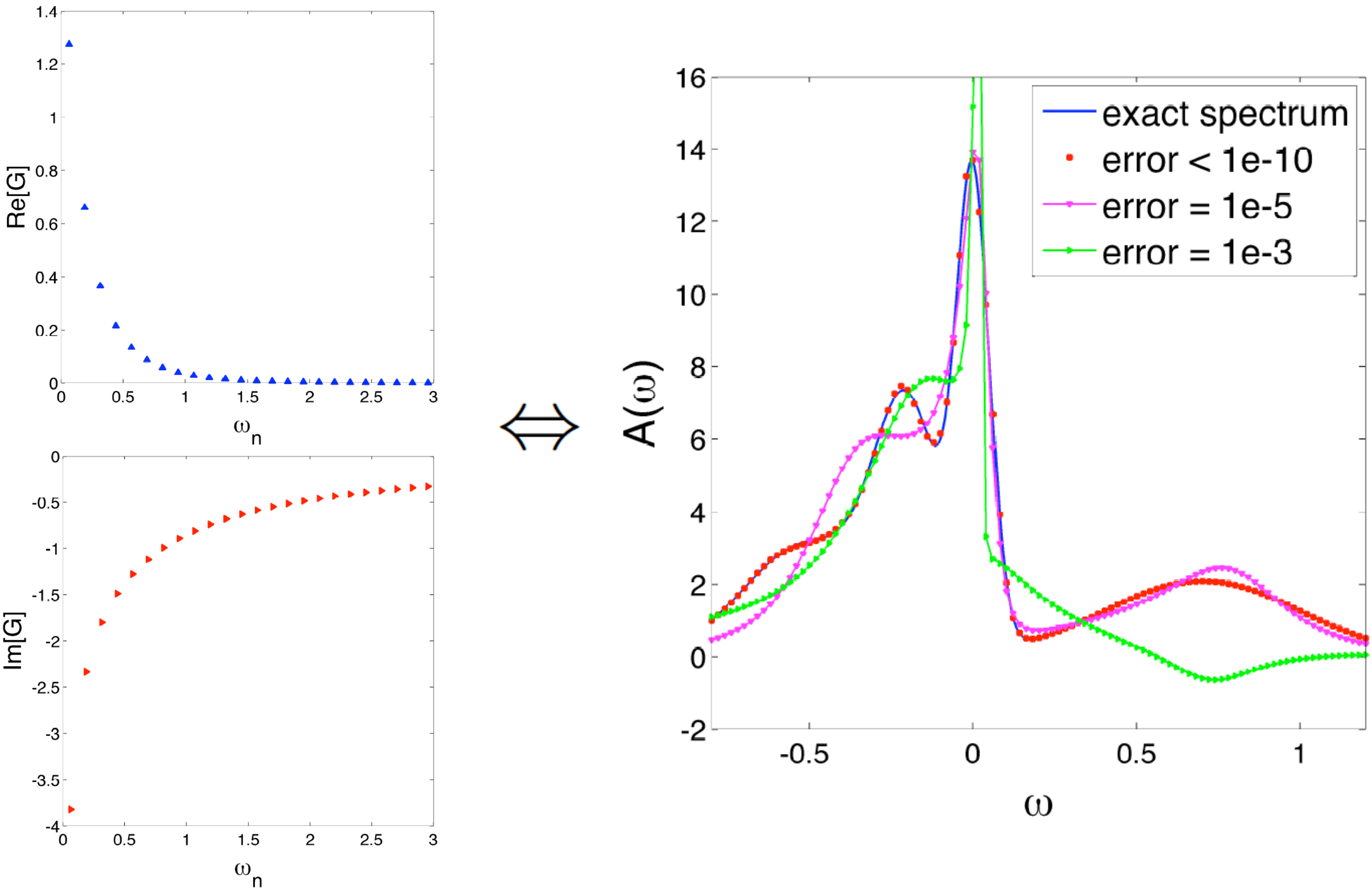
$$B_{n+1}(z) = B_n(z) + a_{n+1}(z - z_n)B_{n-1}(z)$$

$$A_0 = 0,\, A_1 = a_1,\, B_0 = B_1 = 1$$

Then $z \rightarrow \omega + i\eta$ with small finite η

H. J. Vidberg and J. W. Serene, J. Low Temp. Phys. 29, 179 (1977).

Padé approximant : example



Regression using spectral representation

Can we invert $$G(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A(\omega)}{i\omega_n - \omega} .$$

or $$G(\tau) = -\int \frac{d\omega}{2\pi} \frac{e^{-\omega\tau} A(\omega)}{1 \pm e^{-\beta\omega}}$$?

⇒ Problem: discrete approximation $G = \mathbf{K}A$ is ill-conditioned : $\frac{\|\delta A\|}{\|A\|}$ can be large, even if $\frac{\|\delta G\|}{\|G\|}$ is small.

⇒ Regularization required (constraints)

Maximum entropy

Bayes rule:

$$P(A|G) = \frac{P(G|A)P(A)}{P(G)}$$

Likelihood:

$$\boxed{P(G|A) \propto e^{-\frac{\chi^2}{2}}}$$

$$\chi^2 = (G - \mathbf{K}A)^T \mathbf{C}^{-1} (G - \mathbf{K}A)$$

$$\mathbf{C} = \frac{1}{N-1} \sum_{i=1}^{N} (G^i - \bar{G})(G^i - \bar{G})^T$$

Prior:

$$\boxed{P(A) \propto e^{\alpha S}}$$

$$S = -\int \frac{d\omega}{2\pi} A(\omega) \ln \frac{A(\omega)}{D(\omega)}$$

$D(\omega)$: default model

Maximum entropy

$$\Rightarrow \quad P(A|G) \propto e^{\alpha S - \frac{\chi^2}{2}}$$

$$\Rightarrow \quad \boxed{\min_{A} \left(\frac{\chi^2}{2} - \alpha S \right)}$$

Why entropy *S* as regularization?

1) Does not induce false correlations.

2) Imposes $A(\omega) > 0$

Other advantages of MaxEnt:

- high tolerance to noise
- easy inclusion of constraints (Bayesian)

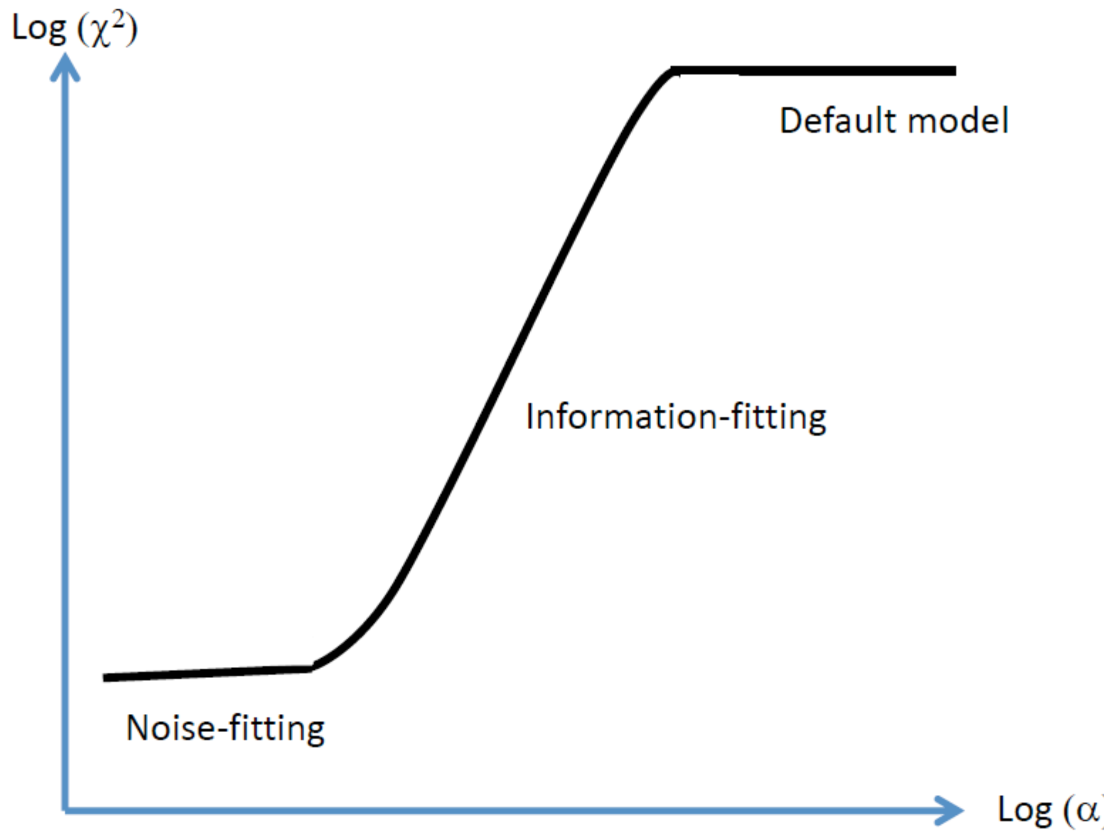
M. Jarrell and J. Gubernatis, Phys. Rep. 269, 133 (1996).

Maximum entropy: choosing α

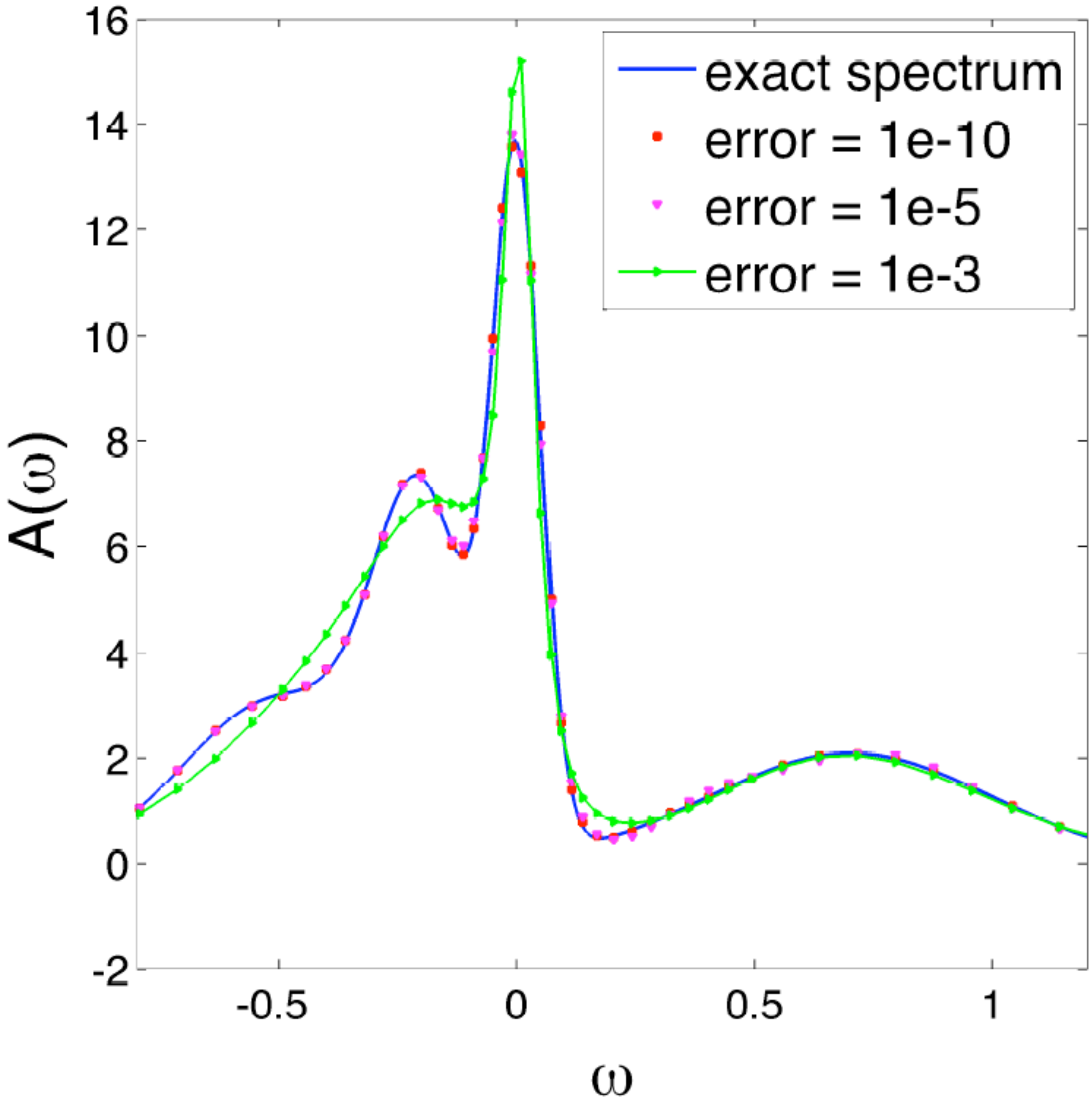
Old method : Bayesian inference

$$\Rightarrow \quad P(\alpha|G) \propto \frac{P(\alpha)}{Z_\alpha^S} \int \mathcal{D}A e^{\alpha S - \frac{\chi^2}{2}}$$

New method :



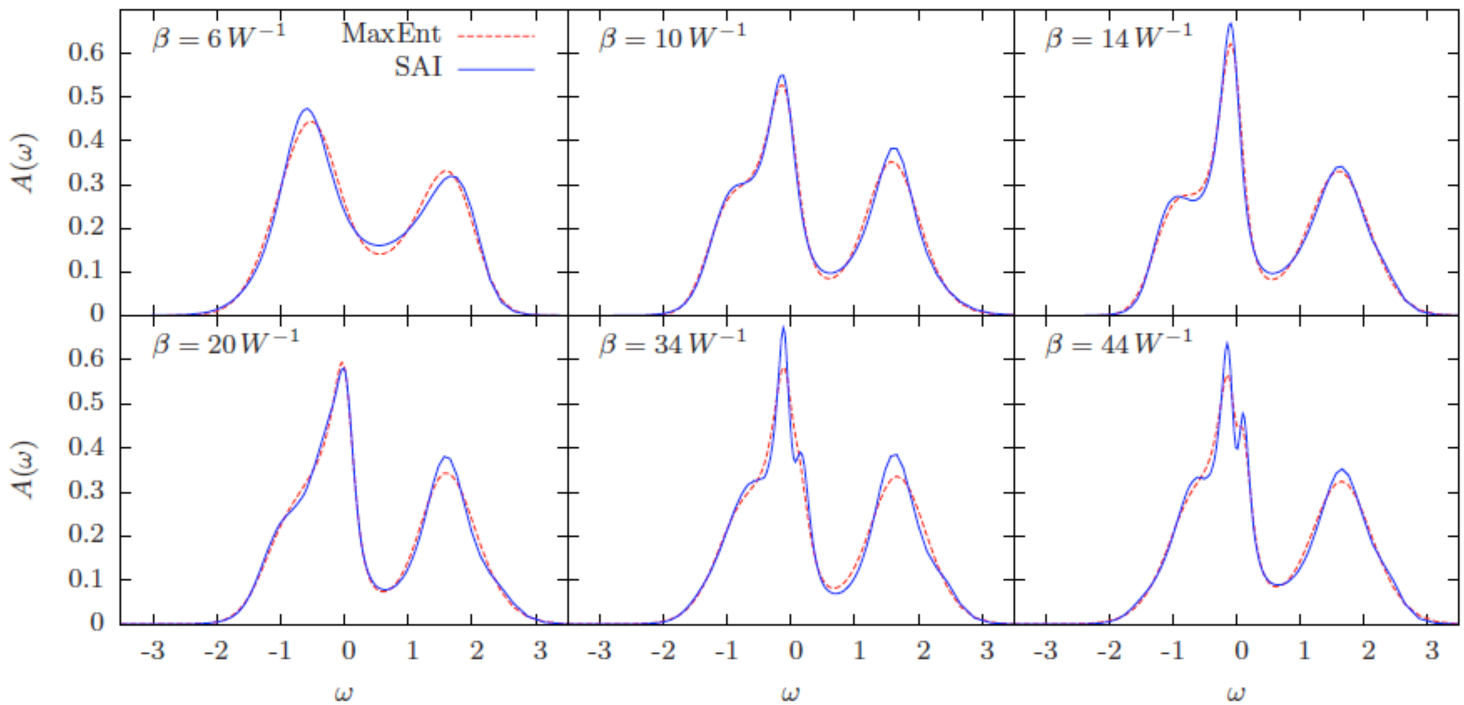
Maximum entropy : example



Stochastic analytic continuation

Use Monte Carlo sampling to compute

$$\boxed{\langle A \rangle = \frac{1}{Z} \int DA\, e^{-\chi^2[A]/\alpha} A} \qquad Z = \int DA e^{-\chi^2[A]/\alpha}$$



S. Fuchs, T. Pruschke, M. Jarrell, Phys. Rev. E 81, 056701 2010

- A. W. Sandvik, Phys. Rev. B 57, 10287 (1998).
- K. Beach (2004), cond-mat/0403055.

Non positive spectral functions

$$C_{AB}(\tau) = -\langle T_\tau A(\tau) B \rangle$$

Fermions : $Im[C^R_{AA^\dagger}(\omega)] < 0$

Bosons : $\frac{Im[C^R_{AA^\dagger}(\omega)]}{\omega} < 0$

$\Rightarrow$ MaxEnt

In general, $Im[C^R_{AB}(\omega)] \nless 0$ (f), $\frac{Im[C^R_{AB}(\omega)]}{\omega} \nless 0$ (b)

$\Longrightarrow$ Direct MaxEnt not possible

Solution : auxiliary Green functions

MaxEntAux

$$O = A + \mu B^\dagger,$$
$$P = A + i\nu B^\dagger.$$

$$\Rightarrow \begin{cases} R(\tau) = C_{OO^\dagger}(\tau) - C_{AA^\dagger}(\tau) - \mu^2 C_{B^\dagger B}(\tau) \\ \qquad = \mu \left[C_{AB}(\tau) + C_{B^\dagger A^\dagger}(\tau)\right] \\ S(\tau) = C_{PP^\dagger}(\tau) - C_{AA^\dagger}(\tau) - \nu^2 C_{B^\dagger B}(\tau) \\ \qquad = -i\nu \left[C_{AB}(\tau) - C_{B^\dagger A^\dagger}(\tau)\right], \end{cases}$$

$$\Rightarrow \quad C^R_{AB}(\omega) = \frac{1}{2}\left[\frac{1}{\mu}R^R(\omega) + i\frac{1}{\nu}S^R(\omega)\right]$$

$$R^R(\omega) = C^R_{OO^\dagger}(\omega) - C^R_{AA^\dagger}(\omega) - \mu^2 C^R_{B^\dagger B}(\omega)$$

$$S^R(\omega) = C^R_{PP^\dagger}(\omega) - C^R_{AA^\dagger}(\omega) - \nu^2 C^R_{B^\dagger B}(\omega)$$

MaxEntAux

$$Im[C^R_{AB}(\omega)] = \frac{1}{2}\left[\frac{1}{\mu}Im[R^R(\omega)] + \frac{1}{\nu}Re[S^R(\omega)]\right] \quad ?$$

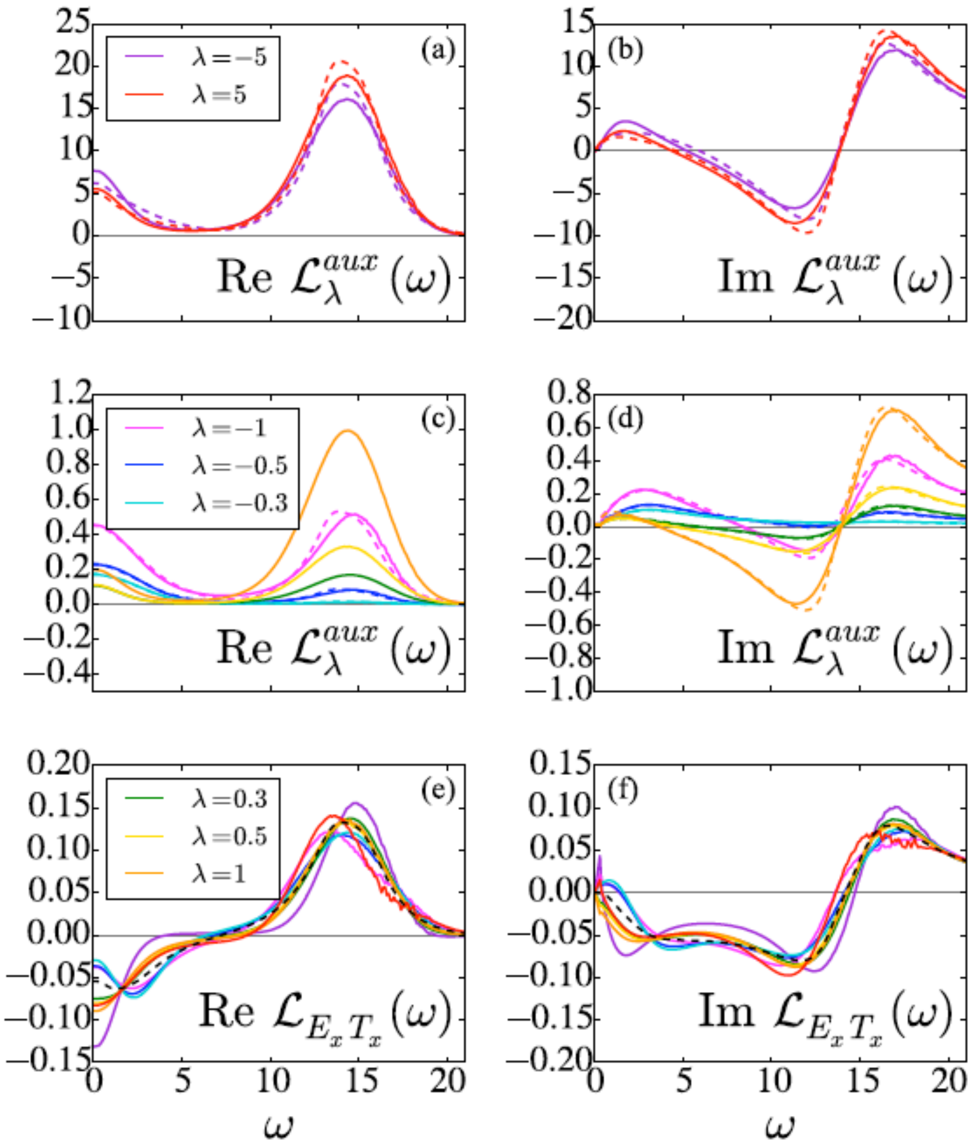
1. Compute $C_{AB}(\tau)$, $C_{B^\dagger A^\dagger}(\tau)$, $C_{AA^\dagger}(\tau)$ and $C_{B^\dagger B}(\tau)$
2. Define μ and ν and compute $C_{OO^\dagger}(\tau)$, $C_{PP^\dagger}(\tau)$
3. Use MaxEnt to compute $Im[C^R_{OO^\dagger}(\omega)]$, $Im[C^R_{PP^\dagger}(\omega)]$, $Im[C^R_{AA^\dagger}(\omega)]$ and $Im[C^R_{B^\dagger B}(\omega)]$, then $Im[R^R(\omega)]$
4. Use Kramers-Krönig to obtain $Re[C_{PP^\dagger}(\omega)]$, $Re[C_{AA^\dagger}(\omega)]$ and $Re[C_{B^\dagger B}(\omega)]$, then $Re[S^R(\omega)]$

- A. Reymbaut, D. Bergeron, and A.-M. S. Tremblay. Phys. Rev. B, 92:060509, Aug 2015.
- A. Reymbaut, A.-M. Gagnon, D. Bergeron, and A.-M. S. Tremblay. Phys. Rev. B, 95:121104, Mar 2017
- OmegaMaxEnt User Guide. https://www.physique.usherbrooke.ca/MaxEnt/index.php/User_Guide

MaxEntAux: Thermoelectric response

$$\mathrm{Re}\,\mathcal{L}_{\gamma\delta}(\omega) = \lim_{\vec{k}\to\vec{0}} \left[\frac{\chi''_{\gamma\delta}(\vec{k},\omega)}{\omega} \right],$$

$$\mathcal{L}_{E_xT_x}(\omega) = \frac{1}{2\lambda}\left[\mathcal{L}^{aux}_{\lambda}(\omega) - \mathcal{L}_{E_xE_x}(\omega) - \lambda^2\mathcal{L}_{T_xT_x}(\omega)\right]$$



A. Reymbaut, A.-M. Gagnon, D. Bergeron, and A.-M. S. Tremblay. Phys. Rev. B, 95:121104, Mar 2017

Ω*MaxEnt*

Input :

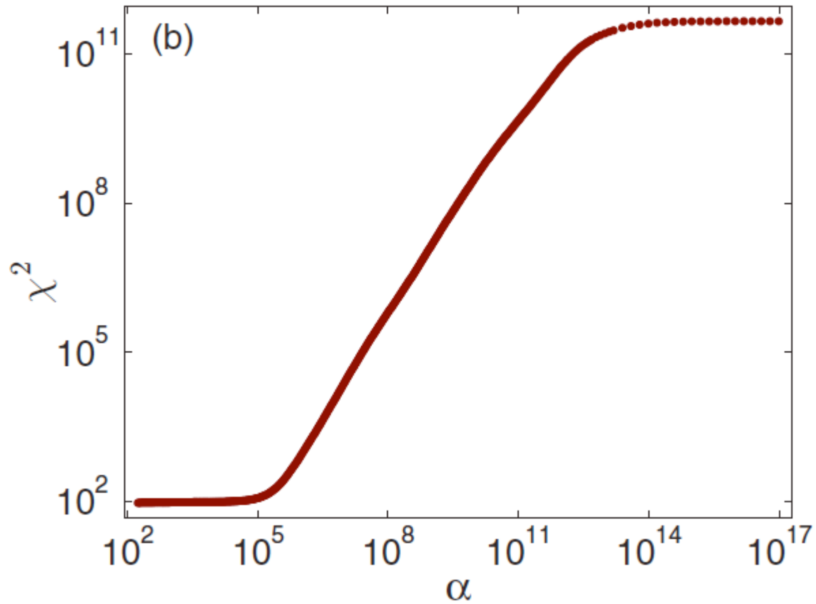
- $G(i\omega_n)$ or $G(\tau)$
- Fermionic ($A(\omega) > 0$) or bosonic ($A(\omega)/\omega > 0$)
- Diagonal or general covariance matrix
- User can modify most parameters

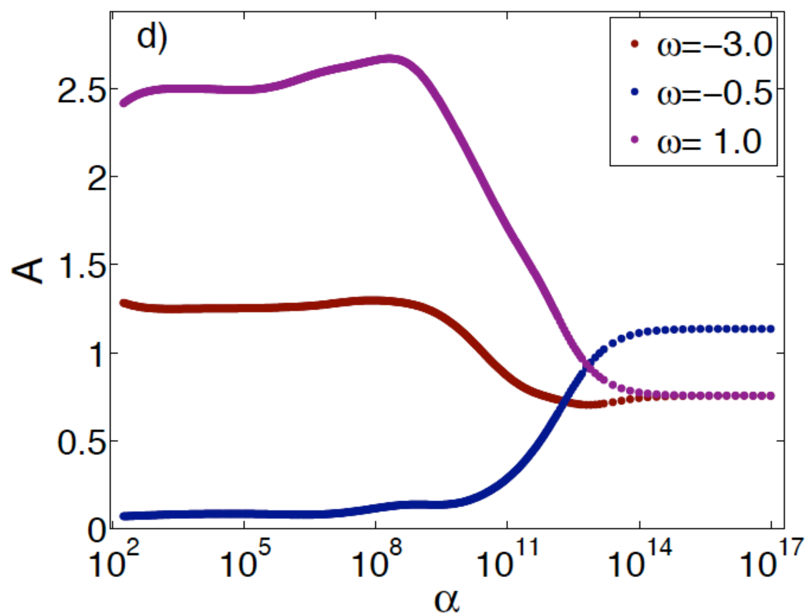
Optimizations:

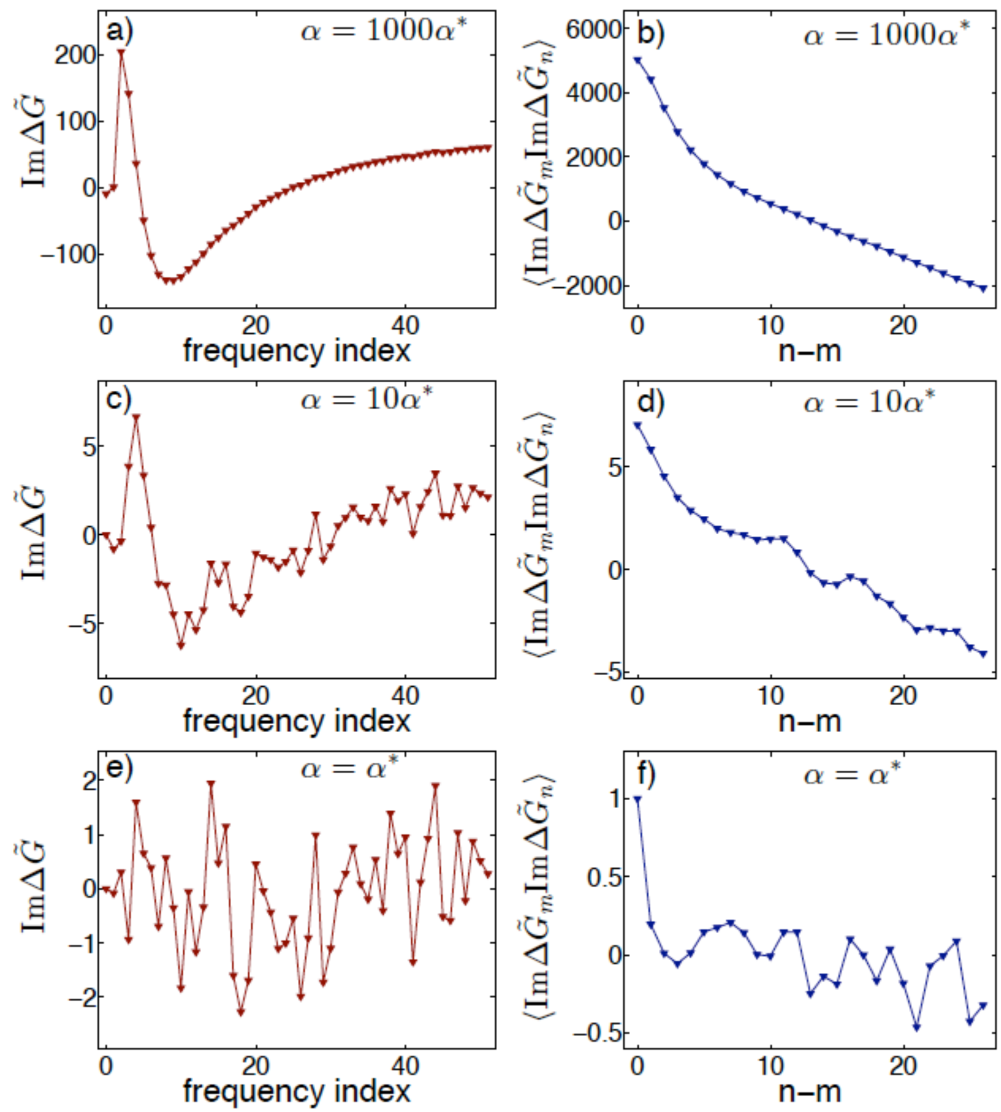
- Adapted ω and ω_n grids
- Spline model for $A(\omega)$ and analytical integration
- Computation complexity weakly dependant on T and spectrum shape
- Robust method of choosing α

-http://www.physique.usherbrooke.ca/MaxEnt
-D. Bergeron and A.-M. S. Tremblay, Phys. Rev. E 94, 023303 (2016)

Ω*MaxEnt* : diagnostic tools







Thanks !