CIFAR
CANADIAN INSTITUTE for ADVANCED RESEARCH

CRSNG NSERC

Fondation canadienne pour l'innovation

Fonds de recherche Nature et technologies Québec

VERITATEM IN CHARITATE

Maximum Entropy analytic continuation with OmegaMaxEnt

D. Bergeron, A.-M.S Tremblay
PRE **94**, 023303 (2016)

UNIVERSITÉ DE SHERBROOKE

USHERBROOKE.CA/IQ

What is the problem?

What is the problem?

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

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

$$\omega_n = \begin{cases} (2n+1)\pi T, & \text{fermions}, \\ 2n\pi T, & \text{bosons}, \end{cases}$$

1) « Standard » approaches

Standard approaches

$$P(A|G) = \frac{P(G|A)P(A)}{P(G)} \sim e^{-(\chi^2/2 - \alpha S)}$$

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

$$\chi^2 = \sum_i \frac{(G_i - \bar{G}_i)^2}{\sigma_i^2}.$$

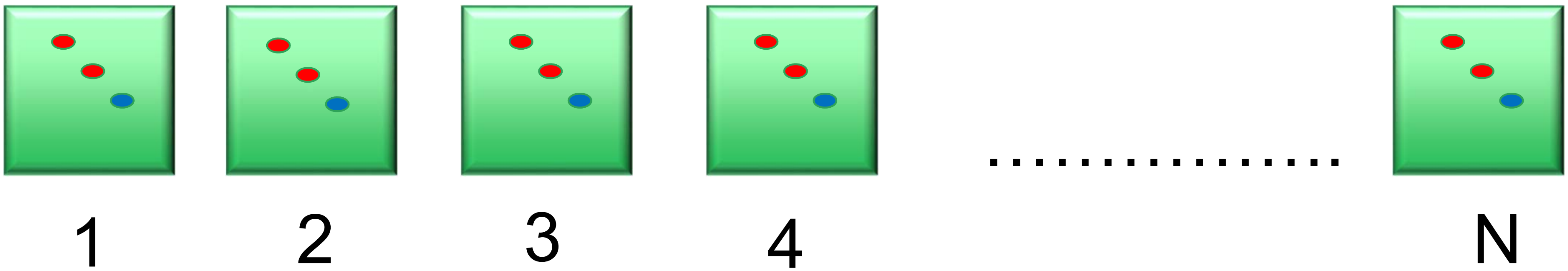
$$\bar{G} = \mathbf{K}A$$

$$P(A) = \frac{e^{\alpha S}}{Z_\alpha^S},$$

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

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

Stochastic Analytic Continuation



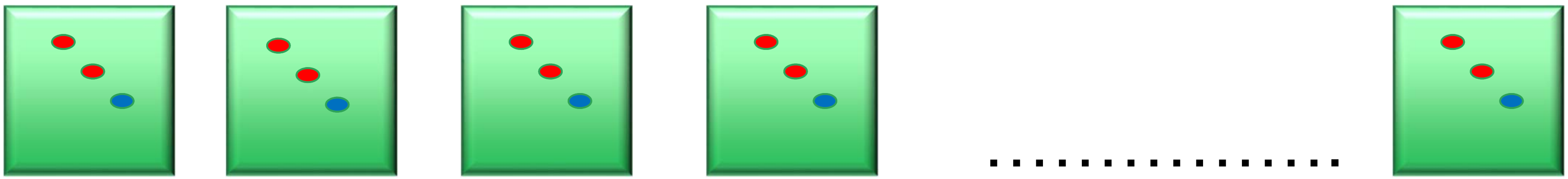
$$\sum_{i-1}^{M} A'(\omega_i)\Delta\omega_i = 1.$$

$$N \to \infty \, (N \gg M),$$

$$P_i \equiv \frac{n_i(N)}{N} = A'(\omega_i)\Delta\omega_i\,,$$

$$\lim_{N\to\infty} P_i = \lim_{N\to\infty} \frac{n_i(N)}{N} = q_i$$

Stochastic Analytic Continuation



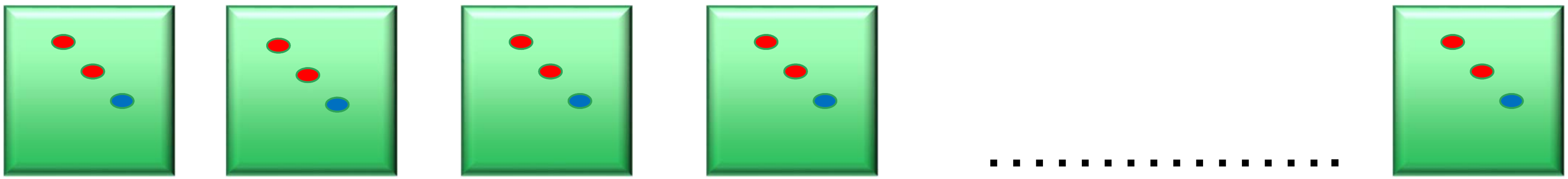
1 2 3 4 N

$$\lim_{N\to\infty} P_i = \lim_{N\to\infty} \frac{n_i(N)}{N}$$

$$\Gamma(n_1,n_2,\ldots,n_M) = \frac{N!}{n_1!n_2!\cdots n_M!}(q_1)^{n_1}(q_2)^{n_1}\cdots(q_M)^{n_M}$$

$$\begin{aligned}\ln\Gamma(n_1,n_2,\ldots) &= \ln N! - \sum_i \ln n_i! + \sum_i n_i \ln q_i \\ &= -N\sum_i P_i \ln\left(\frac{P_i}{q_i}\right),\end{aligned}$$

Stochastic Analytic Continuation



1 2 3 4 .... N

$$\lim_{N\to\infty} P_i = \lim_{N\to\infty} \frac{n_i(N)}{N}$$

Constraints

$$N \sum_i P_i = N \qquad \lim_{N\to\infty} P_i = \lim_{N\to\infty} \frac{n_i(N)}{N} = q_i .$$

If we know expected χ^2 then the value of α is determined

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

Maximum entropy

Stochastic Analytic Continuation

- All *a priori* probabilities equal to 1/M, then the frequency grid determines the model

$$\ln \Gamma(n_1, n_2, \ldots) = -N \sum_i \Delta\omega_i A'(\omega_i) \ln \left[\frac{\Delta\omega_i A'(\omega_i)}{1/M} \right]$$

$$\ln \Gamma(n_1, n_2, \ldots) = -N \sum_i \Delta\omega_i A'(\omega_i) \ln \left[\frac{A'(\omega_i)}{D(\omega_i)} \right],$$

Outline

1) Standard approaches
2) OmegaMaxEnt in a nutshell
3) Algorithms
4) Step by step
5) Benchmarks
6) Discussion

2) OmegaMaxEnt in a nutshell

In a nutshell

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

1. Computation time is almost independent of T and $A(\omega)$
2. Original criterion for choosing α
3. Diagnostic tools to estimate the accuracy of the continuation.

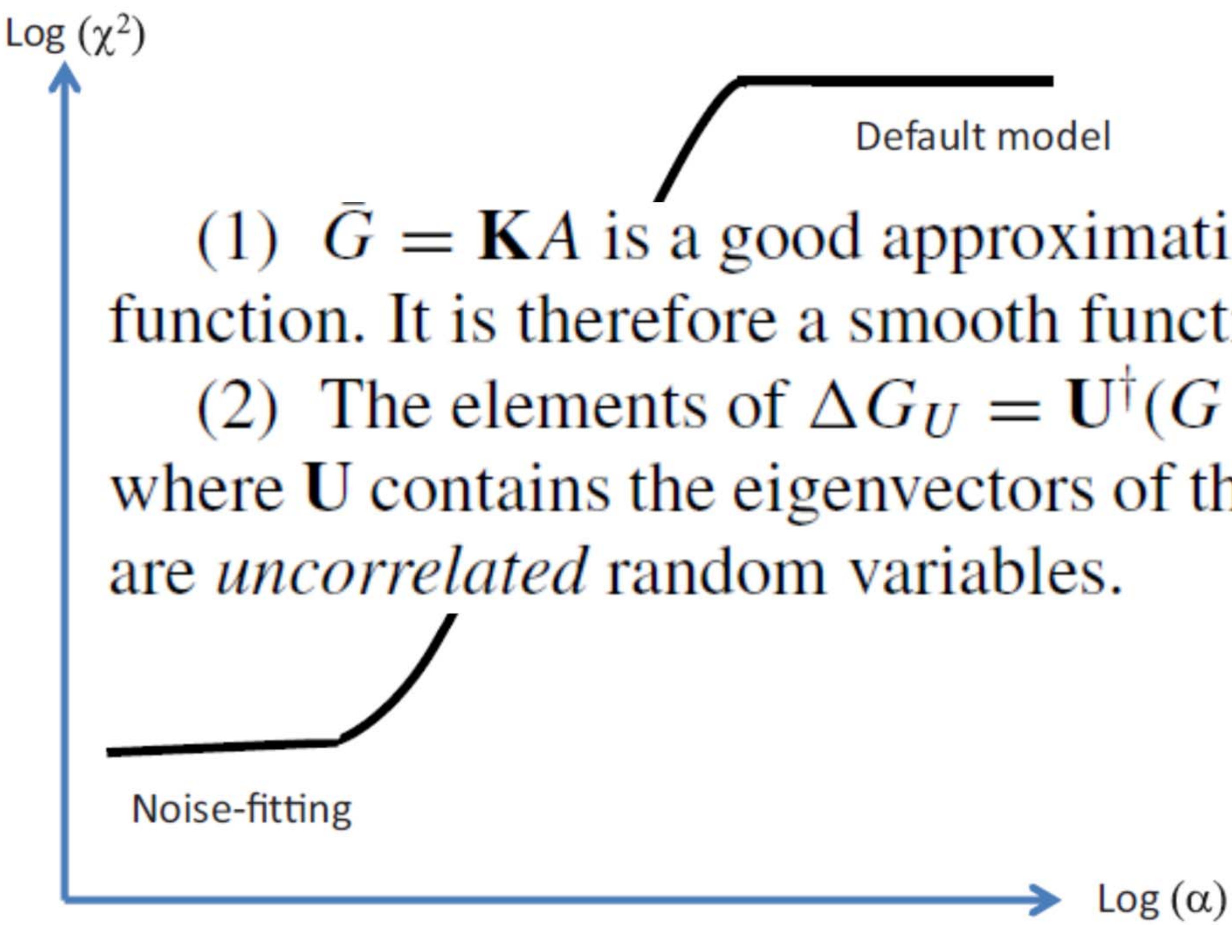
Can be used for

- Fermions
- Bosons (transport quantities)
- Self-energies
- Imaginary-time of Matsubara frequency data

In a nutshell

- Choosing α

$$\sim e^{-(\chi^2/2 - \alpha S)}$$



(1) $\bar{G} = \mathbf{K}A$ is a good approximation to the exact Green's function. It is therefore a smooth function.

(2) The elements of $\Delta G_U = \mathbf{U}^\dagger(G - \bar{G}) = \mathbf{U}^\dagger(G - \mathbf{K}A)$, where $\mathbf{U}$ contains the eigenvectors of the covariance matrix $\mathbf{C}$, are *uncorrelated* random variables.

3) Algorithms

a) Kernel
b) Optimal α
c) Diagnostic tools

Algorithms: a) Kernel

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

- Matsubara Kernel (origin of name)
- Can spline $A(\omega)$ and do piecewise analytic integration
  - Grid adapted to A, not to both kernel and A
  - Similar complexity at low T or with complicated spectrum
- Hybrid spline:

$$u = \begin{cases} \frac{1}{\omega-\omega_{0r}}, & \omega > \omega_r, \\ \frac{1}{\omega-\omega_{0l}}, & \omega < \omega_l. \end{cases}$$

- If $G(\tau)$, then from two moments, spline and go to $G(i\omega_n)$

Algorithms: a) Kernel

- Take care of the high-frequency tails as follows:

$$[G_{\text{in}}(i\omega_n) - K(i\omega_n)A]/\sigma(\omega_n) \text{ with } \omega_n > \omega_{as}$$

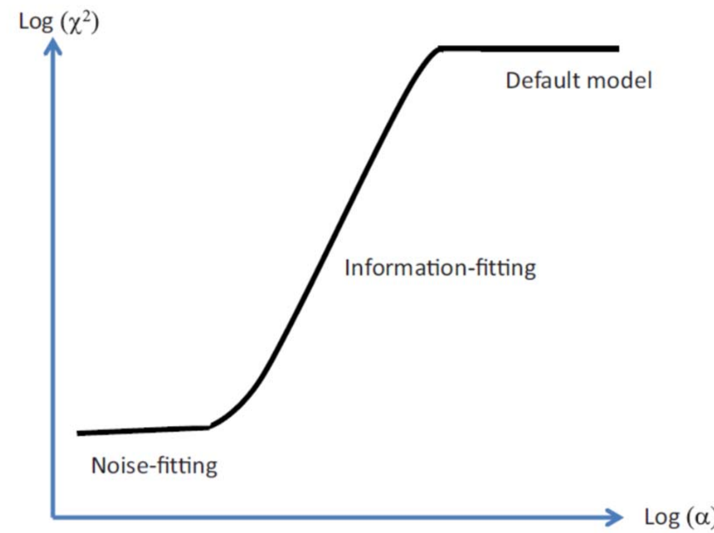
replaced with a few terms of the form $(M_j - m_j A)^2/\sigma_{M_j}$

- Generally, $A(\omega)$ is small at large frequencies, and accordingly, Matsubara grid can be sparse for $G(i\omega_n)$ at large frequencies.

Algorithms: b) Optimal α

- Analog to phase transition in SAC

$$\delta A_j = \Delta\alpha_j\left[\tilde{\mathbf{K}}^T\tilde{\mathbf{K}} + \alpha_j \Delta\omega \mathbf{A}_{j-1}^{-1}\right]^{-1} \times \left[\Delta\omega \ln(\mathbf{D}^{-1} A_{j-1}) + \Delta\omega\right],$$



- $\Delta G(i\omega_n) = G_{\text{in}}(i\omega_n) - K(i\omega_n)A$ equals noise of the data is best solution
- Annealing not necessary (but can be used)
- Curvature is used to find α*
- Reliability does not depend on proximity to model

Algorithms: c) Diagnostic tools

- $\Delta\tilde{G}(i\omega_n) = [G_{\text{in}}(i\omega_n) - G_{\text{out}}(i\omega_n)]/\sigma(i\omega_n)$ is smooth in information fitting region, noisy in noise-fitting region
- $\Delta\tilde{G}^2(\Delta n) \equiv (1/N)\sum_n \Delta\tilde{G}(\omega_n)\Delta\tilde{G}(\omega_{n+\Delta n})$ is like a Kronecker δ in noisy region
- *A*(ω) for a few test frequencies: It must be independent of α as a function of *log* α

4) Step by step procedure

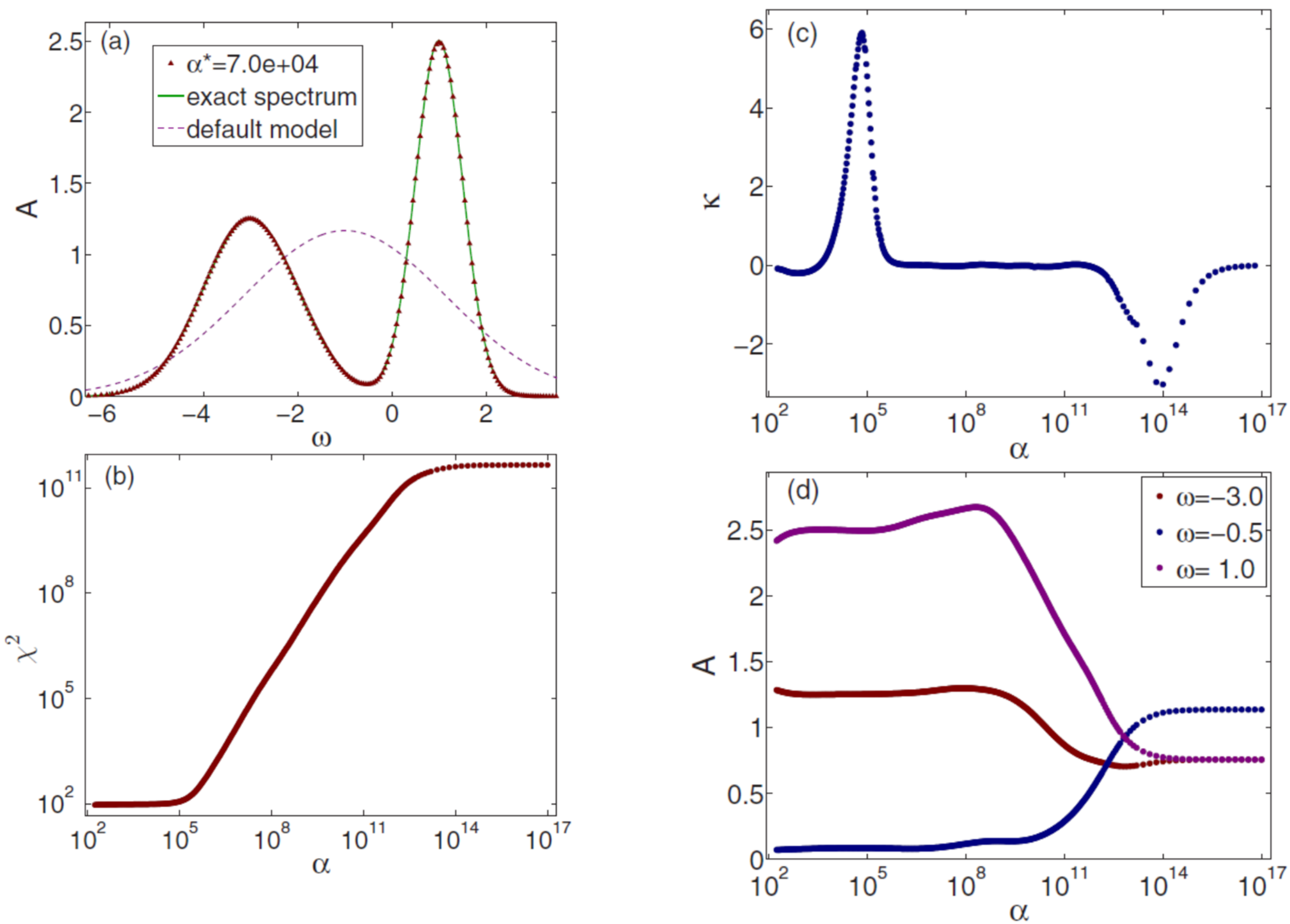
a) Information from input
b) $G(\tau)$
c) Frequency grid and default model
d) Kernel
e) Spectrum as a function of α
f) Optimal α
g) Diagnostics

5) Benchmark applications and diagnostics

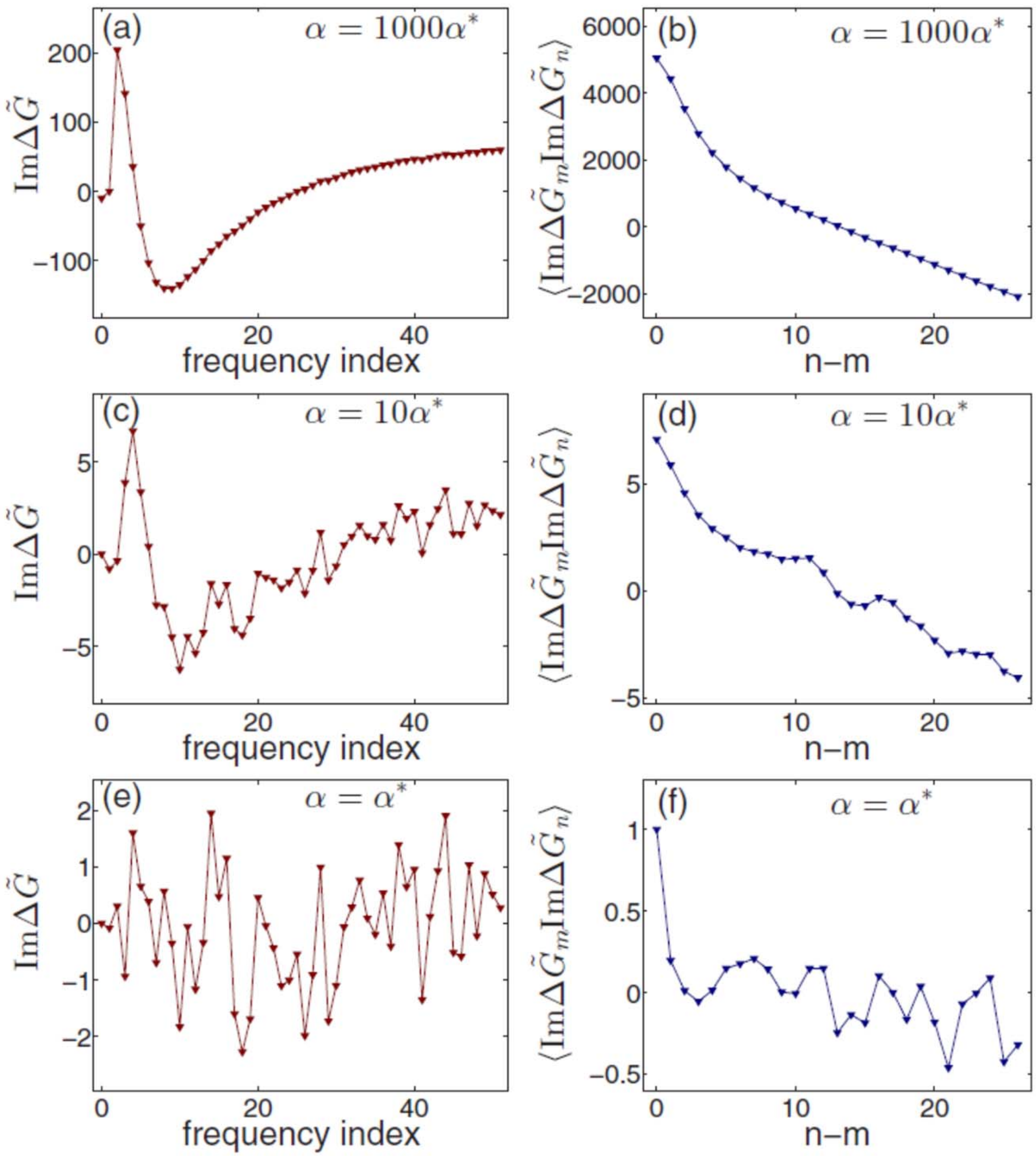
Two artificial cases
Single site DMFT

Benchmarks: a) Toy model

relative error of 10^{-5}, at a temperature $T = 0.05$

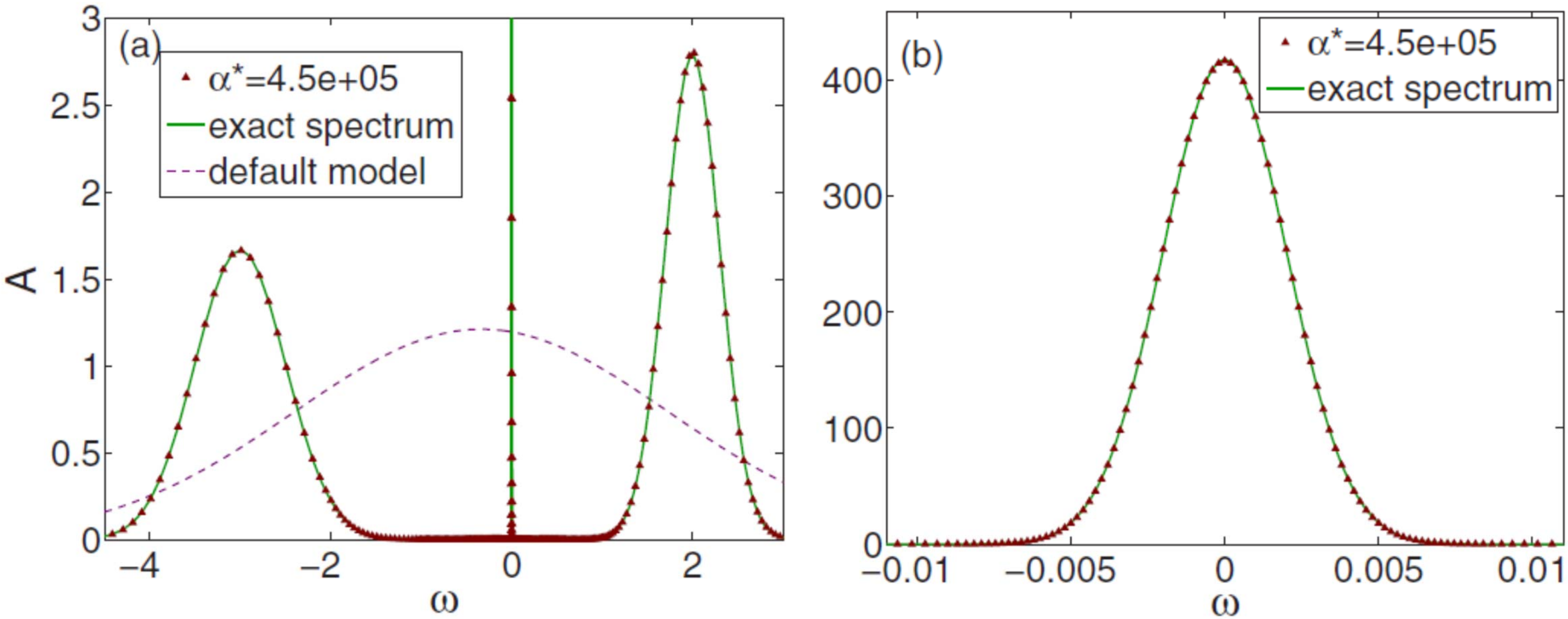


Benchmarks: a) Toy model



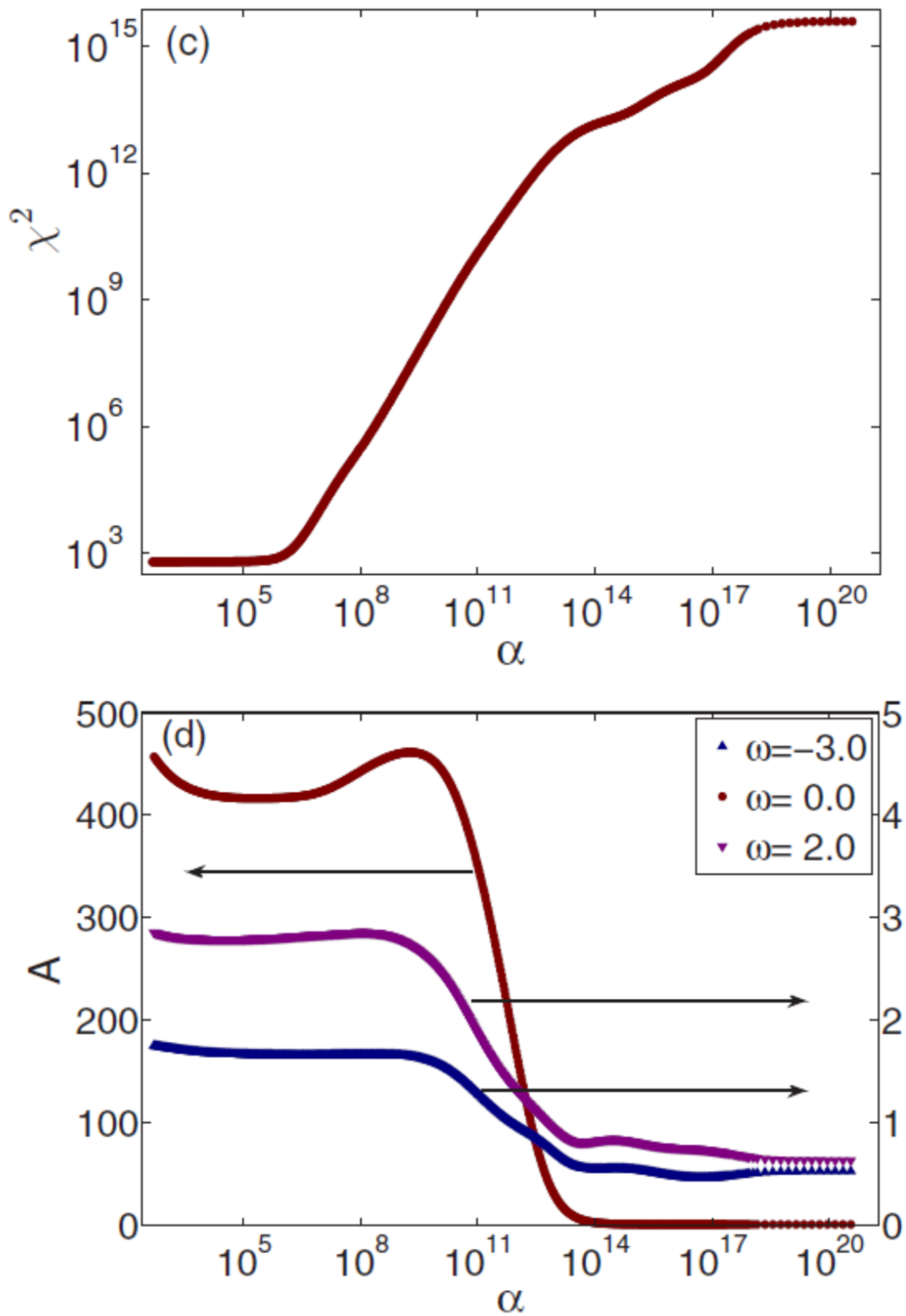
Benchmarks: b) Toy model

$T = 0.002$ constant relative diagonal error of 10^{-6}

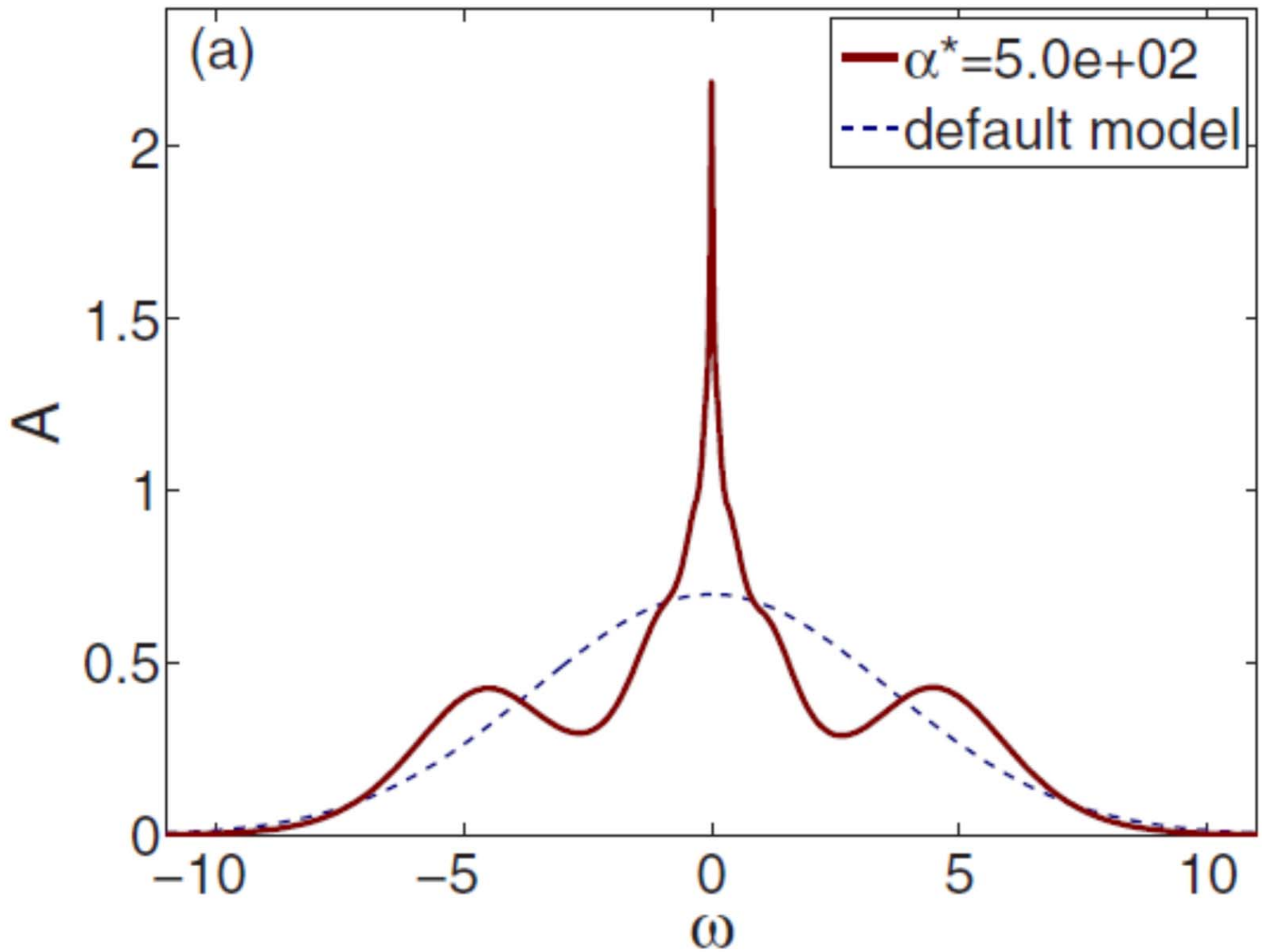


intervals. For the example, in Fig. 4, the step around $\omega = 0$ is $\Delta\omega = 2 \times 10^{-4}$, while $\Delta\omega = 0.1$ for the peak centered on $\omega = -3$ and $\Delta\omega = 0.05$ for the one at $\omega = 2$.

Benchmarks: b) Toy model

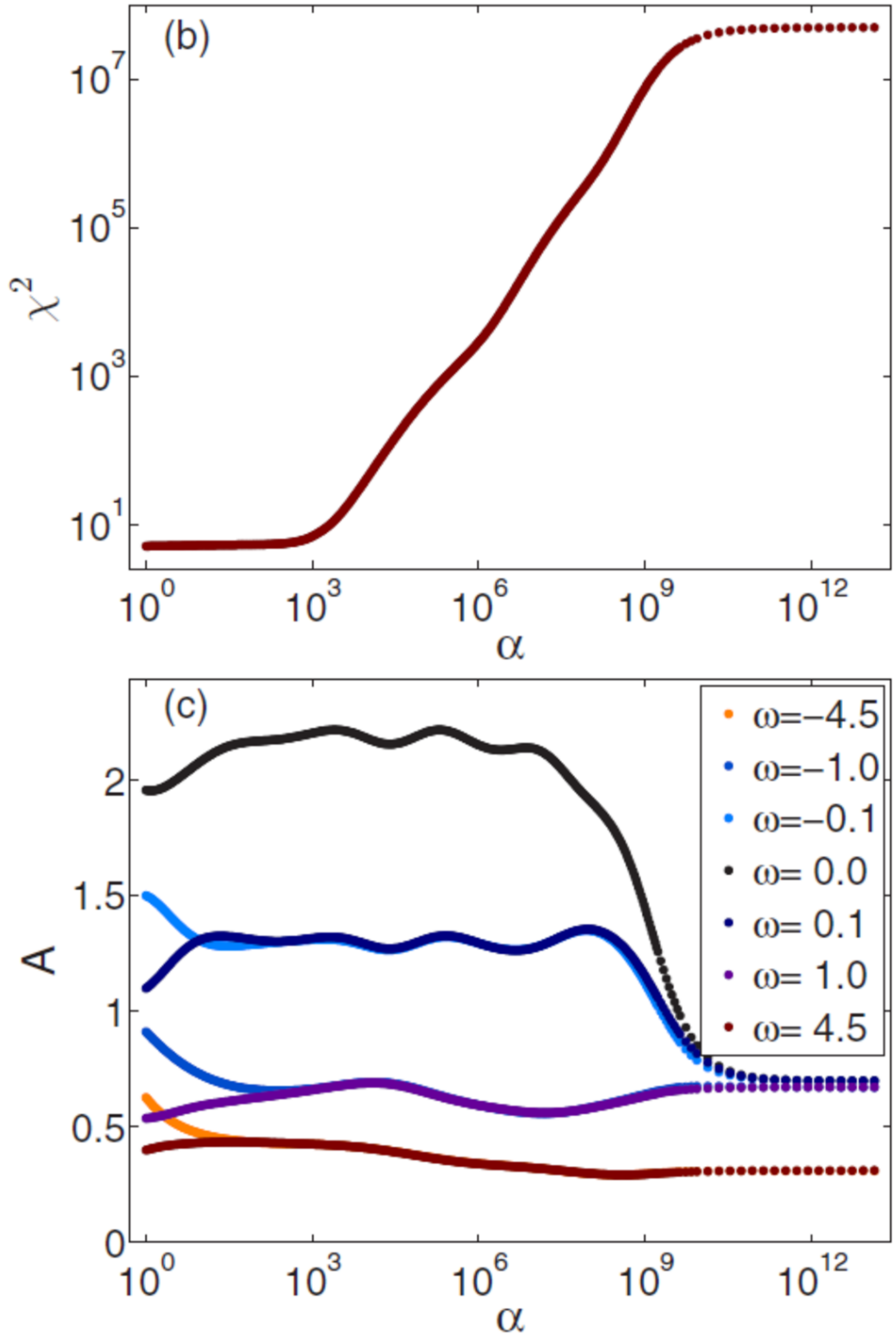


Benchmarks: c) Single site DMFT



Relative error: 5×10^{-4} at most

Benchmarks: c) Single site DMFT



6) Discussion

Discussion

- Splines in Matsubara kernel:
  - Real-frequency grid size can be minimized because of hybrid splines
  - Matsubara frequency grid size also minimized
  - Grid adapted to spectrum because of analytic piecewise integration
  - Large frequencies go into moments
- Overall, little dependence on T or spectrum complexity
- Few minutes computation compared with hours for generic optimization method or SAC

Discussion

- Consistency with assumptions of MaxEnt means
  - α chosen where $d \log \chi^2 / d \log \alpha$ drops
    - Where χ^2 assumption valid
    - In crossover region value of α not so relevant (can be checked) $\log \chi^2$ vs $\gamma \log \alpha$.
    - γ helps putting α^* closer to noise-fitting
- Results independent of default model
- Check with diagnostics
  - ΔG looks like noise
  - ΔG autocorrelation like Kronecker δ
  - Sample values of spectrum

Discussion

- « Accuracy » of error estimate is important
  - Misbehavior of ΔG and its covariance tell us about bad error estimates
  - Possible to have converged results in a frequency range and not in another
- If errors are unknown (roundoff errors) it is preferable to add known gaussian noise artificially and reduce that noise gradually.

Extensions to non-positive spectral weights

A. Reymbaut,[1] A.-M. Gagnon,[1] D. Bergeron,[1] and A.-M. S. Tremblay[1,2]

PRB **95**, 121104(R) (2017)
PRB **92**, 060509(R) (2015)

$$\chi_{\gamma\delta}(\vec{k},\tau) = -\langle \hat{\mathcal{T}}_\tau \, \hat{\mathcal{O}}_{\vec{k}\gamma}(\tau) \, \hat{\mathcal{O}}^\dagger_{\vec{k}\delta}(0)\rangle_{\hat{\mathcal{H}}},$$

$$\chi_{\gamma\delta}(\vec{k},i\omega_n) = \int_0^\beta d\tau \, e^{i\omega_n\tau} \chi_{\gamma\delta}(\vec{k},\tau) = \int \frac{d\omega}{\pi} \frac{\chi''_{\gamma\delta}(\vec{k},\omega)}{\omega - i\omega_n}.$$

$$\frac{\pi}{\mathcal{Z}} \sum_{mm'} e^{-\beta H_m} [e^{\beta\omega} - 1] \langle m|\hat{\mathcal{O}}_{\vec{k}\gamma}|m'\rangle \langle m'|\hat{\mathcal{O}}^\dagger_{\vec{k}\delta}|m\rangle$$

$$\times \delta[\omega - (H_m - H_{m'})]$$

Extensions to non-positive spectral weights

$$\langle m|\hat{\mathcal{O}}_{\vec{k}\gamma}|m'\rangle\langle m'|\hat{\mathcal{O}}^{\dagger}_{\vec{k}\gamma}|m\rangle = |\langle m|\hat{\mathcal{O}}_{\vec{k}\gamma}|m'\rangle|^2 \geqslant 0$$

$$\hat{\mathcal{A}}_{\vec{k}\gamma\delta,\lambda} = \hat{\mathcal{O}}_{\vec{k}\gamma} + \lambda\,\hat{\mathcal{O}}^{\dagger}{}_{-\vec{k}\delta}.$$

$$\chi^{aux\,1}_{\gamma\delta,\lambda}(\vec{k},\tau) = -\langle\hat{\mathcal{T}}_\tau\,\hat{\mathcal{A}}_{\vec{k}\gamma\delta,\lambda}(\tau)\,\hat{\mathcal{A}}^{\dagger}_{\vec{k}\gamma\delta,\lambda}(0)\rangle_{\hat{\mathcal{H}}},$$

$$\chi^{aux\,1}_{\gamma\delta,\lambda}(\vec{k},i\omega_n) = \chi_{\gamma\gamma}(\vec{k},i\omega_n) + \lambda^2\chi_{\delta\delta}(\vec{k},i\omega_n) + \lambda\,\chi_{\gamma\delta}(\vec{k},i\omega_n) + \lambda\,[\chi_{\gamma\delta}(\vec{k},-i\omega_n)]^*$$

$$\hat{\mathcal{B}}_{\vec{k}\gamma\delta,\lambda'} = \hat{\mathcal{O}}_{\vec{k}\gamma} + i\lambda'\,\hat{\mathcal{O}}^{\dagger}{}_{-\vec{k}\delta},$$

Merci

PRE **94**, 023303 (2016)
PRB **95**, 121104(R) (2017)
PRB **92**, 060509(R) (2015)