Introduction to Ω*MaxEnt*, a tool for analytic continuation of Matsubara data

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Analytic Continuation

- $G(\tau)$ or $G(i\omega_n) \Rightarrow A(\omega)$?

$\Rightarrow$ invert

$$G(\tau) = -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{e^{-\omega\tau} A(\omega)}{e^{-\beta\omega} + 1} .$$

or

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

Conditioning Problem:

- If we discretize ω : $G = KA \quad \Rightarrow \quad A = K^{-1}G$
- error on *A*:

$$\frac{1}{\|K\|\|K^{-1}\|}\frac{\|\delta G\|}{\|G\|} \leq \frac{\|\delta A\|}{\|A\|} \leq \|K\|\|K^{-1}\|\frac{\|\delta G\|}{\|G\|}$$

- $\|K\|\|K^{-1}\|$ is large => $\frac{\|\delta A\|}{\|A\|}$ not bounded

- Analytic continuation unique in principle (Baym and Mermin, J.Math.Phys.1961), but unstable numerically

$\Rightarrow$ need constraints on $A(\omega)$

Maximum entropy

- Different strategy: minimize

$$\boxed{Q = \chi^2 - \alpha S}$$

$$\chi^2 = \sum_{mn} (G_m - K_m A)^T C_{mn}^{-1} (G_n - K_n A)$$

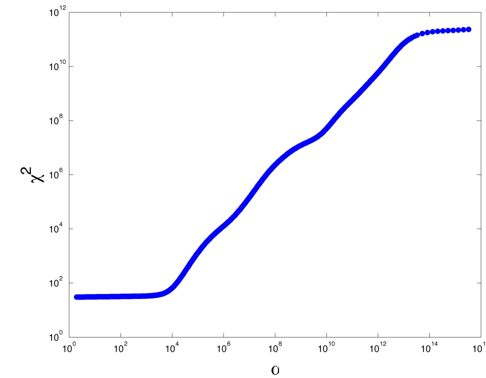
$$S = -\int d\omega A(\omega) \ln \frac{A(\omega)}{D(\omega)}$$

$$C_{mn} = \langle (G_m - \langle G_m \rangle)(G_n - \langle G_n \rangle) \rangle$$

Ω*MaxEnt*

- Use
$$G(i\omega_n) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{A(\omega)}{i\omega_n - \omega} \; .$$
  if $A(\omega)$ is a piecewise polynomial $\Rightarrow$ analytical integration in intervals
- Replace high Matsubara frequencies with contraints on moments
$$M_j = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^j A(\omega)$$
- Use adapted ω grid
- Input can also be $G(\tau)$
- Treats fermionic ($A(\omega) > 0$) and bosonic ($A(\omega)/\omega > 0$) data
- General covariance matrix

Ω*MaxEnt*: how to choose α?



- Compute $A(\omega)$ for large range of α :
  - Three regimes in χ^2 vs α

  $\Rightarrow$ Optimal α located on χ^2 vs α in *log-log*
- Additional diagnostic tools to assess quality of the result:
  - $A(\omega_{sample})$ vs α
  - $\Delta G = (G_{in} - G_{out})/\sigma$ vs ω_n
  - $\langle \Delta G_m \Delta G_{m+n} \rangle$

Why three regimes in χ^2 vs α ?

$$Q = \chi^2 - \alpha S \qquad \nabla_A Q = 0$$

- Large α: $A(\omega) \approx D(\omega) \Rightarrow \chi^2 \approx$ const
- Intermediate: $\alpha \searrow \Rightarrow \chi^2 \searrow$
- Small α: $\chi^2 \searrow$ very slowly (why?)

$$\alpha_j = \alpha_{j-1} - \Delta\alpha \quad \Rightarrow \quad A_j = A_{j-1} + \delta A_j$$

$$\delta A_j = \frac{\Delta\alpha}{2}\left[\tilde{\mathbf{K}}^T\tilde{\mathbf{K}} + \frac{\alpha_j}{2}\mathbf{\Delta}\omega\mathbf{A}_{j-1}^{-1}\right]^{-1}\left(\mathbf{\Delta}\omega\ln\left(\mathbf{D}^{-1}A_{j-1}\right) + d\omega\right)$$

All quantities are smooth in RHS at optimal α ,
but smooth δA_j cannot fit noise

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