

Hi George,

For particle-hole quantities such as spin-spin or charge-charge correlations, you do need a different Kernel. In particular, you have:

$$\langle S(q, \tau) S(-q, 0) \rangle = \frac{1}{\pi} \int d\omega \frac{e^{-\tau\omega}}{1 - e^{-\beta\omega}} \chi''(q, \omega) \quad (1)$$

with in the Lehmann representation:

$$\chi''(q, \omega) = \frac{\pi}{Z} \sum_{n,m} e^{-\beta E_n} |\langle n | S(q) | m \rangle|^2 \delta(\omega + E_n - E_m) (1 - e^{-\beta\omega}) \quad (2)$$

In principle that's it. In practice the setup of the Stochastic MaxEnt is a bit tricky, since as input I need the sum rule. Consider:

$$\coth(\beta\omega/2) \chi''(q, \omega) \quad (3)$$

For this quantity, we have the sum rule since:

$$\int d\omega \coth(\beta\omega/2) \chi''(q, \omega) = 2\pi \langle S(q, \tau = 0) S(-q, 0) \rangle \quad (4)$$

which is just the first point in your data.

Hence,

$$\langle S(q, \tau) S(-q, 0) \rangle = \int d\omega \underbrace{\frac{1}{\pi} \frac{e^{-\tau\omega}}{1 - e^{-\beta\omega}} \tanh(\beta\omega/2)}_{K(\tau, \omega)} \underbrace{\coth(\beta\omega/2) \chi''(q, \omega)}_{A(\omega)} \quad (5)$$

and one extracts with the MaxEnt $A(\omega)$ which one then transforms back to the quantity one wishes. The Kernel and back transformation in the program Max_SAC_ph.f90 does precisely this (This is in your directory FAKHER). If you use this wrapper the output in the files Aom_ps_1 will correspond to $S(q\omega) = \chi''(q, \omega) / (1 - e^{-\beta\omega})$.

Note that the program Max_SAC_ph.f90 uses the fact that $\langle S(q, \tau) S(-q, 0) \rangle = \langle S(q, \beta - \tau) S(-q, 0) \rangle$ so that it reads in only the data for $\tau = 0, \beta/2$. Also since $A(\omega)$ is a symmetric function the omega range you give should be positive.