1 Maximum entropy in the particle-hole channel

1.1 Imaginary time formulation

For particle-hole quantities such as spin-spin or charge-charge correlations, the Kernel reads:

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

This follows directly from the Lehmann representation:

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

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

$$coth(\beta\omega/2)\chi''(q,\omega) \tag{3}$$

For this quantitiy, we have the sum rule since:

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

which is just the first point in the data.

Hence,

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

and one extracts with the MaxEnt $A(\omega)$ which one then transforms back to the quantitiy one wants. In general, the codes will produce the dynamical structure factor:

$$S(q\omega) = \chi''(q,\omega)/\left(1-e^{-\beta\omega}\right) \tag{6}$$

Note 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 can be restricted to positive values.

1.2 Matsubara frequency formulation

Let

$$\chi(q,i\Omega_m) = \int_0^\beta \mathrm{d}\tau e^{i\Omega_m\tau}\langle S(q,\tau)S(-q,0)\rangle = \frac{1}{\pi}\int \mathrm{d}\omega \frac{\chi''(q,\omega)}{\omega - i\Omega_m}. \tag{7}$$

Using the fact that $\chi''(q,\omega) = -\chi''(q,-\omega)$ one obtains:

$$\begin{aligned}\chi(q,i\Omega_m) &= \frac{1}{\pi}\int_0^\infty \mathrm{d}\omega \left(\frac{1}{\omega - i\Omega_m} - \frac{1}{-\omega - i\Omega_m}\right)\chi''(q,\omega) \\ &= \frac{2}{\pi}\int_0^\infty \mathrm{d}\omega \frac{\omega^2}{\omega^2+\Omega_m^2}\frac{\chi''(q,\omega)}{\omega} \equiv \int_0^\infty \mathrm{d}\omega K(\omega,i\Omega_m)A(q,\omega)\end{aligned} \tag{8}$$

with

$$K(\omega, i\Omega_m) = \frac{\omega^2}{\omega^2 + \Omega_m^2} \tag{9}$$

and

$$A(q, \omega) = \frac{2}{\pi} \frac{\chi''(q, \omega)}{\omega} \tag{10}$$

The above definitions are useful since the image satisfies the sum rule:

$$\int_0^\infty \mathrm{d}\omega A(q, \omega) = \frac{1}{\pi} \int_{-\infty}^\infty \mathrm{d}\omega \frac{\chi''(q, \omega)}{\omega} \equiv \chi(q, i\Omega_m = 0) \tag{11}$$