4.6.1 Numerical Procedure for QMC Data

Within the DMFT framework, the optical conductivity may be expressed in the coherent case[48] as [see (4.64) - (4.67)]

$$\mathrm{Re}\,\sigma_{xx}(\omega) = \sigma_0 \int_{-\infty}^{\infty} \mathrm{d}\epsilon\, \tilde{\rho}_{xx}(\epsilon) \int_{-\infty}^{\infty} \mathrm{d}\omega'\, A_\epsilon(\omega') A_\epsilon(\omega'+\omega)\, \frac{n_\mathrm{f}(\omega') - n_\mathrm{f}(\omega+\omega')}{\omega}\,, \tag{4.152}$$

where $\sigma_0 = \frac{2\pi e^2}{\hbar^2}\frac{N}{V}$ and $n_\mathrm{f}(\omega) = \left(1 + \mathrm{e}^{\beta(\omega-\mu)}\right)^{-1}$. Evidently, practical calculations require two basic ingredients: $\tilde{\rho}_{xx}(\epsilon) = \frac{1}{N}\sum_{\boldsymbol{k}} v^2_{\boldsymbol{k}_x}\delta(\epsilon - \epsilon_{\boldsymbol{k}})$ measures the noninteracting density of states weighted with the squared Fermi velocity and thus contains all necessary information about the lattice. For a given model (characterized by its lattice topology and hopping parameters), this function can be determined once and for all, independent of temperature and interaction. For lattices with semi-elliptic Bethe DOS, this task was solved in Sec. 4.4. The remaining problem is the computation of the "momentum-dependent" (i.e., dependent on the noninteracting dispersion ϵ) interacting spectral function

$$A_\epsilon(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G_\epsilon(\omega)\,, \tag{4.153}$$

where

$$G_\epsilon(\omega) = \frac{1}{\omega - \epsilon - \Sigma(\omega)}\,. \tag{4.154}$$

An evaluation for real frequencies ω yields

$$A_\epsilon(\omega) = -\frac{1}{\pi}\,\frac{\mathrm{Im}\,\Sigma(\omega)}{\big(\omega - \epsilon - \mathrm{Re}\,\Sigma(\omega)\big)^2 + \big(\mathrm{Im}\,\Sigma(\omega)\big)^2}\,. \tag{4.155}$$

Once $\Sigma(\omega)$ is known on the real axis, the computation of $\sigma(\omega)$ reduces to the evaluation of a two-dimensional integral (over the variables ϵ and ω'). Note that the "momentum"-dependent spectral functions $A_\epsilon(\omega)$ are strongly peaked in the metallic phase (where $|\mathrm{Im}\,\Sigma(\omega)|$ is small for $\omega \approx 0$; cf. Fig. 4.29) which can in principle cause numerical instabilities; still, this step is straightforward.

In the context of QMC calculations, the real-frequency self-energy $\Sigma(\omega)$ has to be extracted in a multi-step procedure[49] which is summarized in Fig. 4.26 and will be discussed in the remainder of this subsection. All steps will be illustrated on the basis of the spectral function of the Hubbard model with semi-elliptic DOS at $T = 0.05$ and $U = 4.0$ shown as solid line in Fig. 3.77 in Sec. 3.8 (resulting from QMC using $\Delta\tau = 0.1$ and MEM using a flat default model). The corresponding imaginary part of the real-frequency Green function is indicated by circles in Fig. 4.27. It will become apparent later that the frequency grid $\Delta\omega = 0.1$ used in the MEM procedure

[48] For the cases of disorder or a single-link topology which imply incoherent transport, see subsection 4.4.2 and the results presented in subsection 4.6.3.

[49] The QMC method itself and the MEM determination of the local spectral function $A(\omega) = -\frac{1}{\pi}\mathrm{Im}\,G(\omega)$ have already been discussed in Sec. 1.3, Sec. 1.4, and Sec. 3.8.