enough computer time.

3.8 Spectra

The objective of this section is the computation of spectra, i.e., of interacting local spectral functions $A(\omega) = -\frac{1}{\pi}\mathrm{Im}\, G(\omega)$ on the real axis. Since the QMC simulations yield results on the imaginary axis, this requires the use of the maximum entropy method (MEM). In subsection 3.8.1, we discuss advanced aspects of the maximum entropy formalism in the context of spectral functions. A specification of the algorithmic choices made in this work and numerical tests follow in subsection 3.8.2. Finally, numerical results are presented for the half-filled Hubbard model with Bethe DOS at $T = 1/20$ and $T = 1/15$ in subsection 3.8.3.

3.8.1 Maximum Entropy Method for Spectral Functions

Both the basic ideas of the MEM and a simple algorithm have already been introduced in Sec. 1.4. We will in this subsection discuss three potential problems in the application of the MEM for obtaining spectral functions from imaginary-time QMC data: covariance, non-Gaussian distribution of statistical errors, and systematic errors.

Covariance

If a series of measurements is made for a vector of observables and the variance of each component is finite,[58] the probability distribution of the average vector approaches a multivariate Gaussian distribution in the limit of an infinite number of measurements. This distribution is fully characterized by its covariance matrix the estimate of which reads in the case of the imaginary-time Green function

$$C_{kl} = \sum_{i=1}^{N_d} \frac{\left(\bar{G}_k^i - \bar{G}_k\right)\left(\bar{G}_l^i - \bar{G}_l\right)}{N_d(N_d-1)}\,. \tag{3.66}$$

As in (1.61), lower indices l here correspond to time slices $\tau_l = l\Delta\tau$. The l component of the result of the i^{th} measurement (total number: N_d) is denoted by $\bar{G}_l^i$; $\bar{G}_l$ is the corresponding average. In the uncorrelated case, the matrix C_{kl} reduces to its diagonal with elements $\sigma_k^2\delta_{kl}$. This is, in fact, the simplifying assumption made in Sec. 1.4 and used in a program implemented by Sandvik (Sandvik and Scalapino, 1995) which is used in parts of this work. It is the main point of this paragraph to demonstrate that this assumption does not apply in the cases of interest. The covariance matrix for a symmetric case (Bethe DOS with half filling at $T = 1/20$ and $U = 4.6$) is shown in Fig. 3.67 a. Here, crosses indicate matrix elements C_{kl} for $0 \le k \le l \le \Lambda/2$; lines connect elements with the same value of k. Diagonal

[58] The condition of finite variance is trivially met for measurements of the imaginary-time Green function since it is bounded: $0 \le G(\tau) \le 1$.