validity of both results is also supported by the fact that only little spectral weight is predicted in the region $|\omega| > 4.3$ forbidden by (3.68). An additional result for the narrow default model that takes into account the possibility of larger systematic errors (short-dashed line) yields a somewhat more semi-elliptic shape of the Hubbard bands, but is overall consistent with the results discussed so far. In contrast, MEM results based on the exaggerated error derived from unsymmetrized measurements (thinner curves) differ clearly: both the much stronger model dependence and the large weight at high frequencies indicate the poor quality of these results.

As we have pointed out in the beginning of this section, Jarrell's program represents a careful implementation of the Bayesian MEM approach and is in general superior over simplified algorithms as implemented in the code originating from Sandvik. Consequently, it would appear natural to only use the more advanced code for this thesis. However, numerical instabilities were encountered in a direct application of this method to our best QMC data (for $\Delta\tau = 0.1$, i.e., $\Lambda = 200$ time slices), in particular for very accurate data sets with small statistical errors. While some progress could be made when the impact of the systematic iteration error was reduced by combining measurements performed for different impurity models (cf. subsection 3.8.1), consistent results could only be obtained by skipping time slices as illustrated in Fig. 3.73. Here, best results (thick solid and dotted lines) were obtained by using only every 4^{th} time slice (i.e., $\tau_0 = 0$, $\tau_4 = 0.4$ etc.) as can be seen from the relatively small dependence on the default model and from the comparison with the "Sandvik" result (double-dashed line) reproduced from Fig. 3.72. Skipping only every second time slice results in spectra (dashed lines) with additional features or too much weight at large frequencies; for a wide default model, even the analytic constraint $A(\omega = 0) < 1/\pi$ is violated. When using the full QMC data as input, the MEM scheme did not even converge.[66] A welcome side effect of skipping time slices is that the overall impact of covariance is reduced which stabilizes the SVD.

The primary reason for these problems becomes apparent in the main panel of Fig. 3.74. Here, the imaginary-time Green function corresponding to the MEM spectrum obtained from Sandvik's method for a narrow default model (cf. Fig. 3.72) has been subtracted from the measured QMC data. On the resulting magnified scale, an oscillatory behavior with deviations from a smooth curve which alternate on neighboring time slices becomes clearly visible. Since no such short-time oscillations appear in corresponding differences of Green functions associated [via (1.55)] with different MEM spectra (not shown), the phenomenon is recognized as a systematic error of the QMC data. Most likely, this error is associated with remaining deficiencies of the Fourier transformation scheme employed in this work and could be removed by employing a more sophisticated scheme as presented in App. C. While the individual errors are roughly in line with estimated error bars (of about 10^{-4}) for each time slice, the pattern is so strong (in particular for small τ) that the associated unphysical degree of freedom can cause a failure of the full MEM procedure (in Jarrell's code). On the other hand, the short-time oscillations are removed when only every second or every fourth time slice is included in the analysis which explains why the stability

[66] In tests for other parameter sets where numerical convergence could be obtained, additional separated peaks and/or a central dip in the quasiparticle peak appeared in the spectra.