information on the imaginary axis has to be supplemented by a maximum entropy assumption in order to obtain real-frequency spectra. Obviously, the qualitative importance of these errors depends on the final quantity that is calculated. For the PES shown in the previous subsection, the broadening procedure renders details of the initial spectra relatively unimportant. In contrast, the computation of optical conductivity data which we will present in subsection 5.4.3 involves comparisons with the noninteracting DOS and is far less well conditioned: in the computation of $\Sigma(\omega)$, sums can essentially cancel so that the relative error explodes. Thus, reliable results for $\sigma(\omega)$ can only be expected if both the QMC procedure and the MEM algorithms fulfill high standards.

Although the particular algorithm for analytic continuation of imaginary-time QMC data used for obtaining the spectra shown in Fig. 5.5 yields spectra compatible with the measured data, it takes improper account of the associated errors. Consequently, the spectra selected by the algorithm may not be the best maximum entropy spectra. In extensive studies, we implemented more accurate MEM schemes (still using Sandvik's code), which we will characterize below, and also tested a variety of default models.[20] Still, none of the methodological improvements yielded significantly more reliable spectra and derived self-energies. In order to check for convergence, to improve on the statistical accuracy, and to generate enough input data for Jarrell's fully consistent maximum entropy program, we performed additional longer QMC simulations for the same parameter sets. Again, no general improvement was found using the variants of Sandvik's scheme. Jarrell's program failed to yield sensible spectra at all. In our view, the only likely explanation for the fact that an improved treatment of statistical errors did not in general lead to improved spectra is that statistical errors are not the important ones; instead they are dominated by systematic errors. After having established convergence and well thermalized Ising spin ensembles in the QMC simulations, the only remaining candidate as a source for such systematic errors is the finite imaginary-time discretization $\Delta\tau$ in connection with the empirical "smoothing" scheme employed for the discrete Fourier transformation. As discussed in Sec. 3.4, this scheme leads to large errors near a metal-insulator transition in the half-filled single-band case. More generally, one has to expect problems also in the present multi-band case with noninteger filling when correlations become strong. While we cannot test for the influence of the "smoothing" trick alone without rewriting the QMC program, the total systematic error including the unavoidable Trotter error may be estimated from changing the value of $\Delta\tau$, which we will do in the remainder of this subsection.

[20] In the present multi-band case, the choice of a nontrivial appropriate default model is much more difficult than in the symmetric single-band case covered in Sec. 3.8. As an alternative to the previously used flat default model (energy range -20 eV $\leq \omega \leq$ 20 eV with a grid of 0.1 eV) we used Gaussian default models of various widths and with the symmetry axis approximately matched to the band center as well as tighter models derived from a rigid-band assumption which becomes good in the atomic limit. While it is relatively easy to suppress the unphysically long negative-energy tails visible, e.g., in Fig. 5.5 with such default models, a too tight cut-off at high frequencies is likely to lead to artifacts in the main part of the spectrum. For an improved treatment, it seems promising to use QMC estimates for double and triple occupancy for fine-tuning the default model for each particular data set.