are shown as dashed lines in Fig. 3.71 and are specified in its caption.

It is clearly possible to devise default models which represent more accurately expectations about the true spectrum for the given parameter set, i.e., have features like upper and lower Hubbard bands, a quasiparticle peak or a gap at the Fermi energy etc. Such a default model can be obtained, e.g., as a result of approximate theories, by fitting moments, or by using the MEM result of a related parameter set. In particular, Jarrell (1997) describes an annealing method which works at a hierarchy of temperatures: here, an analytic continuation of QMC data is first performed at high temperatures where a default model obtained from perturbation theory is still quite accurate. The MEM result obtained at each temperature step is then used as a default model at the next lower temperature. While such a procedure can be justified from the observation that spectra usually depend smoothly on temperature and show more structure at lower temperatures, it has no Bayesian foundation and may break down near phase transitions. In our view, the use of the annealing method should be limited to cases where the MEM procedure cannot be stabilized by other means, possibly due to lack of sufficient computing resources. As we will see in the following, such a need does not arise within the context of this thesis.

We also will not need to apply generalizations of the MEM for enforcing analytic constraints (i.e., for moments of the spectrum) by adding further terms to the logarithm of the prior probability defined in (1.63) (i.e., in connection with a Lagrange multiplier). While such a procedure does not pose the danger of introducing artifacts, each enforced constraint removes one possible check of the accuracy of the result. For this reason and for the sake of simplicity, we prefer a plain implementation of the MEM (at least for comparison) in connection with sufficiently accurate data.[64] Note that the full band width can also be constrained by an appropriate choice of the default model.

Error Analysis

A first point that we would like to stress is the importance of performing the error analysis in the paramagnetic phase of interest for the spin-averaged data $G(\tau) = (G_\uparrow(\tau) + G_\downarrow(\tau))/2$. By taking this average, the majority of statistical errors is eliminated since in each QMC solution of the impurity problem the estimates of $G_\uparrow(\tau)$ and $G_\downarrow(\tau)$ are highly correlated. Due to the correlations, the alternative procedure of treating both estimates as independent measurements (as previously used in our group) leads to incorrect error statistics; in fact, it grossly overestimates errors for small $\Delta\tau$ (or small $\beta - \Delta\tau$) which are here small due to the symmetry of the half-filled model. This is shown in the inset of Fig. 3.72 for $T = 1/20$ and $U = 4.6$. Here, the lower black solid line represents the true measured statistical error. Treating both

In Jarrell's code, the default model (and even the grid) is completely arbitrary, since it is read from a specified file in tabulated form.

[64] In early stages of this work, we found violations of analytic behavior in MEM results when trying to compute the real-frequency self-energy in antiferromagnetic phases. Here, the numerical MEM procedure can probably only be stabilized when some constraints are enforced. The following necessary conditions for analyticity valid for a Bethe lattice ($W = 4$) may be useful for future work: $\mathrm{Im}\, G_\alpha(\omega)\, ImG_{\bar\alpha}(\omega) \leq 1$ and $\mathrm{Im}\, G_\alpha(\omega)/\mathrm{Im}\, G_{\bar\alpha}(\omega) \geq \mathrm{Re}\, G^2_\alpha(\omega)$. Here, α denotes the sublattice index.