Systematic Errors

It is important to realize that MEM can only yield reliable results when systematic errors are much smaller than statistical errors. For DMFT calculations, systematic errors can be caused by incomplete convergence of the self-consistency cycle and by a finite value of $\Delta\tau$. An accurate solution of the impurity problem and a large number of iterations (possibly using underrelaxation) can control the iteration error or effectively convert it to a statistical error by using completely independent simulation runs. A similar effect is achieved at lesser cost by performing some additional DMFT iterations at very high precision after convergence; measurements of $G(\tau)$ for each of the resulting impurity models can then be combined for analytic continuation. The spectra to be presented in this section will be based on 50 measurements for 6 impurity models (i.e., a total of 300 bins) for each parameter set; this approach brings the iteration error well under control.

In comparison, remaining $\Delta\tau$ errors in $\{\bar{G}_l\}$ are potentially more severe. Since this problem cannot be overcome by extrapolation on the level of spectra, reliable spectra require good algorithms (i.e., programs with minimal $\Delta\tau$ error) using small enough values of $\Delta\tau$. This is more important in the context of DMFT calculations than for the solution of plain SIAMs since for the DMFT even the self-consistency condition itself (which includes discretized Fourier transformations) introduces an error at finite values of $\Delta\tau$ (cf. subsection 3.4.1). For illustration of this point, a comparison of imaginary-time Green functions for the Bethe DOS in the insulating phase ($T = 1/20$ and $U = 5.0$) is shown in Fig. 3.70. In order to resolve the important region of $\tau \approx \beta/2$, we here use a strongly magnified scale (for a more complete picture, see Fig. 3.75). The thick short-dashed line represents our best estimate (for $\Delta\tau = 0.1$) of $G(\tau)$. The thinner dotted line is obtained by transforming back the MEM spectrum to be presented later in Fig. 3.80. The agreement between both curves is excellent for $\tau \lesssim 6$. Since the slight fluctuations visible in the QMC results for $6 \lesssim \tau \leq 10$ (with a local minimum for $\tau \approx 7$) violate analyticity,[62] they are filtered out by the MEM procedure which corresponds to a regularized form of $G(\tau)$ (dotted line). Both curves agree reasonably well with Jarrell's result [for $\Delta\tau = 0.167$ as used in Schlipf et al.'s (1999) paper: long-dashed line]. In contrast, Ulmke's original smoothing trick discussed in subsection 3.4.1 leads to much larger $G(\tau)$ and fails to capture the insulating character of the solution: while the former results are roughly consistent with a gap of 0.5 (here modeled using rigid semi-elliptic Hubbard bands), the Ulmke-code solution implies quite significant spectral weight near $\omega = 0$ (which even exceeds that associated with touching rigid Hubbard bands).

We conclude that the most important prerequisite for computing reliable spectra

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distribution is an ill-conditioned problem. We cannot exclude the possibility that the outliers are artifacts of the QMC method, i.e., arise from the finite number of warm-up sweeps used for each measurement. Up to outliers, all data sets presented in Fig. 3.69 lead to nearly Gaussian histograms of $\log G(\beta/2)$.

[62] The positivity of all even derivatives of $G(\tau)$ can be read off from (1.55); conversely, local extrema for $0 \leq \tau \leq \beta/2$ imply negative regions of the spectrum $A(\omega)$ which is clearly unphysical. A second, weaker form of the violation of analyticity may be detected when the computation of the self energy is attempted (see Sec. 4.6).