Appendix C

Using Splines for Fourier-Transforming Imaginary-Time Green Functions

As discussed in subsection 3.4.1, the Fourier transformations of Green functions from imaginary time to Matsubara frequencies and vice versa that arise in the QMC solution of the DMFT problem are not trivial. All problems can be traced back to the discreteness of the QMC estimates $\bar{G}_l$ for time slices $\tau_l = l\Delta\tau$. However, the true imaginary-time Green function $G(\tau)$ is known to be a smooth curve with continuous derivatives (of all orders) on the interval $[0, \beta]$. Thus, reasonable results can be expected by performing the Fourier transform not for the discrete raw data, but for a fitted smooth curve. In this appendix, we will give a short summary of work carried out recently in collaboration with Knecht. More details can be found in Knecht's (2002) diploma thesis and in upcoming publications.

The simplest practical approach in this context consists of a direct interpolation of the discrete QMC data by a cubic spline (with a continuous second derivative) as implemented by Krauth. While this step suffices for closing the self-consistency equations without any further adjustments (like Ulmke's smoothing trick), it leads to nonanalytic behavior of the self-energy near and beyond the Nyquist frequency as illustrated in Fig. 3.11. In our view, this problem can be traced back to the fact that the natural spline chosen by Krauth is inadequate for this problem: By definition, the second derivative of a natural spline vanishes at its boundaries. However, all even derivatives of the true Green function are maximal at the edges of the interval $[0, \beta]$. The resulting misfit leads to unphysical ringing as illustrated in Fig. C.1. Here, the noninteracting Green function for a semi-elliptic DOS is chosen as an example since it can be computed with arbitrary precision. Furthermore, moderate interactions do not lead to qualitative changes in the Green function so that the example is representative. It is clearly seen that a fit of a discrete set of data points (here for $\Lambda = 40$ and $\beta = 100$, i.e., a large discretization $\Delta\tau = 2.5$) using a natural cubic spline with continuous second derivative leads to a large error oscillating with the Nyquist frequency. While the initial misfit at $\tau = 0$ is similarly large for a natural Akima spline, the oscillation decays significantly faster due to jumps in the second derivative