the ω^{-1} term) which is nonsingular (and purely imaginary) on the imaginary axis is given by

$$\Sigma_{\text{model},\sigma}(\omega) = U\left(\langle \hat{n}_{-\sigma}\rangle - \frac{1}{2}\right) + \frac{1}{2}U^2\,\langle \hat{n}_{-\sigma}\rangle\big(1-\langle \hat{n}_{-\sigma}\rangle\big)\Big(\frac{1}{\omega+\omega_0} + \frac{1}{\omega-\omega_0}\Big). \quad \text{(C.3)}$$

While the quality of the low-frequency part of this fit could be tuned by adjusting the parameter ω_0, the value of this parameter is irrelevant for the following as long as it is not much larger than the bandwidth; we will choose $\omega_0 = 1$. By evaluating Σ_{model} on the imaginary axis, the corresponding Green function G_{model} can be computed for an arbitrary number of Matsubara frequencies. Consequently, the Fourier transformation to imaginary time is unproblematic (when the "free" term $1/(i\omega_n)$ is taken care of analytically). Thus, the difference of the Green functions can be accurately evaluated at all time slices. Since the second derivative of the transformed model Green function at $\tau = 0$ exactly reproduces that of the true Green function, the difference is well represented by a natural spline. The Green function is obtained as a function of Matsubara frequencies by Fourier transforming the oversampled spline and adding the Matsubara-frequency model Green function to the result.

Predictions for the imaginary-time self-energy of the half-filled Hubbard model with semi-elliptic DOS at $T = 0.1$ resulting from the scheme described above for a range of discretizations $0.1 \leq \Delta\tau \leq 0.4$ are shown in Fig. C.2 for the correlated metallic phase at $U = 4.0$ and in Fig. C.3 for the insulating phase at $U = 5.0$. All results show the correct asymptotic behavior at large frequencies. Oscillatory behavior which is initially observed at intermediate frequencies (see insets) becomes undetectable for $\Delta\tau \lesssim 0.2$ in both figures. The convergence at small frequencies is good; it will be further discussed below.

One fundamental difference of the QMC code previously used in our group (based on Ulmke's smoothing trick, cf. subsection 3.4.1) is that it does not make predictions for the self-energy beyond the Nyquist frequency as seen in Fig. C.4 and Fig. C.5. Even worse, the $\Delta\tau$ error is also large at intermediate and small frequencies. In fact, the insulating solutions are even qualitatively wrong at small frequencies for large values of $\Delta\tau$.

In contrast, the results of the improved QMC method developed within this thesis and used throughout chapter 3 depicted in Fig. C.6 and Fig. C.7 show good convergence in the most important small-frequency region. In fact, the $\Delta\tau$ error is asymptotically almost identical to that of the new optimal scheme at small frequencies, at least in the range $\Delta\tau \leq 0.25$ used within this thesis.

This is also seen in Fig. C.8, where the Eliashberg estimate of the quasiparticle weight Z (cf. subsection 3.2.3) is shown as a function of $\Delta\tau^2$. Both in the metallic and in the insulating phase, the new approach yields the smallest errors which are nearly perfectly quadratic in $\Delta\tau$. The systematic errors of the QMC program used in chapter 3 are identical (within statistical errors) at small $\Delta\tau$ and only slightly larger for $\Delta\tau \gtrsim 0.25$. In contrast, Ulmke's method leads to $\Delta\tau$ errors which are larger by a full order of magnitude in the insulating case.

While these results of Knecht's (2002) thesis reproduced in this appendix confirm that the QMC code used in chapter 3 is indeed adequate for studies of the Mott