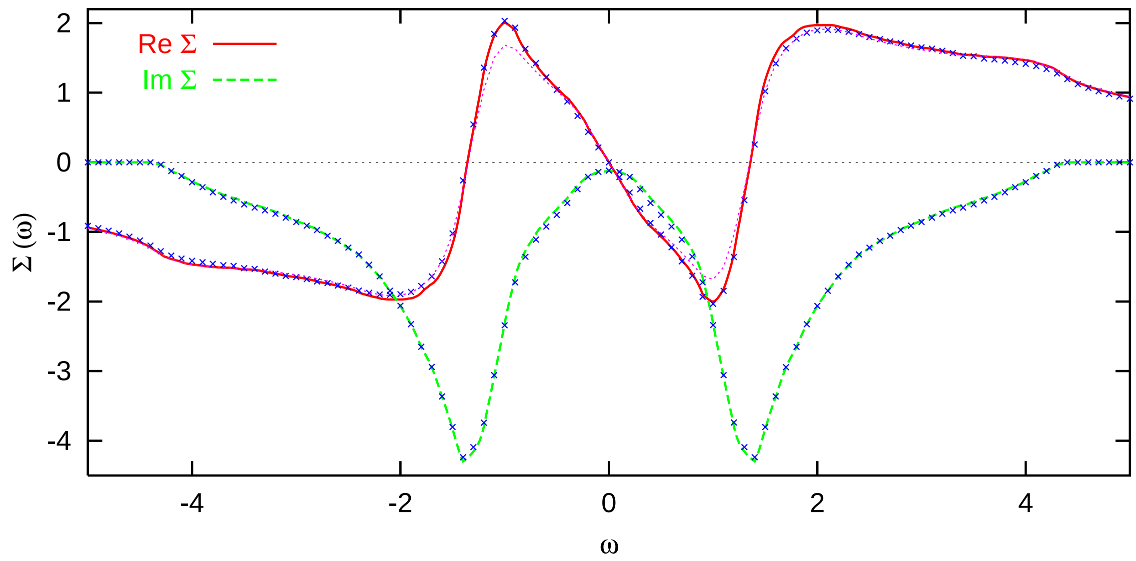

Figure 4.28: QMC results (for $\Delta\tau = 0.1$) at half filling, semi-elliptic DOS, $T = 0.05$, and $U = 4.0$: Real (solid line) and imaginary (dashed line) part of the real-frequency self-energy as derived from the corresponding curves for $G(\omega)$ shown in Fig. 4.27 by inversion of the Dyson equation. Results obtained using a coarse grid (crosses) are seen to violate analyticity: a Kramers-Kronig transform (dotted line) of the "coarse" result for $\mathrm{Im}\,\Sigma(\omega)$ deviates significantly from the direct "coarse" estimate for $\mathrm{Re}\,G(\omega)$.

indication of the high quality of the MEM spectra. For the particular case of the semi-elliptic Bethe DOS studied in this section, the root-finding effort could have been avoided (and was checked) by using the explicit analytic expression. The numerical approach, however, is completely general and will also be used in the LDA+DMFT context in chapter 5 (where it is unavoidable).

The resulting estimates for the self-energy (symmetrized and with a slightly coarser grid resolution $\Delta\omega = 0.025$) are shown as solid and dashed lines for $\mathrm{Re}\,\Sigma(\omega)$ and $\mathrm{Im}\,\Sigma(\omega)$, respectively, in Fig. 4.28. The corresponding results, computed on the coarse grid (crosses) are seen to deviate slightly from these curves. More importantly, the "coarse" results violate analyticity significantly: a Kramers-Kronig transformation of the "coarse" estimate for $\mathrm{Im}\,\Sigma(\omega)$ yields an estimate for $\mathrm{Re}\,\Sigma(\omega)$ (dotted line) which is clearly distinguishable from from the direct "coarse" estimate (and also from the "fine" result). Precise analyticity of $\Sigma(\omega)$, however, is absolutely crucial since otherwise spectral functions computed via the Dyson equation are not properly normalized. "Momentum" resolved spectral functions $A_\epsilon(\omega)$ are shown in the main panel of Fig. 4.29 for $U = 4.0$ and a range of values of $\epsilon \geq 0$. As seen in the inset, the normalization of $A_\epsilon(\omega)$ is correct within 10^{-3} when the fine grid is used, i.e., an interpolation is performed before applying the Kramers-Kronig transformation to $\mathrm{Im}\,G$. Using the nonanalytic self-energy obtained without interpolation, the deviations are about two orders of magnitude larger and would yield clearly visible effects on the level of the momentum distribution function or of the conductivity. Thus, the effort