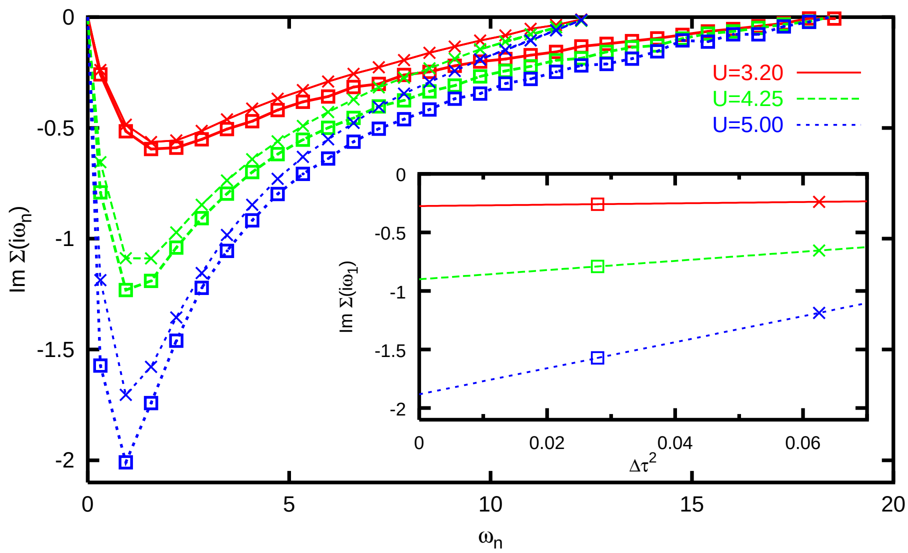

Figure 5.10: Imaginary part of self-energy for $\Delta\tau = 0.25$ (crosses) or $\Delta\tau = 0.167$ (squares). Inset: Extrapolation $\Delta\tau \to 0$ of the value at the first Matsubara frequency $\omega_1 = \pi T$ assuming the best case of a quadratic law. Lines are guides to the eye only.

to an increase of correlation effects.

The discretization error leads to even more prominent changes in the imaginary part of the self-energy on the imaginary axis $\operatorname{Im}\Sigma(i\omega_n)$ shown in Fig. 5.10. On the one hand, the Nyquist cutoff frequency where the computed self-energy unphysically vanishes (instead of decaying like $1/\omega$) is pushed to higher frequencies; on the other hand, the absolute value of $\operatorname{Im}\Sigma$ increases significantly at small frequencies upon decreasing $\Delta\tau$. The latter tendency is, again, a sign that correlation effects are stronger than originally estimated. In fact, the quadratic extrapolation suggests that the quasiparticle weight for $U = 5$ is $Z \approx 0.15$ rather than the value $Z \approx 0.21$ measured for $\Delta\tau = 0.25$.

Due to lack of computing resources in the final stages of this work we could not obtain sufficient data for a controlled application of Jarrell's MEM program. It would also seem more efficient to eliminate systematic errors first before taking details of the statistical error distribution too seriously. Instead, we continued to use the previously applied scheme: for a data set of $50 \lesssim N \lesssim 100$ measurements (bins) of $G^\sigma_\alpha(\tau_i)$ for band index $\alpha \in \{1, 2, 3\}$, spin $\sigma \in \{\uparrow, \downarrow\}$, and time slice $0 \leq i \leq \Lambda = 60$, correlations between measurements at different τ_i and between different spins at the same time slice are neglected when computing averages $G^{\text{av}}_\alpha(\tau_i)$ and the associated errors $\Delta G_\alpha(\tau_i)$ for each band separately.[22] Each band is analytically

[22]Here, a more proper treatment would at least average over spins before calculating errors since the spin-averaged quantities fluctuate much less. In fact, the cleanest approach at this point would involve averaging over spins and orbitals at each time slice before starting the error calculations since we seek information about the paramagnetic phase. On the other hand, the increased error bars generated by the procedures outlined in the text partially mimic systematic errors and can thus limit the impact of unphysical $\Delta\tau$ errors on the resulting spectra.