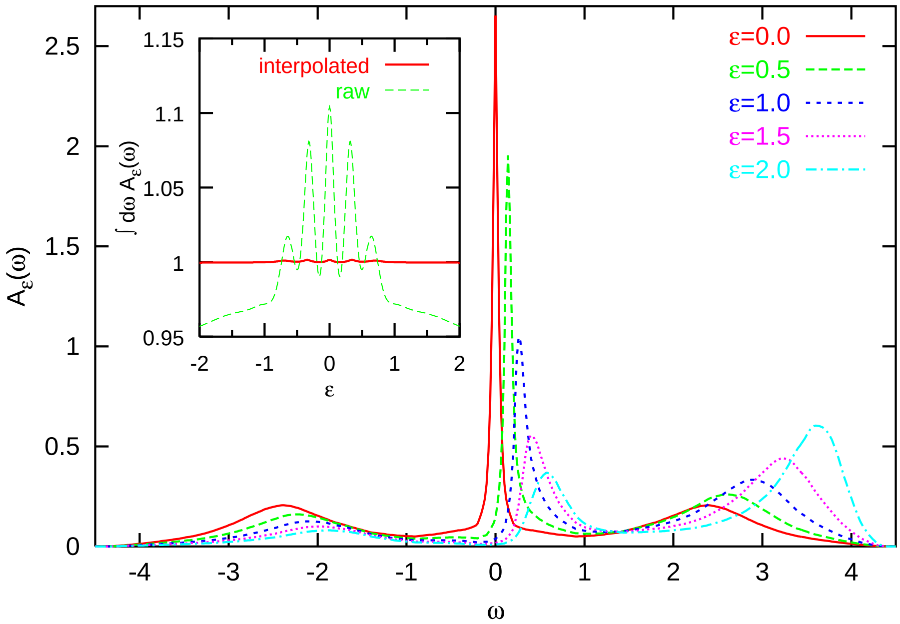

Figure 4.29: Momentum resolved spectral functions $A_\epsilon(\omega)$ for $T = 0.05$ and $U = 4.0$, based on $\Sigma(\omega)$ as presented in Fig. 4.28. $A_\epsilon(\omega)$ shows a three-peak structure for all ϵ; the central resonance is sharpest for $\epsilon = 0$. The inset shows the numerical norm $\int_{-\infty}^{\infty} d\omega A_\epsilon(\omega)$ which should equal 1 for all ϵ. The deviations from this sum rule do not exceed 10^{-3} when the fine grid is used; for a coarse grid, the deviations reach 10^{-1}.

of ensuring fully analytic estimates for $\Sigma(\omega)$ is certainly warranted.[51]

4.6.2 Results: Self-Energy on the Real Axis

In this subsection, we present QMC estimates of the real-frequency self-energy of the half-filled Hubbard model with Bethe DOS for $T = 0.05$. All numerical results are based on the procedure outlined in the previous subsection and on the MEM spectra (corresponding to a flat default model with a frequency grid $\Delta\omega = 0.1$) presented in Fig. 3.77 and Fig. 3.79 in Sec. 3.8.

The self-energy $\Sigma(\omega)$ for the metallic phase is shown in Fig. 4.30. Qualitatively, the overall behavior meets the expectations for a strongly correlated Fermi liquid: $\mathrm{Re}\,\Sigma(\omega)$ is linear near the Fermi energy $\omega = 0$ with negative slope which becomes steeper upon approaching the transition. The imaginary part $\mathrm{Im}\,\Sigma(\omega)$ is nearly quadratic (as a function of ω) in this region. While the curvature increases steadily with increasing U, the offset at $\omega = 0$ is initially almost constant before a relatively rapid increase at $U = 4.7$ signals the breakdown of the Fermi liquid. However, the strong features seen for $U = 4.7$ appear exaggerated: from continuity one would expect that some weight should be shifted from the peaks in $\mathrm{Im}\,\Sigma(\omega)$ to slightly larger

[51] In the following, slight remaining discrepancies in the Kramers-Kronig relations were eliminated by replacing $\mathrm{Re}\,\Sigma(\omega)$ by the Kramers-Kronig transform of $\mathrm{Im}\,\Sigma(\omega)$.