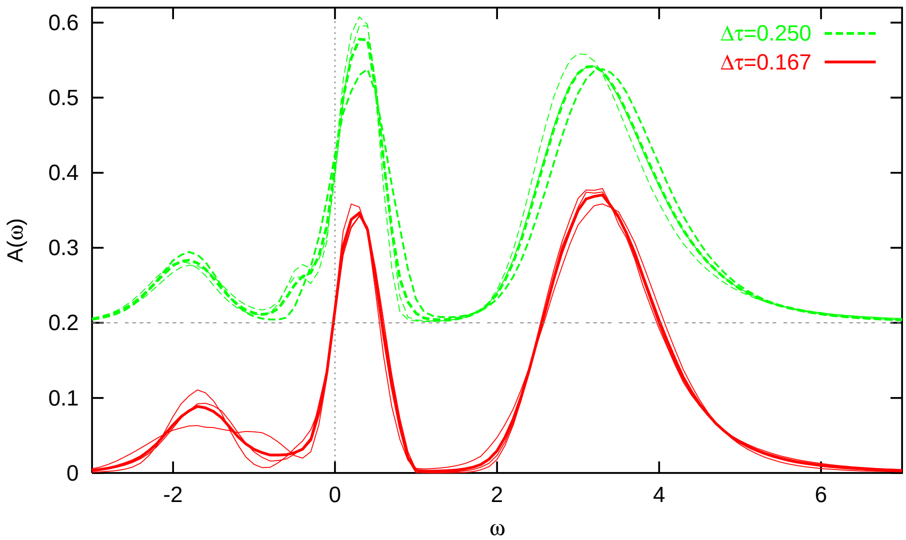

Figure 5.11: Illustration of the MEM strategy "b" used throughout this chapter: data sets (here for $U = 4.25$) for each degenerate t_{2g} band are analytically continued independently to the real axis (thin lines); the partial spectra are then averaged (thick lines). For enhanced clarity of the plot, the ordinate has been shifted for $\Delta\tau = 0.25$ by 0.2.

continued independently. An average over all three bands then defines the final result for each parameter set. As illustrated in Fig. 5.11 for $U = 4.25$ (and $\beta = 10$), the partial spectra (thin lines) show substantial deviations from each other and from the average (thick lines) for both $\Delta\tau = 0.25$ and $\Delta\tau = 0.167$. The observed differences may be regarded as a lower bound on the intrinsic errors. While in general these deviations are not significantly reduced for our new data, the accuracy at small frequencies $|\omega| \lesssim 0.5$ seems improved.

A comparison of the old and new spectra for $U = 3.2$, $U = 4.25$, and $U = 5.0$ is presented in Fig. 5.12. In addition to the data for $\Delta\tau = 0.25$ (same as shown in Fig. 5.5) and data for $\Delta\tau = 0.167$ computed according to the scheme detailed in the last paragraph and denoted as "b", a tighter fit was obtained for comparison by averaging the data over all bands first and applying MEM to the resulting single-band problem ("a"). We stress that the new spectra still leave room for improvement (even for fixed $\Delta\tau = 0.167$); still, the observed changes, i.e., the shift in peak positions and the reduced spectral weight at small frequencies for large U represent genuine improvements over the previously obtained estimates. Unless specified otherwise, we will in the following show results derived from the set "b" of spectra.

Improved Results Figure 5.13 depicts photoemission spectra derived from the new spectral functions with $\Delta\tau = 0.167$ (thick lines) in comparison with those already shown in Fig. 5.5. For the new estimates we also used the temperature $T = 1160$ K in the Fermi function in order to fulfill the sum rule: when the spectra are properly normalized, the integral over the PES computed according to (1.55) equals the band