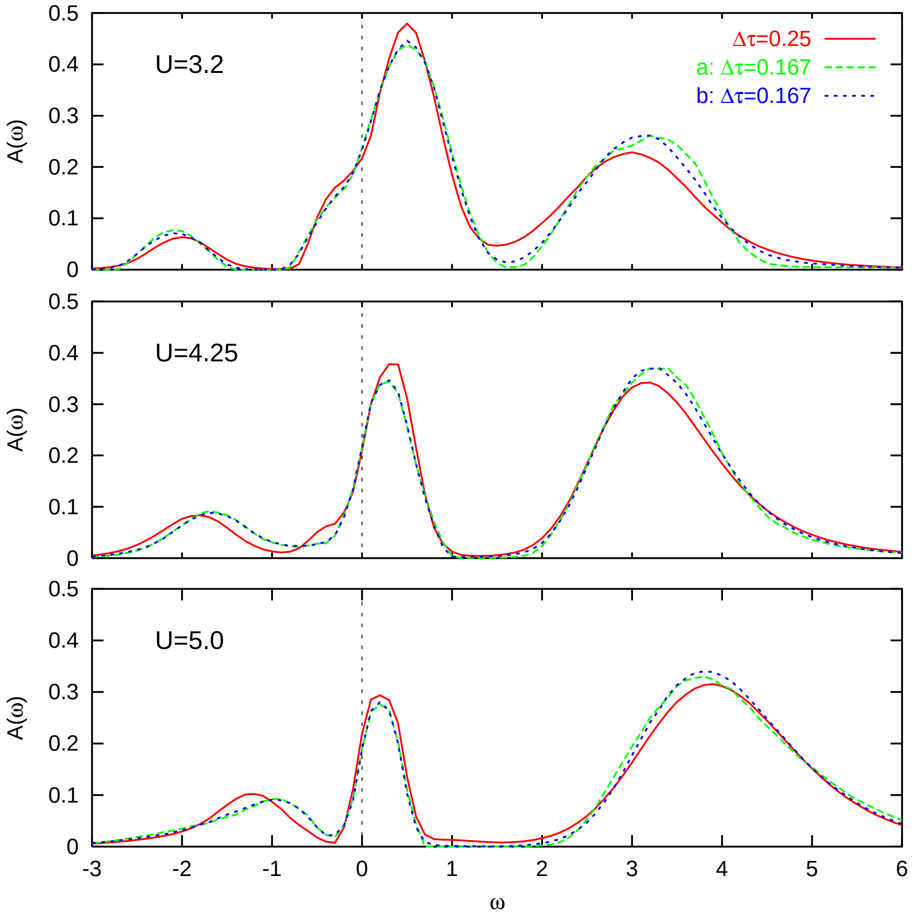

Figure 5.12: Spectra (interacting DOS): new results for $\Delta\tau = 0.167$ using variations of the MEM technique (see text) in comparison to the spectra for $\Delta\tau = 0.25$ shown in Fig. 5.5.

filling to very high accuracy.[23] The increased accuracy makes the peaks at the Fermi energy less prominent; this correlation effect would appear even stronger had both sets of curves been calculated using the same Fermi function. Furthermore, the shape and position of the lower Hubbard bands are modified and the peak positions become more systematic as a function of U.

The upper part of the interacting DOS is in principle also observable experimentally via inverse photoemission, which we model by formally applying (5.23) for negative temperatures. In this case, the noninteracting e_g bands situated above the LDA Fermi energy become very important as is evident in Fig. 5.14. Here, we have used $U = 5.0$ and ignored a possible shift of the Fermi energy, which would also shift the t_{2g} band relative to the remainder of the spectrum. The total PES includes a contribution associated with the O $2p$ band which then fills the gap in the t_{2g} contribution at about 1 eV. In lack of true inverse PES experiments, we compare to

[23]The estimates shown in Fig. 5.7, using $T \ll \Delta\omega = 0.1$ eV in the Fermi function, corresponded to significantly lower band fillings. Therefore, they had been rescaled in (Nekrasov et al., 2000).