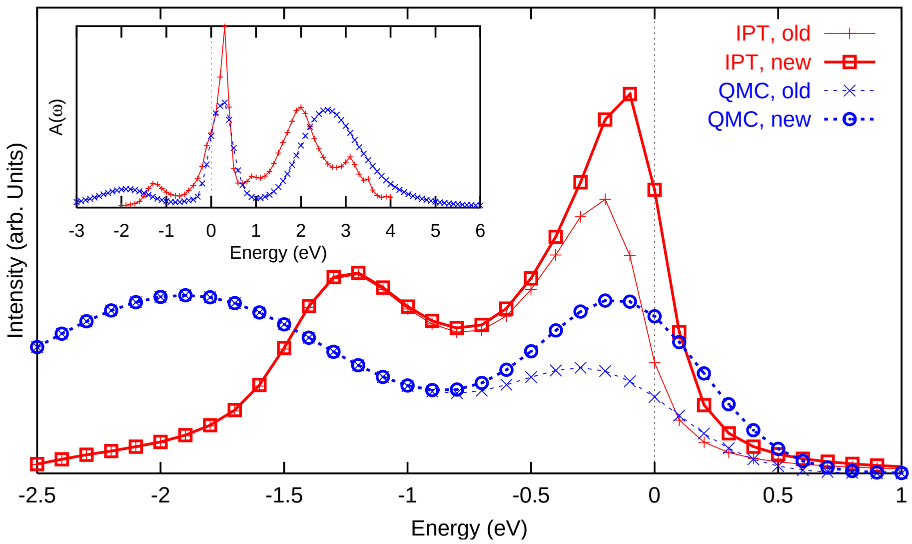

Figure 5.8: Correction of erroneous shift of the chemical potential in (5.23) to -0.1 eV. The "old" IPT PES ($U = 2$ eV, $T = 125$ K) published in (Anisimov et al., 1997) is incorrect, i.e., does not correspond to the DOS computed in the paper (see inset). A corrected curve ("new") shows a much more prominent peak at the Fermi level. A recalculation of the QMC PES for $U = 4$ eV and $T = 1160$ K shown in our preprint (cond-mat/0005207v1) leads to similarly significant changes.

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an error present in the broadening program [i.e., an implementation of (5.23)] used by Anisimov's group, i.e., an erroneous shift of the chemical potential by one grid point, led to strong deviations for the PES when compared to a new (correct) code written as part of this thesis. This observation necessitated new calculations and explains the differences between a first preprint (cond-mat/0005207v1) and the actual publications (Nekrasov, Held, Blümer, Poteryaev, Anisimov, and Vollhardt, 2000; Held, Nekrasov, Blümer, Anisimov, and Vollhardt, 2001) of the work presented in this subsection. While in earlier LDA publications the problem should have been virtually unobservable due to a finer frequency grid, it clearly shows up in the first LDA+DMFT publication (Anisimov et al., 1997). This is seen in Fig. 5.8: both in IPT for $U_{\text{eff}} = 2$ eV, $T = 125$ K and the QMC calculation for $U = 4.0$ eV, $T = 1160$ K the weight of the peak at the Fermi energy was underestimated by about a factor of 2.

5.4.2 Influence of Discretization Errors

While the QMC algorithm used for the treatment of the LDA+DMFT problem in this chapter can in principle yield results of arbitrary precision in the limit of infinite computing resources, it is clear that statistical noise, incomplete convergence of the self-consistency cycle and the Trotter discretization error $\Delta\tau$ in conjunction with approximations made for the Fourier transform (see chapter 3) may impact the results of actual calculations. Even worse, for a finite discretization $\Delta\tau$, the incomplete