prisingly similar to the corresponding plot for $La_{1\text{-}x}Sr_xTiO_3$ shown in Fig. 5.7. This demonstrates that our results may apply to a relatively large class of materials and that, within this class, $La_{1\text{-}x}Sr_xTiO_3$ may not be the system best described by our approach.

5.5 Conclusion

In this chapter, we have given an introduction to the ab initio density functional theory, to its local density approximation (LDA), and to the hybrid LDA+DMFT method in enough detail to expose the various inherent approximations. We have presented published results (Nekrasov et al., 2000) for $La_{1\text{-}x}Sr_xTiO_3$; the relatively good agreement of the computed photoemission data with experiments clearly demonstrates the significant improvement over conventional LDA calculations. We have also discussed some subtleties of the theoretical treatment of photoemission spectra (PES) and have demonstrated the numerical significance of an error in the PES code which we had discovered and corrected.

New results obtained by Nekrasov for the doping dependence of the quasiparticle weight and of the susceptibility of $La_{1\text{-}x}Sr_xTiO_3$ (unpublished) and a planned joint publication (Nekrasov, Blümer, Held, Anisimov, and Vollhardt, 2001) as well as our experiences from treating the metal insulator transition of the half-filled Hubbard model (cf. chapter 3) using the uncorrected QMC code prompted us to question the reliability of the LDA+DMFT(QMC) results in the strongly correlated regime. Therefore, we have repeated all original calculations using an increased number of imaginary time slices in QMC ($\Delta\tau = 0.167$ instead of $\Delta\tau = 0.25$) and testing variations of the maximum entropy method (MEM). As expected, we found significant corrections to the quasiparticle weights and also to the MEM spectra. Our more accurate treatment also leads to a slightly reduced relative weight in the PES near the Fermi energy which is, however, still too high in comparison with experiment. Furthermore, we have computed x-ray absorption (XAS) spectra. While the overall agreement with experiment was seen to be reasonable when including the contributions of Ti e_g and O $2p$ bands (in addition to the Ti t_{2g} bands), the weight at the Fermi energy was again overestimated by theory.

Finally, we have computed the first LDA+DMFT(QMC) estimate of the Ti t_{2g} contribution to the optical conductivity $\sigma(\omega)$ of $La_{1\text{-}x}Sr_xTiO_3$. One prerequisite for this calculation was the development of a program for the inversion of the general $\boldsymbol{k}$-integrated Dyson equation. In lack of momentum resolved LDA data, we also needed to determine the effect of a nonconstant Fermi velocity by application of the general dispersion formalism developed in Sec. 2.3 to the LDA density of states. A detailed comparison of the numerical results with experiment is difficult. On the one hand, experimental results for $\sigma(\omega)$ differ greatly with respect to the presence or width of a Drude peak. On the other hand, contributions of orbitals not included in our theory can be expected to be significant. Taking these uncertainties into account, the overall agreement seems reasonable; again, the most prominent discrepancy is that the theory predicts too much weight at small frequencies.