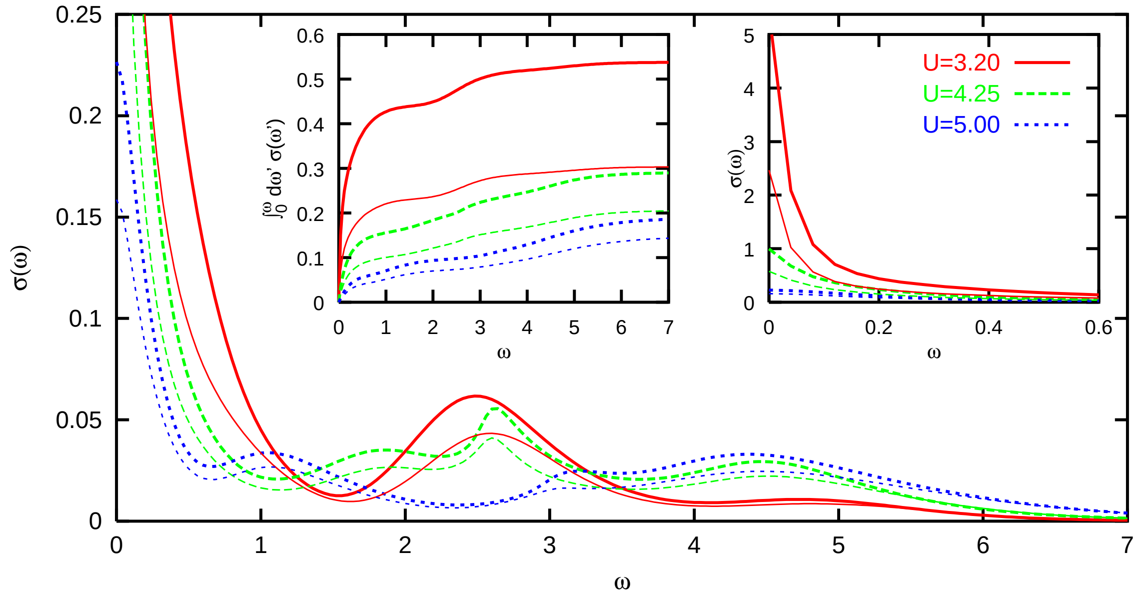

Figure 5.18: QMC estimates for the t_{2g} contribution to the optical conductivity $\sigma(\omega)$ of $La_{1\text{-}x}Sr_xTiO_3$ at $T = 0.1$ (thick lines). For the thin lines, $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$ is set to the constant valid for the hc lattice with NN hopping.

(cf. subsection 3.4.1 and App. C).

When comparing the theoretical transport data to the experimental results reproduced in the following, we also have to keep in mind that interband excitations have been completely neglected so far. A full consistent calculation would require knowledge of the dispersions of all relevant bands and would have to take relative positions of atoms in the unit cell into account (see, e.g., Ahn and Millis, 2000). Then all contributions not involving the correlated t_{2g} band could be calculated using the usual LDA bubble formula for noninteracting electrons. The pure t_{2g} contribution could be evaluated as before, but using the LDA estimate for $\langle|\boldsymbol{v_k}|^2\rangle(\epsilon)$. Finally, transitions between the t_{2g} band and other bands (e.g., the e_g or the O $2p$ bands) would involve both quasiparticles with finite and infinite lifetime. In lack of this data we can only estimate that additional contributions to $\sigma(\omega)$ will appear at least for $\omega \gtrsim 1$ eV.

Since we are not aware of experimental data for the optical conductivity of $La_{1\text{-}x}Sr_xTiO_3$ for the exact doping level $x = 0.06$, we reproduce a set of results obtained for doped $LaTiO_3$ with different stated compositions in chronological order. Measurements of $\sigma(\omega)$ (solid lines) on melt-grown samples over the full Sr doping range (Fujishima, Tokura, Arima, and Uchida, 1992) are shown in Fig. 5.19. An interpolation between the results for "$x = 0.9$" (here "x" denotes the La content) and "$x = 1.0$" or "$x = 0.98$" should be compared to our results. We note that this experiment indicates a minimum in $\sigma(\omega)$ at $\omega \approx 1.2$ eV and that the maximum of $\sigma(\omega)$ at small frequencies exceeds this minimum by a factor of $5-6$. Since the contribution at about 6 eV remains visible in Fig. 5.19 a in the limit $x \to 0$, i.e., for an empty t_{2g}