Only in the last term in (5.20) we have given up generality and thus had to split up the compound orbital index $\alpha$ to single out the strongly correlated Ti $3d$ $t_{2g}$ orbitals.

Both experiment and our LDA calculations (see Sec. 5.4) indicate that the low-temperature properties of $La_{1\text{-}x}Sr_xTiO_3$ are dominated by Ti $3d$ $t_{2g}$ states which hybridize only weakly with other orbitals. Since these states are degenerate, the LDA Hamiltonian is diagonal in this subspace, i.e.,

$$\left(\hat{H}^0_{\mathrm{LDA}}(\boldsymbol{k})\right)_{q_{\mathrm{Ti}} l_{t_{2g}} m, q' l' m'} = \hat{H}^0_{t_{2g}}(\boldsymbol{k})\, \delta_{q_{\mathrm{Ti}} l_{t_{2g}} m, q' l' m'} \,. \tag{5.21}$$

We can thus restrict the explicit treatment to the $t_{2g}$ subspace, in which $G$, $\mathcal{G}$, and $\Sigma$ become diagonal. Due to the special choice $U = V$, $J = 0$, the DMFT problem is then equivalent to a single-band Ising-spin-5/2 Hubbard model, i.e., the derivations of subsection 1.2.3 apply when the replacement $\sigma \to (\sigma, m)$ is made in (1.30)-(1.35). In particular, the LDA input reduces to the $t_{2g}$ DOS (which is supplemented by the estimate for $U$ from constrained supercell LDA calculations).

In this work, we solve the impurity problem using (multi-band) QMC and refer to the resulting general method as LDA+DMFT(QMC). This distinguishes our calculations of photoemission spectra for $La_{1\text{-}x}Sr_xTiO_3$ from earlier work, where analytic approximations have been used for the solution of the impurity problem, i.e., LDA+DMFT(IPT) (Anisimov et al., 1997) and LDA+DMFT(NCA) (Zölfl et al., 2000). The LDA+DMFT(QMC) method was first used by Katsnelson and Lichtenstein (2000) for ferromagnetic iron and applied for the calculation of PES of $Sr_2RuO_4$ by Liebsch and Lichtenstein (2000).

## 5.4 Results for $La_{1\text{-}x}Sr_xTiO_3$

In this section, we present numerical results of the LDA+DMFT(QMC) method applied to $La_{1\text{-}x}Sr_xTiO_3$ for slight doping $x = 0.06$ which drives the system just outside the antiferromagnetic phase and into a paramagnetic strongly renormalized phase. For notational convenience, we will in the following often omit units. Unless stated otherwise, energies are measured in eV, frequencies in eV/$\hbar$, densities of states in $\mathrm{eV}^{-1}$ (or $\hbar$ $\mathrm{eV}^{-1}$), temperatures in eV/$k_{\mathrm{B}}$, imaginary times in $\hbar$ $\mathrm{eV}^{-1}$, and conductivities in arbitrary units.

### 5.4.1 Density of States and Photoemission Spectra

Since the predominant effect of the substitution of La by Sr in $La_{1\text{-}x}Sr_xTiO_3$ is a reduction of the Ti $3d$ $t_{2g}$ band filling while the shape of this band remains essentially unchanged,[14] the LDA spectra were calculated for pure $LaTiO_3$. Furthermore, the orthorhombically distorted crystal structure of this material was replaced by a cubic unit cell. As discussed also in Sec. 5.1, the primary resulting error is an overestimation of the effective bandwidth. The density functional theory problem was solved using

[14] This working hypothesis was later checked by comparison to LDA spectra obtained for doping $x = 0.5$.