noninteracting part of our model. It is neither possible nor necessary to include all possible on-site interactions shown in (1.9). Instead, one has to concentrate on terms which can be treated more accurately in a many-body tight-binding model approach than in LDA and which dominate the correlation physics missed by plain LDA. In a minimal extension of the LDA, one may restrict the treatment to contributions of the density-density type[11]

$$H_{\text{corr}} = \frac{1}{2} \sum_{\substack{ilm,l'm',\sigma\sigma' \\ (lm\sigma)\neq(l'm'\sigma')}} U^{i}_{lm,l'm'}\ \hat{n}_{ilm,\sigma}\ \hat{n}_{il'm',\sigma'}\ . \tag{5.10}$$

For the application to $La_{1\text{-}x}Sr_xTiO_3$, we will only include on-site interactions within the threefold degenerate Ti t_{2g} orbitals, i.e., restrict the sum in (5.10) to $i = i_{\text{Ti}}$ and $l = l' = l_{t_{2g}}$. Furthermore, we crudely approximate intra-orbital and interorbital electron-electron interaction by a common mean parameter, i.e.,

$$U^{i}_{lm,l'm'} = U\delta_{ii_{\text{Ti}}}\delta_{ll'}\delta_{ll_{t_{2g}}}\ . \tag{5.11}$$

The parameter U may be approximately calculated in constrained supercell LDA calculations (Gunnarsson et al., 1989) or estimated from experiment, e.g., high-energy spectroscopy. Note that the LDA estimate depends both on the particular basis set used in LDA and on the selection of interacting orbitals: U decreases if more orbitals (e.g., the Ti $3d$ e_g orbitals) are considered as noninteracting and are thus allowed to participate in screening. In order to avoid double counting, one should in general take into account that the Coulomb interaction (5.11) is already contained in LDA in some averaged way. A guess for the corresponding contribution has been derived from the atomic limit (Anisimov, Poteryaev, Korotin, Anokhin, and Kotliar, 1997),

$$E^{\text{LDA}}_{\text{corr}} = \frac{1}{2}Un_{t_{2g}}(n_{t_{2g}} - 1)\,, \tag{5.12}$$

where $n_{t_{2g}}$ denotes the total occupation of the correlated Ti $3d$ t_{2g} orbitals and which gives rise to a shift of the on-site potential,

$$\Delta\epsilon_{i_{\text{Ti}}l_{t_{2g}}} = U(n_{t_{2g}} - \frac{1}{2})\,. \tag{5.13}$$

We point out that the parabolic interpolation of atomic energies for fractional occupation number $n_{t_{2g}}$ inherent in (5.12) and (5.13) is unphysical, at least for $n_{t_{2g}} < 1$ (where the contribution (5.12) becomes negative). Therefore, the Hartree estimate $E^{\text{Hartree}}_{\text{corr}} = Un_{t_{2g}}(M - 1/2)/(2M)$ (for orbital degeneracy M) might be considered as an alternative.[12] We will in the following consider the Hamiltonian

$$\hat{H}_{\text{LDA+corr}} = \hat{H}^{0}_{LMTO} + U \sum_{\substack{i',m\sigma,m'\sigma' \\ (m\sigma\neq m'\sigma')}} \hat{n}^{t_{2g}}_{i'm\sigma}\hat{n}^{t_{2g}}_{i'm'\sigma'}\,, \tag{5.14}$$

[11] It is also possible to include exchange interactions analogous to the J term in (5.8) on equal footing (Zölfl, Pruschke, Keller, Poteryaev, Nekrasov, and Anisimov, 2000; Held, Keller, Eyert, Vollhardt and Anisimov, 2001) which may lead to further corrections for LDA at the cost of destroying SU(2) symmetry and introducing additional parameters.

[12] For the calculations presented in this chapter, the double counting correction $\Delta\epsilon$ will be irrelevant (see below).