where i' only sums over Ti sites and the double-counting corrected LDA Hamiltonian is assumed as

$$\hat{H}^0_{\mathrm{LDA}} = \hat{H}_{\mathrm{LMTO}} - U(n_{t_{2g}} - \frac{1}{2}) \sum_{i',m\sigma} \hat{n}^{t_{2g}}_{i'm\sigma} \,. \tag{5.15}$$

In lack of exact methods for the solution of the general multi-band Hubbard model, approximative solutions are needed just like for pure model calculations. A treatment within the DMFT seems natural and appropriate since it treats the local dynamics induced by the additional local interactions exactly and was also the first choice historically (Anisimov et al., 1997). Lichtenstein and Katsnelson (1998) used DMFT, the fluctuation-exchange approximation (FLEX), and the Hubbard-I approximation alternatively and named the general approach LDA^{++}. Drchal, Janiš, and Kudrnovský (1999) combined FLEX with the coherent potential approximation (CPA) for the inclusion of disorder effects.

The DMFT solution of (5.14) is best formulated in reciprocal space, where $\hat{H}^0_{\mathrm{LDA}}$ has the matrix elements

$$\big(\hat{H}^0_{\mathrm{LDA}}(\boldsymbol{k})\big)_{qlm,q'l'm'} = \big(\hat{H}_{\mathrm{LDA}}(\boldsymbol{k})\big)_{qlm,q'l'm'} - \delta_{qlm,q'l'm'}\delta_{ql,q_{\mathrm{Ti}}l_{t_{2g}}} U(n_{t_{2g}} - \frac{1}{2}) \,. \tag{5.16}$$

Here, q is an index of the atoms in the elementary unit cell. Generalizing from the 1-band Bravais lattice case discussed in subsection 1.2.3, the lattice problem can be mapped to a multi-band SIAM.[13] Now, on-site lattice Green function G, impurity Green function $\mathcal{G}$, and self-energy Σ are matrices where each index denotes an orbital within the unit cell, $\alpha \equiv (q, l, m)$. The $\boldsymbol{k}$ integrated lattice Dyson equation and the impurity Dyson equation read for (complex) frequency z:

$$G^{\sigma}_{\alpha\alpha'}(z) = \int \frac{\mathrm{d}\boldsymbol{k}}{V_{\mathrm{B}}} \Big[z\delta_{\alpha,\alpha'} - \big(H^0_{\mathrm{LDA}}(\boldsymbol{k})\big)_{\alpha\alpha'} - \Sigma^{\sigma}_{\alpha\alpha'}(z) \Big]^{-1} \tag{5.17}$$

$$\big[G^{\sigma}_{\alpha\alpha'}(z)\big]^{-1} = \big[\mathcal{G}^{\sigma}_{\alpha\alpha'}(z)\big]^{-1} - \Sigma^{\sigma}_{\alpha\alpha'}(z) \,, \tag{5.18}$$

where $[\dots]^{-1}$ denotes matrix inversion (in α, α'). The impurity (or cluster) problem, expressed in mixed notation using imaginary time τ and index n for Matsubara frequency $i\omega_n$ takes the form:

$$G^{\sigma n}_{\alpha\alpha'} = -\frac{1}{Z} \int \mathcal{D}[\psi]\mathcal{D}[\psi^*]\; \psi^{\sigma n}_{\alpha} \psi^{\sigma n *}_{\alpha'} \mathrm{e}^{\mathcal{A}[\psi,\psi^*,\mathcal{G}]} \,, \tag{5.19}$$

with the action

$$\begin{aligned} \mathcal{A}[\psi, \psi^*, \mathcal{G}] &= \sum_{n,\sigma,\alpha,\alpha'} \psi^{\sigma n *}_{\alpha} \big[\mathcal{G}^{\sigma n}_{\alpha\alpha'}\big]^{-1} \psi^{\sigma n}_{\alpha'} \\ &\quad - \frac{U}{2} \sum_{\substack{m,\sigma,m',\sigma' \\ (m\sigma)\neq(m'\sigma')}} \int_0^{\beta} \mathrm{d}\tau\, \psi^{\sigma n^*}_{q_{\mathrm{Ti}}l_{t_{2g}}m}\, \psi^{\sigma n}_{q_{\mathrm{Ti}}l_{t_{2g}}m}\, \psi^{\sigma' n *}_{q_{\mathrm{Ti}}l_{t_{2g}}m'}\, \psi^{\sigma' n}_{q_{\mathrm{Ti}}l_{t_{2g}}m'} \,. \end{aligned} \tag{5.20}$$

[13] In general, the resulting problem appears rather as a finite cluster with on-site interactions and frequency dependent on-site "energies" and "hopping terms" very similar to the systems studied in DCA (cf. App. A.3). Only in absence of hybridization between different orbitals the DMFT mapping leads to a conventional multi-band impurity without mixing terms. Since we will neglect small hybridization terms found in the LDA calculations for $La_{1-x}Sr_xTiO_3$, however, the cluster will indeed reduce to a single impurity in our calculations.