interaction is still local but the valence band is degenerate then contains additional coupling terms[1] (Anderson, 1961; Dworin and Narath, 1970)

$$\begin{aligned}\hat{H}_{m\text{-band}} &= -t \sum_{\langle ij\rangle,\nu\sigma} \hat{c}^\dagger_{i\nu\sigma}\hat{c}_{j\nu\sigma} + U\sum_{i\nu}\hat{n}_{i\nu\uparrow}\hat{n}_{i\nu\downarrow} \\ &\quad + V_0 \sum_{i;\nu<\nu';\sigma\sigma'} \hat{n}_{i\nu\sigma}\hat{n}_{i\nu'\sigma'} + F_0 \sum_{i;\nu<\nu';\sigma\sigma'} \hat{c}^\dagger_{i\nu\sigma}\hat{c}^\dagger_{i\nu'\sigma'}\hat{c}_{i\nu\sigma'}\hat{c}_{i\nu'\sigma},\end{aligned} \tag{A.3}$$

where ν,ν' (with $1 \le \nu \le m$, $1 \le \nu' \le m$) are band indices. The exchange term parameterized by the Hund's rule coupling F_0 can be rewritten as

$$\hat{H}_{F_0} = -2F_0 \sum_{i,\nu<\nu'} \left(\hat{\boldsymbol{S}}_{i\nu} \cdot \hat{\boldsymbol{S}}_{i\nu'} + \frac{1}{4}\hat{n}_{i\nu}\hat{n}_{i\nu'} \right) \tag{A.4}$$

with $\hat{\boldsymbol{S}}_{i\nu} = \frac{1}{2}\sum_{\sigma\sigma'} \hat{c}^\dagger_{i\nu\sigma}\boldsymbol{\tau}_{\sigma\sigma'}\hat{c}_{i\nu\sigma'}$ being the spin operator for orbital ν at site i and the Pauli matrices $\boldsymbol{\tau}_{\sigma\sigma'}$. In quantum Monte Carlo (QMC) simulations, the spin-flipping terms implicit in (A.4) lead to a numeric (minus-sign) problem. Therefore, one here usually replaces the Heisenberg interaction part of (A.4) by an Ising-type interaction at the cost of breaking the SU(2) symmetry (Motome and Imada, 1997; Held and Vollhardt, 1998). Since $\hat{s}^z_{i\nu}\hat{s}^z_{i\nu'} = \sigma\sigma'\hat{n}_{i\nu\sigma}\hat{n}_{i\nu'\sigma'}/4 = (2\delta_{\sigma\sigma'} - 1)\,\hat{n}_{i\nu\sigma}\hat{n}_{i\nu'\sigma'}/4$, one can write this modified multi-band Hubbard Hamiltonian as

$$\hat{H}^z_{m\text{-band}} = \sum_{\langle ij\rangle,\nu\sigma} \epsilon_{\boldsymbol{k}\nu}\hat{c}^\dagger_{\boldsymbol{k}\nu}\hat{c}_{\boldsymbol{k}\nu} + U\sum_{i\nu}\hat{n}_{i\nu\uparrow}\hat{n}_{i\nu\downarrow} + \sum_{i;\nu<\nu';\sigma\sigma'} (V_0 - \delta_{\sigma\sigma'}F_0)\,\hat{n}_{i\nu\sigma}\hat{n}_{i\nu'\sigma'}. \tag{A.5}$$

The interaction U between electrons within each orbital is always larger than the interorbital density-density interaction V_0. The smaller exchange coupling F_0 can trigger ferromagnetic and (possibly coexisting) orbital order.[2]

While in general the inclusion of different nondegenerate bands involves an additional large number of parameters, one can model (and simulate using QMC, e.g., within the DMFT) the influence of a half-filled, locally polarized and relatively inert subband as observed in manganites by adding a Kondo-type interaction between the itinerant electrons and some spin degree of freedom, $-2\sum_\nu\sum_i \hat{\boldsymbol{s}}_{i\nu}\cdot\hat{\boldsymbol{S}}_i$. Here, $\hat{\boldsymbol{s}}_{i\nu}$ are the spin operators for the itinerant twofold degenerate e_g band while $\hat{\boldsymbol{S}}_i$ models a localized spin-3/2 originating from the t_{2g} band (Held and Vollhardt, 2000).

An additional complication in compounds is the presence of several inequivalent ions per unit cell. Such systems can be modeled microscopically by introducing different on-site energies, Coulomb interactions, and hopping matrix elements within a unit cell or more phenomenologically by using renormalized hopping matrix elements between just a subset of orbitals (while others are integrated out). One example of the

[1] Here, an on-site pair hopping term which only contributes when one orbital is doubly and another singly occupied is neglected (Held and Vollhardt, 1998).

[2] In the application of the LDA+DMFT method in chapter 5 we will set $U = V_0$ and $F_0 = 0$; in the absence of long range order and for small filling $n \lesssim 1$ the resulting error is not expected to exceed other sources of errors. In general, local exchange terms only become negligible for extended orbitals (an extreme case being valence molecular orbitals in C_{60} Fullerides).