orbitals, self-interaction corrections can also be applied for transition metal oxides yielding improved predictions for band gaps and moments (Svane and Gunnarsson, 1990). The important advantage of SIC-LDA over LDA (and the reason we mention the method here) is that SIC provides a mechanism which allows the solutions to localize and that it effectively generates a Hubbard-type interaction which may split occupied and unoccupied states.

A similar effect arises in the LDA+U method which explicitly introduces mean-field type local interactions between electrons in correlated orbitals of degeneracy M, e.g., d orbitals (Anisimov, Zaanen, and Andersen, 1991),

$$E_{\mathrm{LDA+U}} = E_{\mathrm{LDA}} + \frac{1}{2} \sum_{m\sigma \neq m'\sigma'} (U - J\delta_{\sigma\sigma'})\,(n_{m\sigma} - \bar{n})(n_{m'\sigma'} - \bar{n}) \tag{5.8}$$

The LDA energy is unchanged in the unpolarized case, when the expectation value $n_{m\sigma}$ of the occupancy of each state equals $\bar{n} := \frac{1}{2M}\sum_{m=1}^{M}\sum_{\sigma} n_{m\sigma}$. Orbital and/or spin order, however, generically lead to negative contributions of the interaction term in (5.8) which may outweigh an concurrent increase of the LDA energy and thus stabilize ordered insulating phases for integer filling. Both interaction parameters U and J can be estimated from constrained supercell LDA calculations (Gunnarsson, Andersen, Jepsen, and Zaanen, 1989). Thus, in contrast to plain LDA, the LDA+U method allows for an "ab initio" modeling of insulating, long-range ordered phases (e.g., antiferromagnetic or orbital order) within the DFT framework, but still cannot describe paramagnetic Mott insulators or strongly renormalized quasiparticle states. Such problems are clearly beyond static effective single-particle theories.

More general approaches which also allow for a microscopic treatment of on-site correlations have to be formulated in terms of a true many-body Hamiltonian. Ideally, one could treat interactions between electrons in some localized orbitals of an open shell explicitly (without resorting to static mean-field approximations) and use LDA for all remaining electron-electron interactions as well as for electron-ion interactions and kinetic energy. In practice, we can at least avoid static mean-field approximations for the explicitly treated interactions and approximately extract a tight-binding model from LDA calculations which we then have to correct approximately for double counting. For this purpose, we interpret the Lagrange parameters ϵ_i of the LDA solution of the Kohn-Sham equations (5.6) for a tight-binding LMTO basis (Andersen et al., 1986; Jepsen and Andersen, 2000) as defining a band structure which may be represented in terms of hopping matrix elements (vanishing on the diagonal: $t_{ilm,ilm} = 0$) and on-site energies,

$$\hat{H}^{\mathrm{LDA}} = \sum_{ilm,jl'm',\sigma} \left(t_{ilm,jl'm'} \hat{c}^{\dagger}_{ilm,\sigma} \hat{c}_{jl'm',\sigma} + \varepsilon_{il} \hat{n}_{ilm,\sigma} \delta_{ilm,jl'm'} \right) . \tag{5.9}$$

Here, the indices i and j label atomic sites, σ labels spin, and l, m, l', m' are orbital indices.[10] Up to double counting corrections, we will regard (5.9) as the

[10] Neither the orbital basis nor the distinction between the index components l and m is unique. Here, we have adopted the convention that degenerate orbitals share a common value of l, but can be distinguished by the index m.