Appendix A

Additions to "Models and Methods"

A.1 Extensions of the Hubbard Model

The one-band Hubbard model represents a highly idealized view of strongly correlated materials. Some of its shortcomings are best characterized by writing down minimal model extensions which could be used for adding the missing physics. While most of the extensions collected in this section will not be used for actual calculations in this thesis, we will discuss the implications of extended hopping in chapter 2 and study a 3-band model based on LDA input data in chapter 5.

The applicability of the one-band Hubbard model to d or f electron systems is a priori questionable since the partially filled bands correspond to atomic orbitals which are 5-fold and 7-fold degenerate (for each spin direction), respectively. While bands in a lattice are more complicated than orbitals of isolated atoms, the remaining degeneracy can be inferred from symmetry considerations alone. Often it is useful to consider a cubic representation of the angular part of atomic d orbitals,

$$\begin{aligned} &|d_{xy}\rangle \propto (|2,2\rangle - |2,-2\rangle)\,, \quad |d_{yz}\rangle \propto (|2,1\rangle + |2,-1\rangle)\,, \quad |d_{zx}\rangle \propto (|2,1\rangle - |2,-1\rangle) \\ &|d_{x^2-y^2}\rangle \propto (|2,2\rangle + |2,-2\rangle)\,, \quad |d_{3z^2-r^2}\rangle \propto |2,0\rangle, \end{aligned} \tag{A.1}$$

expressed in terms of eigenfunctions of the angular momentum operator,

$$\boldsymbol{l}^2|l,m\rangle = \hbar^2 l(l+1)|l,m\rangle, \quad l_z|l,m\rangle = \hbar m|l,m\rangle\,. \tag{A.2}$$

In lattices with cubic symmetry the five d orbitals are energetically split into the t_{2g} orbitals ($|d_{xy}\rangle$, $|d_{yz}\rangle$, $|d_{zx}\rangle$) and the e_g orbitals ($|d_{x^2-y^2}\rangle$, $|d_{3z^2-r^2}\rangle$), which give rise to one threefold degenerate and one twofold degenerate band, respectively. Lower symmetry can lift the remaining degeneracies; e.g., in the trigonal case the t_{2g} orbitals are further split into one nondegenerate a_{1g} and one twofold degenerate e_g^π band. Thus, it is possible that in some d systems only one band crosses or touches the Fermi surface which then justifies the one-band assumption made in subsection 1.1.4 and used in chapter 3. In general, however, the inclusion of several orbitals per site is important. An SU(2)-invariant generalization of the Hubbard model where the