former approach is the "Emery model" or "Varma-Schmitt-Rink-Abrahams model" for electron holes in the copper oxide planes in high-T_c superconductors (Varma, Schmitt-Rink, and Abrahams, 1987; Emery, 1987)[3]

$$\begin{aligned}\hat{H}_{\text{sc}} &= -t_{pd} \sum_{\langle i,j\rangle,\nu,\sigma} (\hat{p}^{\dagger}_{j\nu\sigma}\hat{d}_{i\sigma} + \text{h.c.}) - t_{pp} \sum_{\langle j,j'\rangle,\nu,\sigma} (\hat{p}^{\dagger}_{j\nu\sigma}\hat{p}_{j'\nu\sigma} + \text{h.c.}) + \epsilon_d \sum_i \hat{n}^d_i + \epsilon_p \sum_{j\nu} \hat{n}^p_{j\nu} \\ &\quad + U_d \sum_i \hat{n}^d_{i\uparrow}\hat{n}^d_{i\downarrow} + U_p \sum_{j\nu} \hat{n}^p_{j\nu\uparrow}\hat{n}^p_{j\nu\downarrow} + V \sum_{\langle ij\rangle,\nu} \hat{n}^d_i \hat{n}^p_{j\nu}\,. \end{aligned} \tag{A.6}$$

The latter, more phenomenological approach is used for modeling the compound $La_{1\text{-}x}Sr_xTiO_3$ using an explicit treatment of the Ti $3d$ t_{2g} orbitals only in chapter 5.

Since the restriction to local interactions in the Hubbard model is a crude approximation to the Coulomb interaction, one may expect significant improvements by including nearest-neighbor terms of the Coulomb interaction. For a one-band model, these may be written in the form (Hirsch, 1989; Strack and Vollhardt, 1994)

$$\begin{aligned}\hat{V}^{\text{NN}}_{\text{1-band}} &= \sum_{\langle i,j\rangle} \Big[V\hat{n}_i\hat{n}_j - 2F(\hat{\boldsymbol{S}}_i\hat{\boldsymbol{S}}_j + \frac{1}{4}\hat{n}_i\hat{n}_j) \\ &\quad + X\sum_\sigma (\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.})(\hat{n}_{i\,-\sigma} + \hat{n}_{j\,-\sigma}) + F'(\hat{c}^{\dagger}_{i\uparrow}\hat{c}^{\dagger}_{i\downarrow}\hat{c}_{j\downarrow}\hat{c}_{j\uparrow} + \text{h.c.})\Big]. \end{aligned} \tag{A.7}$$

Here, the V term and the F term are completely analogous to the onsite interactions between orbitals in (A.3), while the additional terms involve density-dependent hopping (X) and pair hopping (F'). These nearest-neighbor contributions of the Coulomb interactions can, e.g., drive ferromagnetism (Hirsch, 1989; Kollar, Strack, and Vollhardt, 1996; Blümer, 1996; Wahle et al., 1998), charge density waves, phase separation, or superconductivity (Hirsch and Marsiglio, 2000).

Disorder is always present to some degree in real materials, in particular in doped systems (as considered in chapter 5), and is potentially very important, e.g., in the context of Anderson localization. A straightforward generalization of the one-band Hubbard model leads to

$$\hat{H}_{\text{disorder}} = \sum_{i\sigma} (\epsilon_i - \mu)\,\hat{n}_{i\sigma} + \sum_{\langle i,j\rangle,\sigma} t_{ij} \left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}\right) + \sum_i U_i(\hat{n}_{i\uparrow} - \frac{1}{2})(\hat{n}_{i\downarrow} - \frac{1}{2}), \tag{A.8}$$

where site-diagonal terms, i.e., the lattice potentials ϵ_i and the Coulomb interaction U_i and/or the (intersite) hopping terms t_{ij} may be allowed to vary [for a treatment within DMFT, see, e.g., Dobrosavljević and Kotliar (1993) and Ulmke (1998)].

The inclusion of phonons is possible in terms of the Holstein-Hubbard model, in which the Hubbard model is supplemented by the electron-phonon interaction plus a phonon energy (Holstein, 1959; Zhong and Schüttler, 1992; Freericks and Jarrell, 1995*b*)

$$\hat{H}_{\text{H-H}} = \hat{H}_{\text{Hub}} + g\sum_i R_i(\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow} - 1) + \frac{1}{2}\sum_i \left(\frac{P_i^2}{M} + M\Omega^2 R_i^2\right). \tag{A.9}$$

[3] Here, i and j denote the unit cell for Cu $3d_{x^2-y^2}$ orbitals and O $2p_x$ or $2p_y$ orbitals, respectively. The orbital index $\nu = x$ or $\nu = y$ distinguishes the oxygen orbitals (living on different sites); unrestricted summation over omitted spin indices is implied.