Several observations can be made at this point: First of all, in contrast to the field-operator representation defined in the continuum, in the Wannier representation even the bare Coulomb interaction not only depends on the densities $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$ but also contains explicit off-diagonal contributions, for example, on-site Hund's rule couplings and Heisenberg nearest-neighbor exchange couplings (see App. A.1). Secondly, when the explicit treatment is restricted to a few valence electrons, the interaction $V^{ee}(\boldsymbol{r}, \boldsymbol{r}')$ cannot be expressed in the translationally invariant form $V^{ee}(\boldsymbol{r} - \boldsymbol{r}')$. This affects symmetry considerations for the matrix elements $\mathcal{V}^{\nu\nu'\mu\mu'}_{ijmn}$.[6] Finally, the matrix elements of the kinetic energy t^{ν}_{ij}, called *hopping amplitudes*, can be expected to fall off rapidly with increasing $|\boldsymbol{R}_i - \boldsymbol{R}_j|$ since the associated atomic orbitals and, consequently, the corresponding Wannier functions hardly overlap, at least for $3d$ or $4f$ valence electrons (see, e.g., Ashcroft and Mermin, 1976).

1.1.4 One-band Hubbard Model

The simplified valence-electron model (1.9) still contains an infinite number of input parameters that cannot be reliably determined from first principles.[7] This situation calls for a minimalistic approach where the number of parameters is chosen to be just large enough to capture the interesting effects, at least qualitatively.

If we restrict the Hamiltonian (1.9) to one valence band ($\nu = \nu' = \mu = \mu' = 1$) with isotropic hopping to nearest neighbors (NN) only[8] and assume "perfect" screening, i.e., choose

$$t^{\nu}_{ij} \equiv t_{ij} = \begin{cases} -t & \text{if } i \text{ NN of } j \\ 0 & \text{otherwise,} \end{cases} \tag{1.12}$$

$$\mathcal{V}^{\nu\nu'\mu\mu'}_{ijmn} \equiv \mathcal{V}_{ijmn} = U\,\delta_{ij}\delta_{im}\delta_{in}\,, \tag{1.13}$$

we arrive at the one-band Hubbard model,

$$\hat{H}_{\text{Hub}} = -t \sum_{\langle i,j\rangle,\sigma} \left(\hat{c}^{\dagger}_{i\sigma}\hat{c}_{j\sigma} + \text{h.c.}\right) + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}\,. \tag{1.14}$$

Here, t parameterizes the kinetic energy, U the Coulomb interaction, and the bracket $\langle i, j\rangle$ restricts the sum to nearest-neighbor pairs i, j. The operator $\hat{n}_{i\sigma} = \hat{c}^{\dagger}_{i\sigma}\hat{c}_{i\sigma}$ measures the occupancy of the site i with electrons of spin σ. Consequently, $\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}$ is the double occupancy, i.e., its expectation value corresponds to the density of doubly occupied sites. Studies of this model, originally proposed for the description of

[6] Formally, higher symmetry can be retained by applying (1.10) and (1.11) to the full unshielded problem. A truncation of the inherent sums over nearest-neighbor shells, however, can only be justified after the divergencies have been removed by renormalization, i.e., shielding.

[7] For an approximate material specific determination of matrix elements using density functional theory, see Sec. 5.3.

[8] Since the methods introduced in the following do not rely on this restriction, we will later also consider extended models with hopping beyond the NN shell. In this context, we refer to the model with NN hopping only as the "pure" Hubbard model.