to the occupation number formalism ("second quantization"; see, e.g., Fetter and Walecka, 1971) in real space, the Hamiltonian for electrons with spin σ takes the form

$$\hat{H} = \hat{H}_0 + \hat{H}_{\mathrm{int}}, \tag{1.4}$$

where

$$\hat{H}_0 = \sum_\sigma \int \mathrm{d}\boldsymbol{r}\; \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) \left[-\frac{\hbar^2}{2m}\Delta + V^{\mathrm{ion}}(\boldsymbol{r}) \right] \hat{\psi}_\sigma(\boldsymbol{r}) \tag{1.5}$$

$$\hat{H}_{\mathrm{int}} = \frac{1}{2} \sum_{\sigma\sigma} \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}'\; V^{\mathrm{ee}}(\boldsymbol{r},\boldsymbol{r}')\, \hat{n}_\sigma(\boldsymbol{r})\, \hat{n}_{\sigma'}(\boldsymbol{r}')\,. \tag{1.6}$$

Here, $\hat{\psi}_\sigma(\boldsymbol{r}), \hat{\psi}^\dagger_\sigma(\boldsymbol{r})$ are field operators which annihilate and create electrons of spin σ at site $\boldsymbol{r}$, respectively; $\hbar = h/2\pi$ is Planck's constant, Δ the Laplace operator, and $\hat{n}_\sigma(\boldsymbol{r}) = \hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r})$ the operator measuring the local density of electrons with spin σ at position $\boldsymbol{r}$.

1.1.3 Wannier Representation

In terms of the lattice momentum $\boldsymbol{k}$ and Bloch eigenfunctions $\phi_{\nu\boldsymbol{k}}(\boldsymbol{r})$ of the non-interacting[5] Hamiltonian (1.5), we may introduce Wannier functions predominantly localized at site $\boldsymbol{R}_i$ by

$$\chi_{i\nu}(\boldsymbol{r}) = \frac{1}{\sqrt{L}} \sum_{\boldsymbol{k}} \mathrm{e}^{-i\boldsymbol{k}\cdot\boldsymbol{R}_i}\; \phi_{\boldsymbol{k}\nu}(\boldsymbol{r})\,, \tag{1.7}$$

where L is the number of lattice sites, and thus construct creation and annihilation operators $\hat{c}^\dagger_{i\nu\sigma}$,$\hat{c}_{i\nu\sigma}$ for electrons with spin $\sigma \in \{\uparrow,\downarrow\}$ in the band ν at site $\boldsymbol{R}_i$ as

$$\hat{c}^\dagger_{i\nu\sigma} = \int \mathrm{d}\boldsymbol{r}\; \chi_{i\nu}(\boldsymbol{r})\; \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) \quad \longleftrightarrow \quad \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) = \sum_{i\nu} \chi^*_{i\nu}(\boldsymbol{r})\hat{c}^\dagger_{i\nu\sigma}\,. \tag{1.8}$$

Using this basis, the Hamiltonian may be written in the lattice representation as (Hubbard, 1963; Hubbard, 1964*a*)

$$\hat{H} = \sum_{i\nu j\sigma} t^\nu_{ij}\, \hat{c}^\dagger_{i\nu\sigma}\; \hat{c}_{j\nu\sigma} + \frac{1}{2} \sum_{\nu\nu'\mu\mu'} \sum_{ijmn} \sum_{\sigma\sigma'} \mathcal{V}^{\nu\nu'\mu\mu'}_{ijmn}\; \hat{c}^\dagger_{i\nu\sigma}\; \hat{c}^\dagger_{j\nu'\sigma'}\; \hat{c}_{n\mu'\sigma'}\; \hat{c}_{m\mu\sigma}\,, \tag{1.9}$$

where the matrix elements are given by

$$t^\nu_{ij} = \int \mathrm{d}\boldsymbol{r}\; \chi^*_{i\nu}(\boldsymbol{r}) \left[-\frac{\hbar^2}{2m}\Delta + V^{ion}(\boldsymbol{r}) \right] \chi_{j\nu}(\boldsymbol{r}) \tag{1.10}$$

$$\mathcal{V}^{\nu\nu'\mu\mu'}_{ijmn} = \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\boldsymbol{r}'\; V^{ee}(\boldsymbol{r},\boldsymbol{r}')\, \chi^*_{i\nu}(\boldsymbol{r})\; \chi^*_{j\nu'}(\boldsymbol{r}')\; \chi_{n\mu'}(\boldsymbol{r}')\; \chi_{m\mu}(\boldsymbol{r})\,. \tag{1.11}$$

[5] In principle, we mean by "noninteracting" the absence of interaction between electrons. In practice, however, it is often necessary to assume that at least a long-range Hartree part of the interaction between the valence electrons is also included as a part of the kinetic energy and used for the definition of the Wannier orbitals (Gebhard, 1997) which then better justifies a very short-ranged form of the remaining explicit interaction. In any case, however, we want to assume that the external potential need not be determined self-consistently (which might affect conclusions about phenomena such as phase separation).