4.9.1 Mean-Field-Approximation for the description of the Coulomb-Coupling

For a two atoms containing molecule there is a quite simple and illustrative way to include Coulomb repulsion of the electrons without leaving the one electron approximation:

Each electron only "feels" the mean charge of all other electrons

This additional charge is added to the Hamiltonian (4.64). This can simply be interpreted as a shielding of the core charges. Since the efficiency of the shielding is not known a priory, this additional charge is used as a variable and calculated self consistently:

- We start with a Hamiltonian $H(\rho(x,y,z),...)$, including an arbitrary density distribution $\rho(x,y,z)$ of the electrons.
- For this Hamiltonian we determine the Eigenvector system ψ_i.
- Using this Eigenvector system we calculate the expectation value of the electron density

$$\rho'(x,y,z) = \sum_i |a_i|^2 \langle \psi_i | e | \psi_i \rangle \tag{4.81}$$

- Self consistent solution means $\rho'(x,y,z) = \rho(x,y,z)$, i.e. we have to change the electron density until this condition is fulfilled.

This method can be generalized for solids; e.g. in the LDA (Local Density Approximation) a variational function $\varrho(x,y,z)$ for the mean electron density at each position of the solid is calculated self consistently for the whole solid. Using this approach even magnetic ordering is described by defining two different spin dependent variational functions $\varrho_\sigma(x,y,z)$). This allows to calculate magnetic moments and its expectation values. This self consistent "mean field" approach is often used in solid state theory to calculate approximations.
The "mean field" method correctly describes the Coulomb coupling of electrons; but it is a poor description for properties which are directly coupled to the Pauli principle since one electron (handled as an operator) only "sees" the mean effect of other electrons (handled as a number). This suppresses the quantum mechanical character of the electron-electron-interaction at least partly.
For high temperature superconductors the mean field approach does not sufficiently take into account the strong spin-spin interaction due to the Pauli-Principle which only can be described by more complicating solutions like in Eq. ((4.80). The explicit calculation gets extremely complicating since two opposing tendencies exist in these materials:

1. The periodic lattice and a quite large overlap integral would "prefer" free electron like solutions, i.e. k-dependent energy bands.
2. The Pauli exclusion principle and the strong coulomb interaction suppress the hopping of electrons through the solid and thus prefer localized states.