tations are listed in App. A.1. While most of these extensions are beyond the scope of this thesis, the multi-band model (A.5) will be central to chapter 5.

### 1.1.1 Solid State Theory for Crystals

The typical condensed matter system contains a macroscopic number (usually $10^{20}$ or more) of atomic nuclei and electrons.[1] In this situation, a complete description of a particular system for given initial conditions is not possible. In fact, it might not be desirable since the truly interesting information would be hidden in an extensive amount of details. It is the concept of *statistical physics* to abstract from some specific system and view it as a realization of an ensemble of systems which share only some important features like the atomic constitution exactly but are allowed to differ in others. Among the observations that can be made for such ensembles are not only those that pertain to each individual realization (like energy conservation), but also others that involve averages over the ensemble, over time, and/or over space (like density-density pair correlation functions).[2] All results of this work will apply to the thermodynamic limit of a *(grand) canonical ensemble* of unbounded systems with no net charge.

Neglecting intra-nuclear effects and the gravitational, "weak", and "strong" forces (which are extremely small on typical condensed matter length scales of $10^{-10}$ m to 1 m), we assume that condensed matter systems are composed of inert pointlike atomic nuclei and electrons which interact by the Coulomb $1/r$ potential (for a distance $r$) and have no internal degrees of freedom other than (possibly) spin. Although, in general, relativistic effects are important for the systems under consideration, they often contribute only a constant energy offset to the solid-state problem (e.g., for core states of heavy nuclei) or can be treated approximately in a nonrelativistic framework (e.g., spin-orbit coupling for valence electrons; see App. A.1). Thus, the usual starting point for condensed matter theory is *nonrelativistic quantum statistical mechanics* for charged electrons and ions with the Hamiltonian[3]

$$H = \sum_{i=1}^{N_e} \frac{\boldsymbol{p}_i^2}{2m} + \sum_{k=1}^{L} \frac{\boldsymbol{P}_k^2}{2M_k} + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} + \sum_{k<l} \frac{Z_k Z_l e^2}{|\boldsymbol{R}_k - \boldsymbol{R}_l|} - \sum_{i,k} \frac{Z_k e^2}{|\boldsymbol{r}_i - \boldsymbol{R}_k|} \tag{1.1}$$

Here, $\boldsymbol{r}_i$ ($\boldsymbol{R}_k$), $\boldsymbol{p}_i$ ($\boldsymbol{P}_i$), and $m$ ($M_k$) label the positions, momenta, and masses of electrons (ions), respectively; $e$ is the electronic charge, $N_e$ the total number of electrons, $L$ that of ions, and $Z_k$ the atomic number of the ion with index $k$. Charge neutrality requires that $N_e = \sum_k Z_k$. In the Gaussian system of units, $4\pi\varepsilon_0 = 1$ drops out of the expressions for the Coulomb energy.

[1] Exceptions to this rule are, e.g., mesoscopic systems where the physics may be dominated by finite-size effects like in the single-electron transistor.

[2] Note that for ergodic systems, the infinite-length limit of the time average by definition agrees with the ensemble average.

[3] The discussion of couplings to external electromagnetic fields is deferred to Sec. 4.2. We note at this point, however, that the assumption of instantaneous Coulomb interaction used here and in the following is exact within the Coulomb gauge.