

# I Physical and Computational Basics

## I.1 The electronic structure problem

In solid state physics, one general problem we are concerned with is finding the properties of the ground state of an isolated system of  $N$  interacting electrons in an external potential. The system is described by the Schrödinger equation

$$\hat{H}\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N) \quad (\text{I.1})$$

with the Hamiltonian

$$\hat{H} = \hat{T}_e + \hat{V}_{n-e} + \hat{V}_{e-e} + \hat{V}_{n-n} \quad (\text{I.2})$$

$$= -\sum_i \frac{1}{2} \nabla_i^2 - \sum_i \sum_{\alpha} \frac{Z_{\alpha}}{|\mathbf{r}_i - \mathbf{R}_{\alpha}|} + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2} \sum_{\alpha\beta} \frac{Z_{\alpha} Z_{\beta}}{R_{\alpha\beta}} \quad (\text{I.3})$$

where:

- $\hat{T}_e$  is the kinetic energy of the electrons
- $\hat{V}_{n-e}$  is the potential energy of the electrons in the field of the nuclei
- $\hat{V}_{e-e}$  is the Coulomb interaction between the electrons and
- $\hat{V}_{n-n}$  is the Coulomb interaction between the nuclei

The wavefunction  $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$

## I.2 Density Functional Theory

A direct solution to the electronic structure problem, this meaning obtaining the ground-state many-body wavefunction  $\Psi(\mathbf{r}_1, \dots, \mathbf{r}_N)$  for a given potential is analytically impossible even for a small number of electrons. As such, the need for good approximations to obtain results for real world systems is high. One particularly successful approach is *Density Functional Theory* (DFT).

### I.2.1 Hohenberg-Kohn theorems

The basis for DFT lies in the exact reformulation of the outlined electronic structure problem by Hohenberg and Kohn [1]. This reformulation uses the ground state density of the electronic system as the basic variable. [Missing]

Hohenberg-Kohn theorems:

- I The external potential (and by extension the ground state wave function and the ground state energy) are unique functionals of the ground state density (except for an additive constant).
- II The ground state energy minimizes the energy functional,

$$E[n(r)] > E_0 \quad \forall n(r) \neq n_0(r)$$

.

### **I.2.2 Kohn-Sham equations**

One way of approximating the functional  $F[n]$  was given by Kohn and Sham [2]. The idea is to use a non-interacting auxiliary system of electrons and introduce a correction potential.

## **I.3 Parallel computing**

The following section will give an overview of the technical aspects of running computer code (such as QUANTUM ESPRESSO) on massively parallel computing environments (such as the PHYSnet compute cluster). The information presented can be found in any textbook on parallel or high-performance computing [3].

### **I.3.1 On scalability**

In scientific computing, one can identify two distinct reasons to distribute workloads to multiple processors:

- The execution time on a single core is not sufficient. The definition of sufficient is dependent on the specific task and can range from "over lunch" to "multiple weeks"
- The memory requirements grow outside the capabilities of a single core

In order to judge how well a task can be parallelized, usually some sort of scalability metric is employed, for example:

- How fast can a problem be solved with  $N$  processors instead of one?
- What kind of bigger problem (finer resolution, more particles, etc.) can be solved with  $N$  processors?
- How much of the resources is used for solving the problem?

The speedup by using  $N$  workers to solve a problem instead of one is defined as  $S = \frac{T_1}{T_N}$ , where  $T_1$  is the execution time on a single processor and  $T_N$  is the execution time on  $N$  processors.