I Physical and Computational Basics

I.1 The Schrödinger Equation

$$\hat{H}\Psi(\mathbf{r_1}, \ldots, \mathbf{r_N}) = E\Psi(\mathbf{r_1}, \ldots, \mathbf{r_N}) \tag{I.1}$$

The Hamiltonian for an isolated system of N interacting electrons in an external potential, so the

I.2 Density Functional Theory

A direct solution to the electronic structure problem, this meaning obtaining the ground-state many-body wavefunction $\Psi(\mathbf{r_1}, \ldots, \mathbf{r_N})$ 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

I.2.2 Kohn-Sham equations

One way of approximating the functional $F[n]$ was given by Kohn and Sham [1]. The idea is to use a non-interacting auxiliary system of electrons and introduce a correction potential.