

I Physical and Computational Basics

I.1 The Schrödinger Equation

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

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

I.2.2 Kohn-Sham equations

The success of DFT