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Kurzzusammenfassung

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Conventions

Throughout the text of this thesis scalars are written in italic s, vectors in bold italic $\boldsymbol{v}$ and matrices in bold $\mathbf{M}$ fonts. The summation/multiplication over nearest neighbour sites i and j is $\langle ij \rangle$ as a subscript to $\sum/\prod$. Furthermore, Hartree atomic units are used in general and only in selected instances it is deviated from this: $\hbar = m_\mathrm{e} = \mathrm{e} = {}^{4\pi}/_{\varepsilon_0} = 1$.

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) Density Functional Theory

I.2.1 Hohenberg-Kohn theorems

I.2.2 Kohn-Sham equations

The success of DFT