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Kurzzusammenfassung

Danksagung

Motivation

Inhaltsverzeichnis

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 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

$$\hat{H}\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \tag{I.1}$$

with the Hamiltonian

$$\hat{H} = \hat{T}_e + \hat{V}_{n-e} + \hat{V}_{e-e} + \hat{V}_{n-n} \tag{I.2}$$

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

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
- $\hat{U}_{e-e}$ is the Coulomb interaction between the electrons and
- $\hat{W}_{n-n}$ is the Coulomb interaction between the nuclei

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

I.2 Density Functional Theory

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

The basis for DFT lies in the excact 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,

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

.

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 over technical aspects of running computer code (such as Quantum ESPRESSO)

Literatur

[1] P. Hohenberg und W. Kohn. „Inhomogeneous Electron Gas“. In: *Phys. Rev.* 136.3 (Nov. 1964). Publisher: American Physical Society, B864–B871. DOI: 10.1103/PhysRev.136.B864.

[2] W. Kohn und L. J. Sham. „Self-Consistent Equations Including Exchange and Correlation Effects“. In: *Phys. Rev.* 140.4 (Nov. 1965). Publisher: American Physical Society, A1133–A1138. DOI: 10.1103/PhysRev.140.A1133.