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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 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 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-perfomance computing [3].

I.3.1 On scalabilty

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 parallelized, usually some sort of scalabilty 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. In the ideal case, where all the work can be perfectly distributed among the processors, all processors need the same time for their respective workloads and don't have to wait for others processors to finish their workload to continue, the execution time on N processors would be $\frac{T_1}{N}$, so the speedup would be $S = \frac{T_1}{\frac{T_1}{N}} = N$.

In reality, there are many factors either limiting or in some cases accelerating parallel code execution. Limiting factors include:

- *Algorithmic limitations*:
- *Bottlenecks*:
- *Startup Overhead*:
- *Communication*:

On the other hand, faster parallel code execution can come from:

- *Better caching*: when the data the program is working with is distributed among processors,

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.

[3] G. Hager und G. Wellein. *Introduction to High Performance Computing for Scientists and Engineers*. 0. Aufl. CRC Press, 2. Juli 2010. ISBN: 978-1-4398-1193-1. DOI: 10.1201/EBK1439811924.