Chapter 2
Ab-Initio Calculations

Abstract Due to the difficulties found in the direct solution of the Schrödinger equation, different simplified approaches were proposed and are nowadays widely used. Among them, those most usually employed are the Hartree–Fock and the Density Functional Theory, which we revisit in the present chapter. The former makes use of nonstandard numerical approximations in order to calculate the wavefunction while circumventing the curse of dimensionality, whereas the latter involves the electronic density that is now defined in three dimensions but requires deeper analyses to retain the most relevant features present in the wavefunction description in a coarse 3D model.

Keywords Hartree-Fock · Hohenberg and Kohn Theorems · Density Functional Theory

2.1 The Hartree–Fock Description

2.1.1 The Orbital Model

The set of all the solutions to the one-electron Schrödinger equation reads as

$$\hat{\mathscr{H}}\ \phi_i = \hat{E}_i\ \phi_i, \tag{2.1}$$

where $\hat{\mathscr{H}}$ represents the one-electron Hamiltonian hermitian operator. The eigenfunctions ϕ_i, known as spatial orbitals, related to the eigenvalues $\hat{E}_i$ (energies), define a complete basis of the 3D space, such that any 3D function can be written as

$$f(\mathbf{r}) = \sum_{j=1}^{\infty} c_j\ \phi_j(\mathbf{r}), \tag{2.2}$$

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where $\mathbf{r}$ denotes the space coordinates, after eliminating the spin coordinate in expression (1.129), i.e., $\mathbf{r} = (x, y, z)$.

If we define the spin-orbitals $\varphi_j(\mathbf{x})$ as

$$\varphi_j(\mathbf{x}) = \phi_j(\mathbf{r}) \cdot \alpha(s), \tag{2.3}$$

or

$$\varphi_j(\mathbf{x}) = \phi_j(\mathbf{r}) \cdot \beta(s), \tag{2.4}$$

then the solution $\Psi(\mathbf{x}_1, \mathbf{x}_2)$ of the two-electrons Schrödinger equation could be approximated as follows: fixing the value of one of the coordinates, e.g., $\mathbf{x}_2$, and using the rationale just described, it results that

$$\Psi(\mathbf{x}_1; \mathbf{x}_2) = \sum_{j=1}^{\infty} c_j(\mathbf{x}_2)\, \varphi_j(\mathbf{x}_1), \tag{2.5}$$

and considering

$$c_j(\mathbf{x}_2) = \sum_{k=1}^{\infty} d_k^j\, \varphi_k(\mathbf{x}_2), \tag{2.6}$$

it ultimately results that

$$\Psi(\mathbf{x}_1, \mathbf{x}_2) = \sum_{j=1}^{\infty} \sum_{k=1}^{\infty} c_{jk}\, \varphi_j(\mathbf{x}_1) \cdot \varphi_k(\mathbf{x}_2), \tag{2.7}$$

where $c_{jk} = d_k^j$.

This expression can be generalized to the many-electrons distribution function.

2.1.2 Accounting for the Pauli Exclusion Principle

In order to ensure verification of the Pauli exclusion principle, we define the determinants

$$\Phi_k(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}) = \begin{vmatrix} \varphi_{m_1^k}(\mathbf{x}_1) & \cdots & \varphi_{m_1^k}(\mathbf{x}_{N_e}) \\ \vdots & \ddots & \vdots \\ \varphi_{m_{N_e}^k}(\mathbf{x}_1) & \cdots & \varphi_{m_{N_e}^k}(\mathbf{x}_{N_e}) \end{vmatrix}, \tag{2.8}$$

where k refers to a particular choice of the N_e indexes $m_1^k, \cdots, m_{N_e}^k$.

Thus, the multi-electronic wavefunction can be approximated as

$$\Psi(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}) = \sum_{k=1}^{\infty} D_k\, \Phi_k(\mathbf{x}_1, \cdots, \mathbf{x}_{N_e}). \tag{2.9}$$

A permutation in the label of two electrons implies the exchange of two columns of the different determinants involved in Eq. (2.9), and then a change of the sign in agreement with Pauli exclusion principle.

2.1.3 The Variational Principle

In order to compute the wavefunction approximate given by Eq. (2.9), we must prove the existence of a variational principle whose minimization will result in the desired wavefunction.

The eigenproblem related to the multi-electronic system reads as

$$\mathscr{H}\ \Psi = E\ \Psi, \tag{2.10}$$

which results in the eigenfunctions Ψ_i verifying the orthonormality condition

$$\int \overline{\Psi_i}\ \Psi_j\ d\mathbf{r} = \delta_{ij}, \tag{2.11}$$

where $d\mathbf{r} = d\mathbf{r}_1 \cdot d\mathbf{r}_2 \cdots d\mathbf{r}_{N_e}$. It is important to note that since the Hamiltonian is independent of the spin, the resulting eigenfunctions only depend on the space coordinates.

Although Ψ_i are and remain unknown, their formal properties ensure that they form a complete basis for the expression of any function. Thus, if we write

$$\Psi' = \sum_{j=1}^{\infty} B_j\ \Psi_j, \tag{2.12}$$

where B_j are arbitrary coefficients, then the associated energy (according to (Eq. 1.83)), results in

$$E' = \frac{\int \overline{\Psi'} \mathscr{H} \Psi' d\mathbf{r}}{\int \overline{\Psi'} \Psi' d\mathbf{r}}, \tag{2.13}$$

where the denominator accounts for the non-normality of Ψ'.

Introducing the approximation (2.12) into the expression (2.13) and taking into account Eq. (2.11), it results that

$$E' = \frac{\sum_{j=1}^{\infty} |B_j|^2 E_j}{\sum_{j=1}^{\infty} |B_j|^2}, \tag{2.14}$$

which subtracting the lowest energy E_1 (ground state), yields

$$(E' - E_1) = \frac{1}{\sum_{j=1}^{\infty} |B_j|^2} \sum_{j=1}^{\infty} |B_j|^2 \,(E_j - E_1) \geq 0, \tag{2.15}$$

implying that

$$E' \geq E_1, \tag{2.16}$$

which means that whatever function of N_e electronic coordinates one chooses, the mean value of the Hamiltonian operator is always greater than the lowest true energy of the associated Schrödinger equation, giving the procedure for finding numerical solutions. It suffices to minimize the Hamiltonian operator applied to the test wavefunction approximate as described in the next section.

2.1.4 A Direct Solution Procedure

If the expression of Ψ' is written as a linear combination of a finite number M of determinants, i.e.,

$$\Psi'(\mathbf{x}_1, \ldots, \mathbf{x}_{N_e}) = \sum_{j=1}^{M} D_j \;\Phi_j(\mathbf{x}_1, \ldots, \mathbf{x}_{N_e}), \tag{2.17}$$

then the associated energy results in

$$E' = \frac{\sum_{j=1}^{M} \sum_{k=1}^{M} \overline{D_j} D_k \int \overline{\Phi_j} \mathscr{H} \Phi_k d\mathbf{r}}{\sum_{j=1}^{M} \sum_{k=1}^{M} \overline{D_j} D_k \int \overline{\Phi_j} \Phi_k d\mathbf{r}}. \tag{2.18}$$

Introducing the notation

$$\begin{cases} H_{jk} = \int \overline{\Phi_j} \mathscr{H} \Phi_k \; d\mathbf{r} \\ S_{jk} = \int \overline{\Phi_j} \Phi_k \; d\mathbf{r} \end{cases}, \tag{2.19}$$

Equation (2.18) reads as

$$\left(\sum_{j=1}^{M} \sum_{k=1}^{M} \overline{D_j} D_k S_{jk} \right) E' = \sum_{j=1}^{M} \sum_{k=1}^{M} \overline{D_j} D_k H_{jk}, \tag{2.20}$$

whose minimization leads to

$$\left(\sum_{k=1}^{M} D_k S_{jk}\right) E = \sum_{k=1}^{M} D_k H_{jk}, \qquad \forall j, \tag{2.21}$$

which can be written in the matrix form

$$\begin{pmatrix} H_{11} & \dots & H_{1M} \\ \vdots & \ddots & \vdots \\ H_{M1} & \dots & H_{MM} \end{pmatrix} \begin{pmatrix} D_1 \\ \vdots \\ D_M \end{pmatrix} = E \begin{pmatrix} S_{11} & \dots & S_{1M} \\ \vdots & \ddots & \vdots \\ S_M & \dots & S_{MM} \end{pmatrix} \begin{pmatrix} D_1 \\ \vdots \\ D_M \end{pmatrix}, \tag{2.22}$$

or

$$\mathbf{H}\,\mathbf{D} = E\,\mathbf{S}\,\mathbf{D}. \tag{2.23}$$

The main difficulties in this numerical approach are as follows:

- How many determinants M should be considered in the expansion (2.12)?
- How to quantify the solution quality?
- What are the most appropriate spin-orbitals $\varphi_i(\mathbf{x})$ for performing the development?
- What are the best determinants to consider, that is, the best choices of indices m_i^k, $\forall k$?
- Despite the fact that coefficients H_{jk} and S_{jk} are known, in principle, because everything is known about the integrals, they still remain formidable technical problems, being integrals of $3N_e$ spatial variables. The integrals can be separated as a sum of products of integrals defined in the 3D spaces. However, the separated form of integrals H_{jk} requires the integration in 6D spaces, because of the electron-electron potential that appears in the Hamiltonian.

2.1.5 The Hartree–Fock Approach

As the general expansion (2.17) is computationally too expensive, one could try to capture the main features of the solution by assuming that this sum reduces to a single term. Of course, if one uses

$$\Psi'(\mathbf{x}_1, \dots, \mathbf{x}_{N_e}) = D\,\Phi(\mathbf{x}_1, \dots, \mathbf{x}_{N_e}), \tag{2.24}$$

there would be no chance of defining an acceptable solution, except by considering that the determinant $\Phi(\mathbf{x}_1, \dots, \mathbf{x}_{N_e})$ is defined from a set of separate unknown orbitals that should be computed from the minimization that the variational principle imposes. Thus, the Hartree–Fock approach considers the Hartree–Fock wavefunction $\Phi^{HF}(\mathbf{x}_1, \dots, \mathbf{x}_{N_e})$ defined from

$$\Phi^{HF}(\mathbf{x}_1, \ldots, \mathbf{x}_{N_e}) = \begin{vmatrix} \chi_{m_1}(\mathbf{x}_1) & \ldots & \chi_{m_1}(\mathbf{x}_{N_e}) \\ \vdots & \ddots & \vdots \\ \chi_{m_{N_e}}(\mathbf{x}_1) & \ldots & \chi_{m_{N_e}}(\mathbf{x}_{Ne}) \end{vmatrix}, \tag{2.25}$$

in which, as just indicated, orbitals χ_i are approximated from m spin-orbitals (previously introduced) according to

$$\chi_i(\mathbf{x}) = \sum_{r=1}^{m} C_{ri}\ \varphi_r(\mathbf{x}). \tag{2.26}$$

Coefficients C_{ri} are computed by using the variational formulation associated with the energy

$$E\left[\Phi^{HF}\right] = \frac{\int \overline{\Phi}^{HF}\,\mathscr{H}\,\Phi^{HF}\,d\mathbf{r}}{\int \overline{\Phi}^{HF}\,\Phi^{HF}\,d\mathbf{r}}, \tag{2.27}$$

where $E\left[\Phi^{HF}\right]$ indicates that the energy is a functional of the Hartree–Fock wavefunction, which could also be written as $E[\chi_i]$. The interested reader can refer to [1] for additional details on the calculation procedure.

2.1.6 Post-Hartree–Fock Methods

Note that Eq. (2.26) involves $N_e \cdot m$ unknown complex coefficients. Thus, the computational complexity scales in $N_e \cdot m$, that is, linearly with the dimension of the space (number of electrons N_e) or with the number m of functions used in the approximation of the orbitals χ_i. This scalability is characteristic of separated representations [2].

The main limitation of the Hartree–Fock method lies in the single-determinant expansion used in the approximation of the wavefunction solution of the multi-electronic Schrödinger equation. If the main features present in this solution cannot be expressed from a single-determinant expansion, the Hartree–Fock solution could be inaccurate.

To circumvent this crude approximation, different multi-determinant approaches have been proposed. Interested readers can refer to [3], as well as to the different chapters of the handbook on computational chemistry [4]. The simplest alternative consists in writing the solution as a linear combination of some Slater determinants, built by combining m orbitals, with $m > N_e$. These orbitals are assumed as being known (e.g., the orbitals related to the hydrogen atom) and the weights are searched to minimize the electronic energy. When the molecular orbitals are built from the Hartree–Fock solution (by employing the ground state and some excited eigenfunctions), the technique is known as the Configuration Interaction method (CI).

A more sophisticated technique consists in writing this multi-determinant approximation of the solution by using a number of molecular orbitals m (with $m > N_e$) that are assumed to be unknown. Thus, the minimization of the electronic energy leads to simultaneous computation of the molecular orbitals and the associated coefficients of this multi-determinant expansion. Obviously, each one of these unknown molecular orbitals is expressed in an appropriate functional basis (e.g., Gaussian functions, ...). This strategy is known as a Multi-Configuration Self-Consistent Field (MCSCF).

All of the just-mentioned strategies (and others like the coupled cluster or the Moller–Plesset perturbation methods) belong to the family of wavefunction-based methods. They can only be used to solve quantum systems composed of a moderate number of electrons, because the number of terms involved in the determinants scales with the factorial of the number of electrons, i.e., with $N_e!$ (the factorial of N_e).

2.2 Density Functional Theory

Solid physics deals with multi-electron systems implying billions of particles, not just dozens as in molecular theories. This means that methods based on electron density are much more widely used. The constant efforts to develop such methods have been rewarded by a series of amazing theorems showing that it is possible to obtain the exact electron density without using the wavefunction.

Density functional theory–DFT–is based on two major results, the so-called Hohenberg and Kohn theorems.

2.2.1 *The First Hohenberg and Kohn Theorem*

The first Hohenberg and Kohn theorem states that the electronic density uniquely determines the external potential, the one created by the nuclei.

We start by defining the electronic density in the context of the single-determinant approach (which implies operating with space-spin coordinates)

$$\rho(\mathbf{r}) = N_e \int \overline{\Phi}(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_{N_e}) \Phi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_{N_e})\, d\mathbf{r}_2 \ldots d\mathbf{r}_{N_e}, \tag{2.28}$$

or

$$\rho(\mathbf{r}) = N_e \int |\Psi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_{N_e})|^2\, d\mathbf{r}_2 \ldots d\mathbf{r}_{N_e}. \tag{2.29}$$

We assume the following Hamiltonian partition:

$$\mathscr{H} = \mathscr{T} + \mathscr{V} + \mathscr{G}, \tag{2.30}$$

where $\mathscr{T}$ represents the kinetic energy operator, $\mathscr{V}$ the external potential operator (the one created by the nuclei) and $\mathscr{G}$ the inter-electron repulsions potential.

In order to prove that the electronic density uniquely determines the external potential, we assume that two different external potentials correspond to the same electronic density. This fact implies different Hamiltonians that only differ due to the difference in the external potentials because the kinetic energy part and the one corresponding to the inter-electron interactions are the same as soon as the number of electrons is the same. We denote the two different external potentials by $\mathscr{V}$ and $\mathscr{V}'$, and their corresponding Hamiltonians by $\mathscr{H}$ and $\mathscr{H}'$, respectively. As the Hamiltonian determines the wavefunction, these will be denoted by Ψ and Ψ'.

Now, the variational principle introduced in Sect. 2.1.3 states

$$\begin{cases} \int \overline{\Psi'} \mathscr{H} \Psi' \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} > E \\ \int \overline{\Psi} \mathscr{H}' \Psi \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} > E' \end{cases}, \tag{2.31}$$

with

$$\begin{cases} E = \int \overline{\Psi} \mathscr{H} \Psi \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} \\ E' = \int \overline{\Psi'} \mathscr{H}' \Psi' \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} \end{cases}. \tag{2.32}$$

Thus, considering the first expression in Eq. (2.31), it results that

$$\begin{gathered} E < \int \overline{\Psi'} \mathscr{H} \Psi' \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = \\ \int \overline{\Psi'} \mathscr{H}' \Psi' \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} + \int \overline{\Psi'} (\mathscr{H} - \mathscr{H}') \Psi' \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = \\ E' + \int \overline{\Psi'} (\mathscr{V} - \mathscr{V}') \Psi' \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = E' + \int (v(\mathbf{r}) - v'(\mathbf{r})) \rho(\mathbf{r}) \, d\mathbf{r}, \end{gathered} \tag{2.33}$$

where $v(\mathbf{r})$ refers to the one-electron potential (see Sect. 1.9).

Now, applying the same rationale to the second expression in Eq. (2.31), we obtain

$$\begin{gathered} E' < \int \overline{\Psi} \mathscr{H}' \Psi \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = \\ \int \overline{\Psi} \mathscr{H} \Psi \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} + \int \overline{\Psi} (\mathscr{H}' - \mathscr{H}) \Psi \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = \\ E + \int \overline{\Psi} (\mathscr{V}' - \mathscr{V}) \Psi \, d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = \\ E + \int (v'(\mathbf{r}) - v(\mathbf{r})) \rho(\mathbf{r}) \, d\mathbf{r} = E - \int (v(\mathbf{r}) - v'(\mathbf{r})) \rho(\mathbf{r}) \, d\mathbf{r}. \end{gathered} \tag{2.34}$$

By adding Eqs. (2.33) and (2.34), it results that

$$E' + E < E' + E, \tag{2.35}$$

from which we conclude that $\mathscr{V}' = \mathscr{V}$ and $\mathscr{H}' = \mathscr{H}$. Since the wavefunction depends on the Hamiltonian, we can affirm that the wavefunction is uniquely determined by the electron density, and consequently $\Psi' = \Psi$.

2.2.2 The Second Hohenberg and Kohn Theorem

Now, in order to determine the electronic density, the second Hohenberg and Kohn theorem establishes a variational principle whose minimization results in the desired electronic distribution.

From a given electronic density $\rho'(\mathbf{r})$, we can write

$$E' = \int \overline{\Psi'} \mathscr{H} \Psi' d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = W[\rho'(\mathbf{r})]. \tag{2.36}$$

The variational principle introduced in Sect. 2.1.3 implies that

$$E' = W[\rho'(\mathbf{r})] \geq E = \int \overline{\Psi} \mathscr{H} \Psi d\mathbf{r}_1 \cdots d\mathbf{r}_{N_e} = W[\rho(\mathbf{r})], \tag{2.37}$$

with $\mathscr{H}\Psi = E\Psi$, which establishes the desired result

$$\begin{cases} W[\rho'(\mathbf{r})] \geq W[\rho(\mathbf{r})] \\ \int \rho'(\mathbf{r}) d\mathbf{r} = N_e \end{cases}. \tag{2.38}$$

2.2.3 The Hohn–Sham Equations

In the density functional theory, two conceptual difficulties remain:

- How to quantify the electron's kinetic energy solely with the knowledge of their distributions in space?
- What is the role of antisymmetry (Pauli exclusion principle) requirements in the electron density function?

We start by approximating the unknown function, the trial density, within a single-determinant approach

$$\rho(\mathbf{r}) = N_e \int \overline{\Phi}(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_{N_e}) \Phi(\mathbf{x}, \mathbf{x}_2, \ldots, \mathbf{x}_{N_e})\, d\mathbf{r}_2 \ldots d\mathbf{r}_{N_e}, \tag{2.39}$$

where the determinant Φ involves the unknown orthonormal spin-orbitals $\chi_i(\mathbf{x}_i)$, an approximation that is in agreement with the Pauli exclusion principle and that verifies the N_e-representability

$$\int \rho(\mathbf{r})d\mathbf{r} = N_e. \tag{2.40}$$

The total energy $W[\rho(\mathbf{r})]$ can be decomposed into three contributions, one related to the kinetic energy $T[\rho(\mathbf{r})]$, one that considers the external potential (electron-nuclei interactions) $V[\rho(\mathbf{r})]$ and finally one representing the electron-electron interactions $J[\rho(\mathbf{r})]$, with the last two contributions reading as

$$V[\rho(\mathbf{r})] = \int v(\mathbf{r})\rho(\mathbf{r})d\mathbf{r}, \tag{2.41}$$

and

$$J[\rho(\mathbf{r})] = \int \rho(\mathbf{r}_1)\frac{1}{||\mathbf{r}_1 - \mathbf{r}_2||}\rho(\mathbf{r}_2)d\mathbf{r}_1 d\mathbf{r}_2. \tag{2.42}$$

For the kinetic energy, we assume an initial contribution $\hat{T}$ by assuming non-interacting electrons

$$\hat{T}[\rho(\mathbf{r})] = \sum_{i=1}^{N_e} \int \overline{\chi_i} \left(\frac{1}{2}\nabla^2\right) \chi_i \, d\mathbf{r}_i, \tag{2.43}$$

where χ_i are the orbitals considered in the expression of the determinant Φ.

The remaining contribution to the kinetic energy and the non-Coulomb effects are grouped in the exchange-correlation-residual-kinetic energy $E_{XCKE}[\rho(\mathbf{r})]$. The main difficulty concerns the expression of the exchange-correlation-kinetic-residual energy that is not known. In general, this term is obtained through a combination of heuristic arguments, because more accurate techniques exploiting the self-consistency are too expensive to be used.

Now, the solution procedure consists of the following steps

- Associate a variation in the density with linearly independent variations in χ_i and $\overline{\chi}_i$;
- Generate the form of the variations of each functional involving χ_i and $\overline{\chi_i}$: $\hat{T}$, V, J and E_{XCKE};
- Add a Lagrange multiplier to enforce the N_e-representability;
- Enforce optimality conditions of the variational principle.

The interested reader can refer to [1] for additional details on the calculation procedure.

2.3 Concluding Remarks on the Quantum Scale

After this brief analysis of the quantum scale, we reach the following conclusions:

- Schrödinger formalism represents the finest contemporary level of description. In the formalism introduced here, there is no mention in the Hamiltonian of spin-dependent magnetic interactions. These effects, as well as the relativistic ones, taken into account in Dirac's equation, are neglected. The consideration of very heavy nuclei requires the introduction of such relativistic effects.
- The wavefunction involved in the Schrödinger equation is spatially continuous, and its evolution is governed by a PDE.
- The Schrödinger equation is defined in a multidimensional space leading to the curse of dimensionality issues. It has been solved exactly for systems containing a reduced number of electrons.
- The ab-initio approximations, density functional and Hartree–Fock theories just summarized seem sometimes to be crude, but they are the only valuable route for addressing multi-electronic systems.
- The solution of the Schrödinger equation could provide an excellent description of the world at the nanometric scale, as well as accurate interatomic potentials to be used in molecular dynamics simulations.
- There are some quantum systems in which the solution explores the whole multi-dimensional configuration space, and thus remain almost intractable despite all the possible advances in the computational performances.

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