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Introduction

The theoretical study of atomic nuclei provides a bridge between nuclear physics and nuclear engineering. Starting from a framework consistent with quantum mechanics, the strong interaction, and its underlying symmetries, modern nuclear theory aims to construct models characterized by a limited number of free parameters and capable of predicting both nuclear structure and reactions across a wide range of systems. While experimental data have long provided invaluable insight into nuclear properties and processes, only a coherent theoretical description allows for systematic extrapolations toward regions of the nuclear chart or physical conditions that remain beyond current experimental reach, thus playing an essential role in applications relevant to nuclear engineering.

In particular, nuclear fission, despite its massive importance in nuclear engineering, remains only partially understood from a microscopic standpoint. Current models that use empirical approaches [59, 61], successfully reproduce global quantities like fission barrier heights, fragment mass distributions, and average neutron multiplicities for well studied nuclei. However, these models may rely on a huge number of parameters, which limit their predictive power when extrapolated to systems which are less investigated experimentally. A fully microscopic understanding of the collective dynamics leading from the compound nucleus to scission, the treatment of quantum many-body correlations [76], and the description of fragment excitation and emission remain among the major open challenges, particularly relevant for the simulation of next-generation reactors, which require the accurate description of nuclei and fuel materials – far less explored than those employed in traditional thermal systems – to be correctly predicted.

In this regard, the approach to the microscopic description of nuclei, is the one of the many-body theory, which starting from the interacting nucleons, aims at building a complete description of the nucleus. The use of phenomenological potentials based on the Woods-Saxon one is still relevant, thanks to its computational feasibility and its capability to include shell effects in a simple manner, but it cannot account for many-body effects. At the moment, there are two competing frameworks that try to tackle the microscopic description of nuclei,

i the *ab-initio* approach [41], where the interaction is in principle exact, derived from controlled approximations of quantum chromodynamics; and

ii the use of effective interactions and nuclear Density Functional Theory[3, 27].

Ab-initio methods, while technically speaking more rigorous, are still limited as of now, since they can only account for light nuclei or medium-heavy nuclei that can be considered as spherical. Energy density functionals and effective interactions, such as the Skyrme force, on the other hand are more flexible and less computationally expensive, enabling a much wider representation of nuclei across the whole chart, including heavy nuclei and processes such as fission, fusion, reactions and decays, which are of crucial importance in nuclear engineering.

D Vautherin and D M Brink laid the foundations of the nuclear Hartree-Fock theory using the Skyrme interaction in 1972 [88], through spherically symmetric calculations, which are unable to account for nuclear deformations, essential for nuclei far from magic numbers. Over the years, thanks to the increase in computational performance of modern hardware, codes that are able to represent more coordinates have been written, mainly using basis expansions on the harmonic oscillator [56, 77], which have the downside of not being able to account for near drip line nuclei, due to the different asymptotic behavior of the Gaussian basis in the harmonic oscillator and quasi-resonant states.

In the past twenty years, the use of Cartesian meshes to better account for such extremal cases has been introduced [14, 24, 58, 73], often times assuming certain approximations, such as plane reflection symmetries [72] and axial symmetry [58]. The use of fully unconstrained Hartree-Fock methods, of critical importance for exotic deformations, is still a novel endeavour that only a handful of implementations have tackled, due to the high computational cost.

The aim of this work is to explore a new computational approach, the Generalised Conjugate Gradient method, to efficiently solve spatially unconstrained Skyrme functionals. This thesis is organised as follows:

- In chapter 1, a short, comprehensive introduction to nuclear physics and its open problems is given, as to prime the reader on the essential physical properties of atomic nuclei, starting from phenomenological facts and empirical models. A formal description of nuclear deformations and fission is also given, to highlight the importance of symmetry breaking.
- In chapter 2, the motivations and objectives of this work are presented, along with a summary of the methods used to achieve them.

- In chapter 3, the theoretical framework used in the present work is reviewed, by introducing aspects of Hartree-Fock theory, Density Functional Theory and the effective interaction used in this work.
- In chapter 4, the numerical methods used in this work are presented, along with actual implementations in writing the code.
- In chapter 5, results for the spherically symmetric case are presented as a way of benchmarking the new implementation of this thesis, along with a description of the main physical quantities we compare.
- In chapter 6, benchmarks for the deformed nucleus ^{24}Mg are shown, after which novel results regarding... are presented.

1 | Nuclear structure and deformations

In this chapter, a concise introduction to nuclear structure physics is provided, as a way to understand the essential physical quantities, terminology, and phenomenology of atomic nuclei to then have the necessary background to tackle nuclear deformations within the microscopic framework in later sections. The reader may refer to introductory textbooks on nuclear physics, such as ref. [9, 63] for a more in-depth treatment of the subject and ref. [69] for a focus on many-body theory.

This chapter is organised as follows, first, in section 1.1, we will review the main empirical facts about nuclides, such as particle density distribution, binding energies and phenomenological models employed to describe them. Moving on to more advanced topics, that are able to complete the general description of nuclear structure, which are nuclear pairing in section 1.2 and nuclear deformations in section 1.3. Lastly, in section 1.4, we will review the nuclear fission process, derive a simple model to describe it, and discuss the importance of deformations to accurately describe it.

1.1. Nuclear structure models

The study of low energy hadron physics, has always been a challenging task. This is due to the known fact that the strong force, which is responsible for the interaction between nucleons, is not perturbative at low energies, as opposed to the atomic case for the Coulomb interaction, whose coupling can be assumed as constant at low energies, while the one for the strong interaction cannot. Nevertheless, both problems have in common the fact that they are related to many-body theory, thanks to which they share some challenges and the corresponding solutions, when present.

1.1.1. Phenomenology of the NN interaction

It is possible to obtain a good insight on nuclear structure, by using empirical data obtained experimentally on the bulk properties of nuclei, such as the binding energy and the particle density.

Binding energies

Let us start with the binding energy. We can define it as the mass defect of the nucleus with respect to the constituents – protons and neutrons – isolated from each other. If Z is the number of protons, N the number of neutrons, and $A = N + Z$ the nuclear mass, then the binding energy E_B is given by

$$E_B = (Zm_p + Nm_n - M)c^2, \quad (1.1)$$

where m_p is the proton mass, m_n the neutron mass, and M the nucleus mass.

In figure 1.1, the binding energy per nucleon E_B/A as a function of A is presented. As shown in the figure, the binding energy per nucleon rapidly saturates and stalls around 7 MeV just after $A = 4$, this striking behaviour is due to nucleons interacting only with near neighbours, since the strong force is a short-range interaction. Otherwise, the trend would follow a behaviour similar to $\sim (A-1)$ as in the Coulomb interaction case, meaning the binding energy per nucleon would be linear with the mass number.

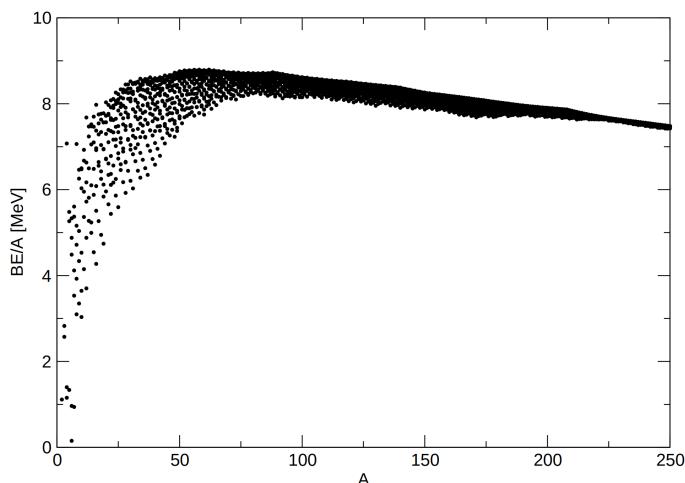


Figure 1.1: Binding energy per nucleon as a function of A . Due to the short range of the strong force, this value saturates around 7 MeV, with a steady, dim decrease after ^{56}Fe . Figure taken from [27].

Nuclear density

An important aspect of nuclear phenomenology that can be accessed experimentally is the nuclear density, most notably through elastic electron-nucleus scattering [42]. The measured form factor can be related to the Fourier transform of the charge density, from which the spatial distribution is reconstructed. The resulting densities are well reproduced by a Fermi-like distribution of the form

$$\rho(r) = \frac{\rho_0}{1 + e^{(r-R_0)/a}}, \quad (1.2)$$

where R_0 is the nuclear radius, which can be parametrized as $R_0 \approx 1.2A^{1/3}$, and a is the diffusivity, whose value determines how sharp the density drops from its saturation value $\approx \rho_0$ to ≈ 0 . The saturation density ρ_0 is generally universal for all nuclei, amounting to $\approx 0.16 \text{ fm}^{-3}$.

1.1.2. Structure models

The theoretical description of nuclear structure has been proven to be a difficult task over the years. Due to the extremely rich phenomenology of nuclei and the challenges brought by the strong force, as we shall see, many models and further approximations to give a satisfactory description of all nuclides have been proposed.

Liquid drop model

One, if not the first successful model, is the liquid drop model. It is based on the assumption that the nucleus behaves as a liquid droplet, where forces among constituents saturate. This hypothesis, formulated by G. Gamow, culminated in the formalization of the semi-empirical mass formula (SEMF) by N Bohr and C F von Weizsäcker in 1935 [89], which reads

$$E_B = a_V A - a_S A^{2/3} - a_C \frac{Z(Z-1)}{A^{1/3}} - a_A \frac{(N-Z)^2}{A} + \delta_P \quad (1.3)$$

where E_B is the binding energy of the nucleus. Each term has a different physical meaning:

- $a_V A$ is the volume energy of the nucleus, given by the approximately constant binding energy per nucleon, which makes the total energy proportional to A ;
- $a_S A^{2/3}$ is the surface energy, a correction to the volume energy due to outer nucleons interacting with fewer nucleons than those in the inner bulk, meaning that a_S is of the same order of a_V ;
- $a_C Z(Z-1)/A^{1/3}$ is the approximation to the Coulomb energy repulsion of the

nucleus, assuming the protons are uniformly distributed;

- $a_A(N - Z)^2/A$ is the asymmetry energy, which is due to the Pauli exclusion principle, since protons and neutrons occupy their respective states, a high imbalance of one species or the other implies loosely bound nucleons, thus a higher energy contribution of those states; and
- $\delta_P = a_P A^{-1/2}$ refers to the pairing contribution, due to the increase in binding energy of an even number of neutrons and/or protons, more details on the pairing energy are given in section 1.2.

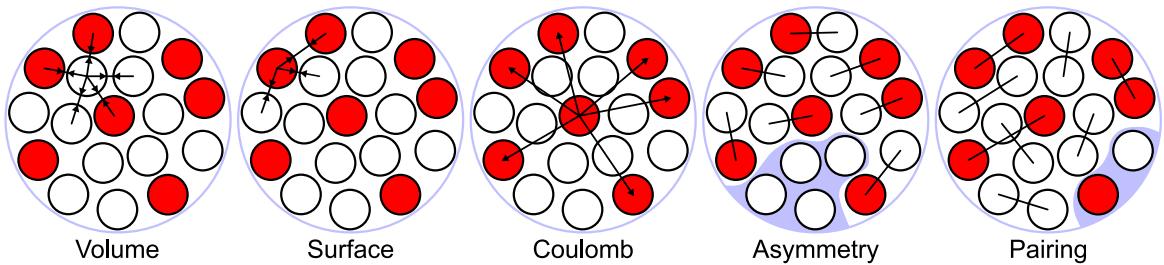


Figure 1.2: Visual representation of the liquid drop model. Figure taken from [35].

The SEMF can be fitted on experimental data to get a good estimate of binding energies [6], but it still lacks the ability of describing many aspects of nuclear structure, mainly, the nuclear shell structure, which can account for magic numbers and nuclear deformations.

An example of the SEMF parametrization is given in table 1.1, values are taken from [70].

Coefficient	a_V	a_S	a_C	a_A	a_P
Value [MeV]	15.8	17.8	0.711	23.7	11.2

Table 1.1: A typical parametrization of the coefficients in the SEMF (1.3). Values from [70].

Shell corrections

The liquid drop model, while being a good approximation for the description of the nuclear binding energy, it only accounts for the Pauli exclusion principle and the saturation of the strong force, providing only a partial description of the full quantum mechanical nature of the nucleus, thus the need to account for shell effects. Unfortunately, unlike the ‘atomic’

case, there is no single source of the field to which nucleons are subject to, since it's generated by the nucleons themselves; nonetheless, the formulation of an empirical mean-field potential which reproduces experimental data has been proven to be successful in providing useful corrections.

The so called Woods-Saxon potential is an empirical field used for modelling the average field to which an independent nucleon would feel in a nucleus. It is formulated as to follow the shape of the nuclear density (1.2), and it reads

$$U(\mathbf{r}) = -\frac{U_0(A, N)}{1 + e^{\frac{r-R}{a}}}, \quad (1.4)$$

where U_0 is the potential depth

$$U_0(A, N) = U_0 \left(1 \pm \kappa \frac{2N - A}{A} \right), \quad (1.5)$$

and the $+$ and $-$ signs refer to protons and neutrons respectively. R refers to the radius of the nuclear surface, parametrized as

$$R = r_0 A^{1/3} \quad (1.6)$$

and a is the surface diffuseness, as in the density expression (1.2).

Spin-orbit coupling The success of the shell model is mainly due to the possibility of accounting for spin-orbit coupling, which is included through a term that reads

$$U_{LS}(\mathbf{r}) = U_0^{LS} \left(\frac{r_0}{\hbar} \right)^2 \frac{1}{r} \frac{d}{dr} \left(\frac{1}{1 + e^{\frac{r-R}{a}}} \right). \quad (1.7)$$

A typical parametrization of the values in the Woods-Saxon potential and the spin-orbit term is given in table 1.2, values are taken from [79].

U_0 [MeV]	κ	r_0 [fm]	a [fm]	U_0^{LS} [MeV·fm ²]
52.1	0.639	1.260	0.662	22.0

Table 1.2: Typical Woods-Saxon potential parameters. Values from [79].

As shown in table 1.2, the spin-orbit coupling strength is high, compared to the atomic case, this causes a bigger splitting of the energy levels, leading to the formation of stable closed shells when the magic numbers 8, 20, 28, ... are reached, as shown in figure 1.3.

Coulomb interaction In the spherical case, the coulomb interaction can be taken as the energy potential produced by a sphere of charge Z and radius R , which reads

$$U_C(r) = Ze^2 \begin{cases} \frac{3-(r/R)^2}{2R} & r \leq R, \\ \frac{1}{r} & r > R. \end{cases} \quad (1.8)$$

The complete Hamiltonian then reads

$$\hat{H} = \hat{T} + U + U_{\text{LS}} + U_C, \quad (1.9)$$

where U_C is present only when solving for the proton shells. The solution to the eigenvalue problem $\hat{H}\psi = E\psi$ is of the form

$$\psi_{nljm_j} = \frac{u_{nl}(r)}{r} [Y_{nl}(\hat{\mathbf{r}}) \otimes \chi_{1/2}]_{jm_j} \quad (1.10)$$

where $Y_{nl}(\hat{\mathbf{r}})$ is the spherical harmonic function of degree l and order m , the $\hat{\mathbf{r}}$ notation is used to denote dependence on the azimuthal and polar angles of \mathbf{r} , the symbol \otimes takes the meaning of the angular momentum coupling with the spinor $\chi_{1/2}$, and $u_{nl}(r)$ satisfies the reduced Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + \frac{\hbar l(l+1)}{2mr^2} + U(r) \right) u_{nl} = Eu_{nl}. \quad (1.11)$$

The effect of the spin-orbit coupling U_{LS} and the Coulomb repulsion U_C could be accounted for by using first order perturbation theory.

Harmonic oscillator

A small digression on the harmonic oscillator is in order. The solution of the spherical potential

$$U_{\text{HO}}(\mathbf{r}) = \frac{1}{2}m\omega^2 r^2, \quad (1.12)$$

produces the spherical harmonic oscillator basis, which is very similar to the basis one would get solving for the Woods-Saxon potential, provided that ω is taken as $41/A^{1/3}$ MeV. As a matter of fact, the harmonic oscillator basis is often used to perform calculations in nuclear physics. We will see in section 4.3 that a harmonic oscillator basis is used as starting guess for the numerical solution of a Woods-Saxon potential.

Shell structure

A graphical representation of the shells for a harmonic oscillator is shown in figure 1.3, where the contribution of the spin-orbit coupling is also accounted for; compared to the atomic case, shells whose total angular momentum is higher are lowered in energy, viceversa for lower total angular momentum, due to the sign of the spin-orbit coupling U_0^{LS} of $U_{\text{LS}}(\mathbf{r})$ in equation (1.7).

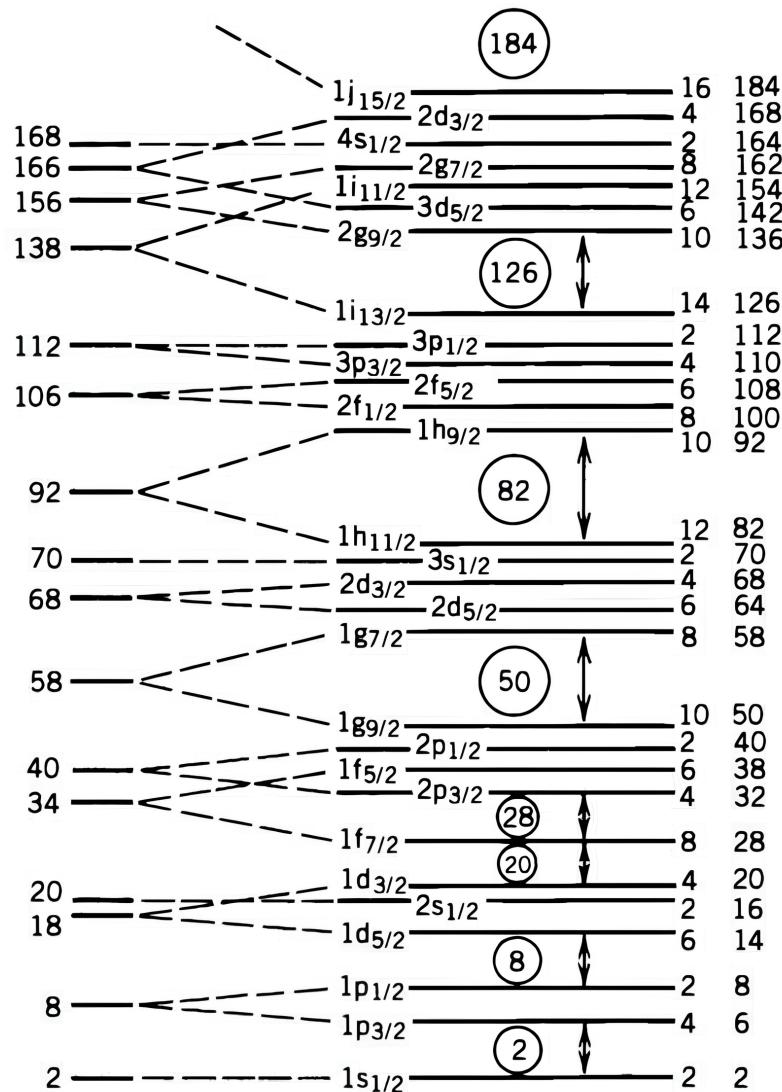


Figure 1.3: Graphical representation of a harmonic oscillator shells, together with the spin-orbit coupling. Shells whose total angular momentum is higher are lowered in energy, viceversa for lower total angular momentum. Figure adapted from [36].

1.2. Nuclear pairing

In the semi-empirical mass formula (1.3), the δ_p term can be parametrised as

$$\delta_p = \begin{cases} +\delta_0 & \text{if } N \text{ and } Z \text{ are even,} \\ 0 & \text{if } A \text{ is odd,} \\ -\delta_0 & \text{if } N \text{ and } Z \text{ are odd,} \end{cases} \quad (1.13)$$

hence having an even number of neutrons and/or protons increases the binding energy of the nucleus. A common choice for δ_0 is

$$\delta_0 = a_P A^{-1/2} \text{ MeV.}$$

A typical value for a_P is reported in table 1.1. This is a phenomena closely related to superconductivity, as nucleons of the same type form pairs that lie in higher energy states. An experimental evidence of this fact is known as odd-even staggering, where the separation energy

$$S_n = E_B(A+1, Z) - E_B(A, Z), \quad (1.14)$$

is higher for even A , an increase that corresponds to the energy necessary to break a pair. A graphical representation of the odd-even staggering for Sn isotopes is shown in figure 1.4. We will see in section 3.2 the two main methods to account for pairing at a microscopic level.

1.3. Nuclear deformations

If we were to observe the ratio between the first and second excited states energies of even-even nuclei, respectively $E(2^+)$ and $E(4^+)$, we would find that for nuclei where both N and Z are far from magic numbers, the ratio could be well approximated as

$$\frac{E(4^+)}{E(2^+)} \approx 3.33. \quad (1.15)$$

The ratio (1.15) can be explained by the collective rotation of the nucleus, when rotational symmetry is broken. Denoting by J the total angular momentum of this rotation, the quantized rotor energy reads

$$E_{\text{rot}} = \frac{\hbar^2}{2I} J(J+1), \quad (1.16)$$

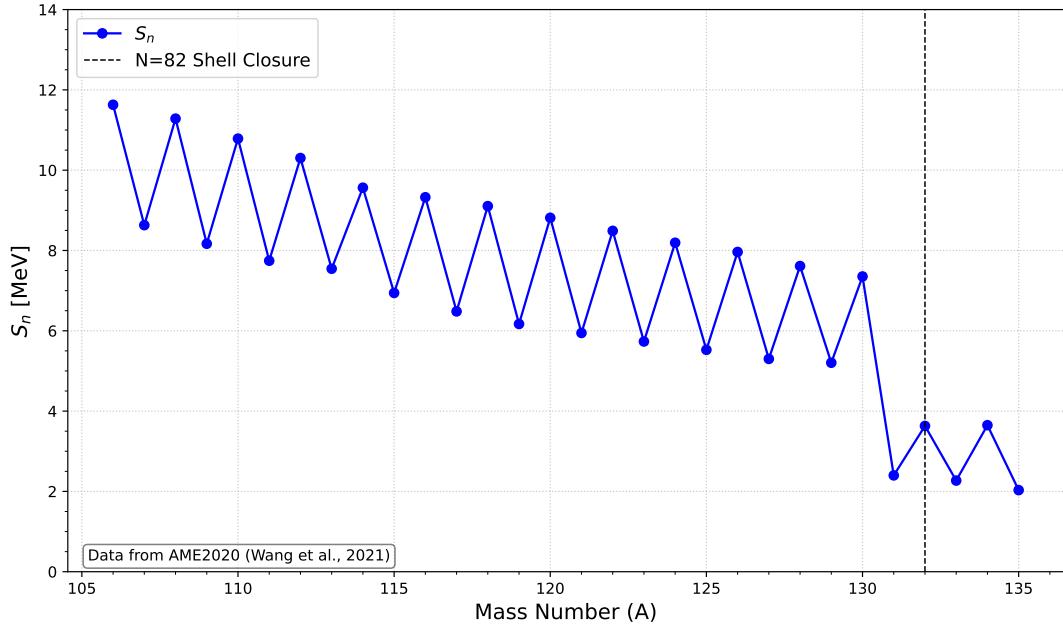


Figure 1.4: Odd-even staggering for Sn isotopes. Data taken from [1].

where \mathcal{I} is the nuclei's moment of inertia. Taking the ratio of equation (1.16) when $J = 4$ and $J = 2$, yields

$$\frac{20}{6} \approx 3.33. \quad (1.17)$$

Since there are many nuclei that display this property, it becomes obvious that nuclear deformations play a central role in the description of nuclear structure; as such, we shall now give a description of the nuclear shape in a formal framework. We will start by expanding the nuclear radius in terms of spherical harmonics and develop the case of an axial deformation. After that, we will briefly discuss the more general case of triaxial, octupole, and parity breaking configurations.

1.3.1. Quadrupole deformation

Let us suppose to consider variations of the nuclear radius R in terms of spherical harmonics

$$R(\theta, \phi) = R_0 \left[1 + \sum_{\lambda\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta, \phi) \right], \quad (1.18)$$

where the moments $\alpha_{\lambda\mu}$, defined as

$$\alpha_{\lambda\mu} = \int Y_{\lambda\mu}^*(\theta, \phi) R(\theta, \phi) d\Omega \quad (1.19)$$

are considered small, in the sense that $|\alpha_{\lambda\mu}|^2 \ll |\alpha_{\lambda\mu}|$, so that the volume of the system

$$V = \iint_0^{R(\theta,\phi)} R^2 dR d\Omega = \frac{4}{3}\pi R_0^3 \left[1 + \frac{3}{4\pi} \sum_{\lambda\mu} |\alpha_{\lambda\mu}|^2 \right] \quad (1.20)$$

is conserved. Since Y_{00} is constant, including it in the expansion changes the total volume (1.20), we then set $\alpha_{00} = 0$. If we consider only frames of reference where the nucleus has a center of mass fixed at the origin, we get vanishing $\alpha_{1\mu}$ coefficients.

Now, let us consider only $\alpha_{2\mu}$ coefficients and neglect higher order terms, so that the deformation is purely quadrupolar, then the radius reads

$$R(\theta, \phi) = R_0 \left[1 + \sum_{\mu=-2}^2 \alpha_{2\mu} Y_{2\mu}(\theta, \phi) \right]. \quad (1.21)$$

If we assume to be in the reference frame in which the inertia tensor, proportional to the coefficients $\alpha_{2\mu}$, is diagonal, which is called intrinsic frame, then the sum

$$\alpha_{21} Y_{21}^* + \alpha_{2-1} Y_{2-1}^*$$

vanishes. Since R is a real valued function, we have the relation

$$\alpha_{\lambda\mu} Y_{\lambda\mu} + \alpha_{\lambda-\mu} Y_{\lambda-\mu} = 2 \operatorname{Re}\{\alpha_{\lambda\mu} Y_{\lambda\mu}\}, \quad (1.22)$$

as a consequence, the resulting expansion reads

$$\begin{aligned} R(\theta, \phi) &= R_0 \left[1 + a_{20} Y_{20} + 2 \operatorname{Re}\{a_{22} Y_{22}\} \right] \\ &= R_0 \left[1 + \sqrt{\frac{5}{16\pi}} \left(a_{20}(3 \cos^2 \theta - 1) + 2a_{22}\sqrt{3} \sin^2 \theta (\cos^2 \phi - \sin^2 \phi) \right) \right]. \end{aligned} \quad (1.23)$$

If we perform the substitution

$$a_{20} = \beta \cos(\gamma) \quad (1.24)$$

$$a_{22} = \beta \sin(\gamma) \quad (1.25)$$

and express the variation of R along the cartesian axes, we get

$$R_x - R_0 = \delta R_x = \sqrt{\frac{5}{4\pi}} \beta R_0 \cos \left(\gamma - \frac{2\pi}{3} \right), \quad (1.26)$$

$$R_y - R_0 = \delta R_y = \sqrt{\frac{5}{4\pi}} \beta R_0 \cos \left(\gamma + \frac{2\pi}{3} \right), \quad (1.27)$$

$$R_z - R_0 = \delta R_z = \sqrt{\frac{5}{4\pi}} \beta R_0 \cos \gamma. \quad (1.28)$$

Assuming the value of β to always be positive, in the case $\gamma = 0$, $\delta R_x = \delta R_y < \delta R_z$, meaning the nucleus is in a *prolate* configuration; while in the case of $\gamma = \pi/3$, $\delta R_x = \delta R_y > \delta R_z$, meaning the nucleus has an *oblate* shape. A general convention is to write β with a negative sign in the oblate case, and a positive sign in the prolate case.

By using trigonometric identities, it is trivial to show that unique shapes are found only for $\gamma \in [0; \pi/3]$, if γ takes a value different from 0 or $\pi/3$, the shape is said to be triaxial, meaning $\delta R_z \neq \delta R_x \neq \delta R_y$, the nucleus has no more rotational symmetries and is only symmetric for reflections along the (x, y) , (x, z) and (y, z) planes, which also induces parity symmetry.

1.3.2. Nilsson model

To understand the effect on single-particle motion of a deformed potential, we can consider the case of an axially deformed harmonic oscillator potential, for which $\omega_z \neq \omega_x = \omega_y = \omega_{\perp}$, meaning the oscillator frequency takes on a different value on the z axis than in the x and y axes.

To treat the deformation perturbatively, we can assume that the various frequencies deviate from the unperturbed $\omega_0 = 41/A^{1/3}$ MeV, in which case they may read

$$\omega_z = \omega_0 - \frac{2}{3}\varepsilon, \quad (1.29)$$

$$\omega_{\perp} = \omega_0 + \frac{1}{3}\varepsilon, \quad (1.30)$$

this definition of the frequencies satisfies the conservation of volume, at lowest order in ε , assumed to hold for

$$\omega_0^3 = \omega_z \omega_{\perp}^2. \quad (1.31)$$

We can thus write the single-particle Hamiltonian in the deformed potential as

$$H = H_0 + \varepsilon H_1, \quad (1.32)$$

$$H_0 = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} m \omega_0^2 r^2, \quad (1.33)$$

$$\varepsilon H_1 = \frac{1}{3} \omega_0^2 \varepsilon (x^2 + y^2 - 2z^2) = -\frac{1}{3} \sqrt{\frac{16\pi}{5}} m \omega_0^2 \varepsilon r^2 Y_{20}. \quad (1.34)$$

H_0 is the usual spherical harmonic potential, for which the eigenfunctions, expressed through the usual quantum numbers $|nljm_j\rangle$ are known. Assuming ε to be small, we can evaluate the first order correction of H_1 to the system, which reads

$$\Delta E = \langle nljm_j | \varepsilon H_1 | nljm_j \rangle, \quad (1.35)$$

$$= -\frac{1}{3} \sqrt{\frac{16\pi}{5}} \varepsilon m \omega_0^2 \int r^2 u_{nl}(r) \langle jm_j | Y_{20} | jm_j \rangle dr, \quad (1.36)$$

$$= \frac{\varepsilon}{6} m \omega_0^2 \int r^2 u_{nl}(r) \frac{3m_j^2 - j(j+1)}{j(j+1)} dr, \quad (1.37)$$

thus in the limit of large j , states with the maximum total angular momentum projection m_j are shifted upwards, while states with the minimum m_j are shifted downwards; moreover, eigenstates with $\pm m_j$ are degenerate, as expected by the reflection symmetry of the Hamiltonian if the z axis is inverted.

Adding further empirical terms to reproduce experimental data, and the spin-orbit coupling, results in the formulation of the Nilsson model [60]. In figure 1.5, a graphical representation of the energy levels in the Nilsson model is shown [91].

Deformed Woods-Saxon

Recent studies of deformed nuclei have been carried out using empirical potentials such as deformed Woods-Saxon potentials [32, 44]. In these models, the nuclear shape is expanded as

$$R(\theta) = R_0 \left[1 + \sum_{\lambda}^L \beta_{\lambda} Y_{\lambda 0} \right], \quad (1.38)$$

so that the solution is axially symmetric and the problem is reduced to just the (r, θ) coordinates, in which we can write the potential as

$$U_{WS}(r, \theta) = -\frac{U_0(A, N)}{1 + e^{\frac{r-R(\theta)}{a}}}. \quad (1.39)$$

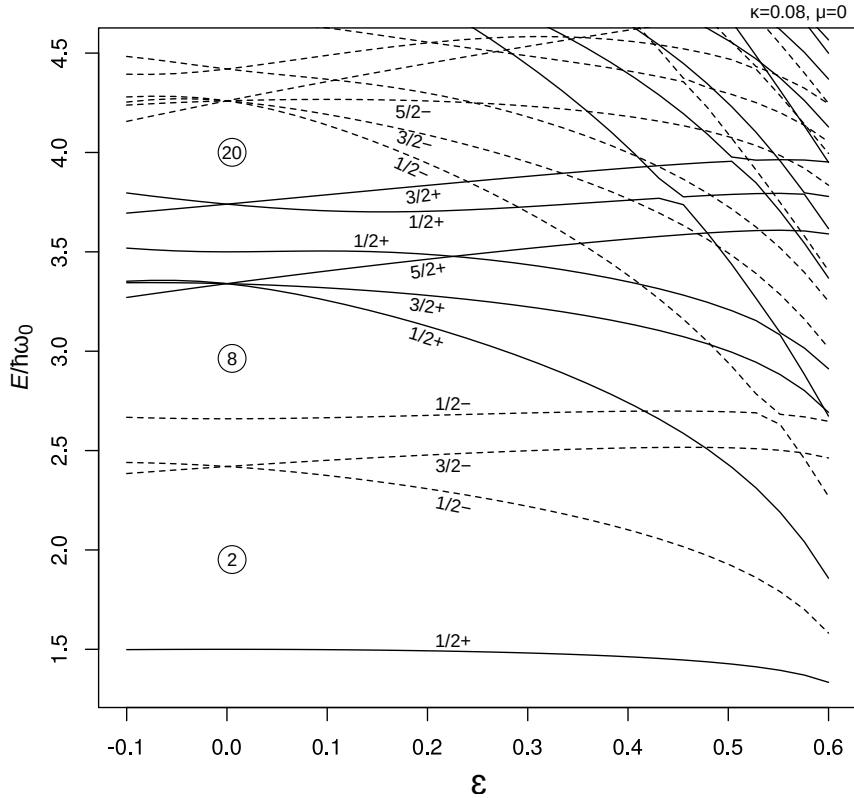


Figure 1.5: Nilsson model energy levels trends, as a function of ε . Figure taken from [91].

1.3.3. Octupole deformations and parity breaking

While quadrupole deformations concern nuclei across the whole chart, octupole deformations are much less common, being found in ground states only for heavier nuclei. The evidence for such deformations is mainly provided by the large electric octupole transition probability $B(E3)$, which reads

$$B(E3; 3^- \rightarrow 0^+) = \frac{1}{2J_i + 1} |\langle 0^+ | e r^3 \hat{Q}_3 | 3^- \rangle|^2, \quad (1.40)$$

where J_i is the initial total angular momentum of the nucleus and \hat{Q}_3 is the octupole operator defined as

$$\hat{Q}_3 = r^3 Y_{30}(\hat{r}). \quad (1.41)$$

Evidence of such strong coupling was initially found in neutron-rich Barium isotopes, ^{144}Ba [17] and ^{146}Ba [18], and a while later in Radium isotopes [20] and other heavy nuclei as well [19].

Expansions on spherical harmonics, under the parity operation $\mathcal{P} : \mathbf{r} \mapsto -\mathbf{r}$, transform as

$$\mathcal{P}\alpha_{\lambda\mu} = (-1)^\lambda \alpha_{\lambda\mu}, \quad (1.42)$$

hence a nuclear octupole deformation, whose order $\lambda = 3$, would break the parity symmetry of the mean-field. In figure 1.6 a graphical representation of the spherical harmonics for $\lambda = 3$ and $\mu = 0, 2$ is shown.



Figure 1.6: Graphical representation of possible octupole deformations. On the left, the axially symmetric Y_{30} deformation, on the right, the non-axial octupole deformation Y_{32} .

1.4. Nuclear fission

Nuclear fission is the process by which a nucleus splits into two – sometimes three – nuclei, whether spontaneously or when induced by a reaction. The physics that governs nuclear fission is that of a many-body, large-amplitude collective mode that gradually elongates the nuclear shape until the so-called *fission barrier* is surmounted and the energetically favoured path leads the nucleus to fragment. In figure 1.7, a graphical representation of the fission path and corresponding barrier is shown.

Although the basic idea of a nucleus dividing into two pieces may appear simple, the underlying dynamics is remarkably rich and involves several stages. Historically, the first theoretical interpretation of fission was given by Bohr and Wheeler in 1939 [12], who formulated the liquid-drop model description and introduced the concept of the fission barrier, determined by the competition between Coulomb repulsion and surface

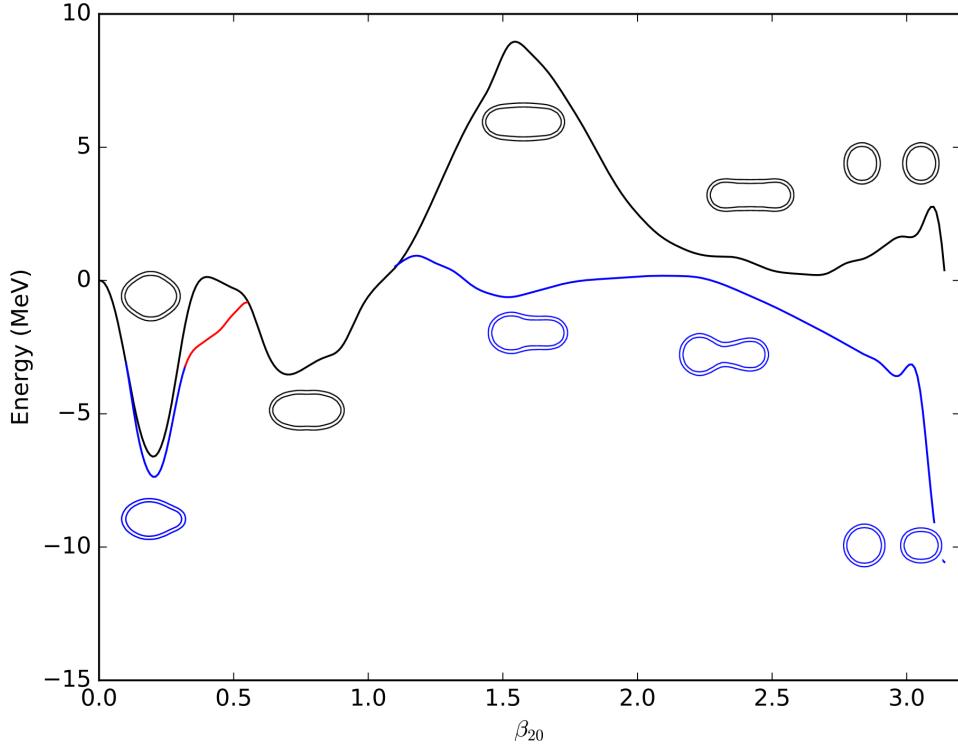


Figure 1.7: Fission path of ^{226}Ra , blue lines indicate axial octupole configurations, black lines indicate axial quadrupole and parity conserving configurations, red lines indicate triaxial, parity conserving configurations.

tension. Their framework already suggested that nuclei may experience intermediate configurations, multiple saddle points, and shape isomerism along the fission path.

Subsequent developments incorporated more detailed descriptions of the collective degrees of freedom and the role of shell effects, leading to the recognition that the fission landscape is often characterised by multiple barriers, intermediate minima, and highly deformed transition states [15, 87]. Modern microscopic approaches, based on energy-density functionals, have further clarified that fission dynamics involves a sequence of slow, dissipative shape evolutions, interspersed with possible gamma-decay pathways, and culminating in the formation of two (or more) pre-fragments connected by a narrowing neck. As the system evolves beyond the outer saddle, exotic spatial configurations appear, and the fragments themselves may exhibit deformation or even reflection asymmetry before scission. A visual representation of the overall fission process is shown in figure 1.8.

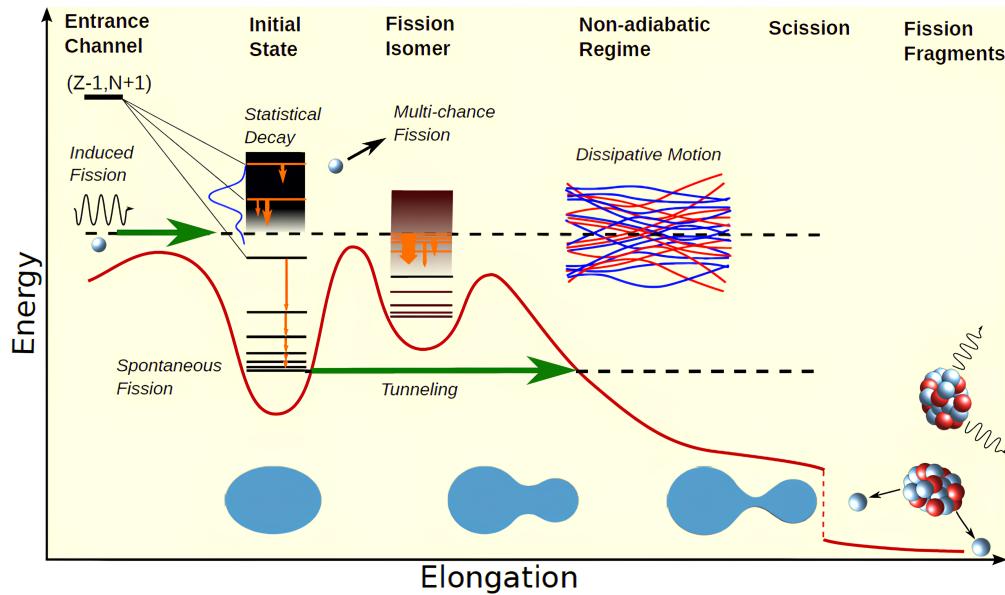


Figure 1.8: Visual representation of the fission process. Figure taken from [5].

Spontaneous fission model

It should be obvious that a formal treatment of deformations and collective modes is necessary to give a theoretical description of fission reactions. We can derive a simple spontaneous fission model by studying the effect of an axial quadrupole deformation on the semiempirical mass formula 1.3.

Let us assume that the nuclear radius may be expanded, as previously done in section 1.3, as

$$R = R_0[1 + \alpha_{20}Y_{20}]. \quad (1.43)$$

Assuming the nuclear volume is conserved across the fission path, the volume energy will not change. As for the surface energy, its variation can be expressed at the lowest order in α_{20} as

$$\Delta E_{\text{surf}} = E_{\text{surf}} - E_{0,\text{surf}} = E_{0,\text{surf}} \frac{2}{5} \alpha_{20}^2. \quad (1.44)$$

Regarding the Coulomb energy, the variation is given by

$$\Delta E_{\text{coul}} = E_{\text{coul}} - E_{0,\text{coul}} = -E_{0,\text{coul}} \frac{1}{5} \alpha_{20}. \quad (1.45)$$

Since the neutron and proton numbers does not change, the surface and Coulomb energies are the only contributions to the total energy difference. We can write

$$\Delta E = \frac{2}{5} \alpha_{20}^2 a_s A^{2/3} - \frac{1}{5} \alpha_{20}^2 a_c Z^2 A^{-1/3}, \quad (1.46)$$

if we set equation (1.46) to zero, we get, other than the undeformed solution for $\alpha_{20} = 0$,

$$\frac{Z^2}{A} = \frac{2a_s}{a_c}, \quad (1.47)$$

where the ratio $2a_s/a_c$ amounts to ≈ 50 in typical parametrizations of the SEMF. Equation (1.46), shows that for values of the so called *fissility parameter* Z^2/A larger than 50, the energy change becomes negative, favouring a configuration in which the nucleus fragments due to the spontaneous fission.

1.4.1. Symmetry breaking and microscopic approaches to fission

Microscopic theory

The use of phenomenological macroscopic-microscopic models has long provided valuable insight into fission processes, allowing for the prediction of barrier heights and fragment yields through parametrised shape degrees of freedom and empirical shell corrections [11, 16, 49]. In these models, the total energy is expressed as

$$E_{\text{tot}}(\mathbf{q}) = E_{\text{LD}}(\mathbf{q}) + \delta E_{\text{shell}}(\mathbf{q}) + \delta E_{\text{pair}}(\mathbf{q}), \quad (1.48)$$

where E_{LD} is the macroscopic liquid-drop term depending on deformation coordinates \mathbf{q} , while δE_{shell} and δE_{pair} account for shell and pairing corrections, respectively. While such models reproduce many global observables, they lack a true microscopic foundation. In particular, the collective coordinates \mathbf{q} are not derived from the underlying many-body dynamics, and the empirical shell corrections cannot describe the self-consistent rearrangement of the mean field along the fission path.

A more fundamental understanding is achieved within self-consistent mean-field approaches such as the Hartree-Fock or Hartree-Fock-Bogoliubov formalisms. The use of nuclear Density Functional Theory [3, 76] allows one to define a universal EDF $E[\rho, \kappa]$ that encapsulates both mean-field and pairing correlations. The resulting constrained HFB calculations produce the potential energy surface (PES) $E(\mathbf{q})$, mapping the energy of the system as a function of collective deformations such as the quadrupole (Q_{20}), octupole (Q_{30}), and triaxial (Q_{22}) moments. The minima and saddle points of this multidimensional PES determine the fission barriers and shape isomeric states [31, 78].

However, static mean-field approaches are limited by their single-reference character: the HFB vacuum represents only one configuration at a time, typically corresponding to a local minimum of the PES. In the vicinity of the fission barrier, where several configurations

with different intrinsic quantum numbers coexist, this approximation breaks down. The wave function should instead be expressed as a superposition of several self-consistent configurations $\{|\Phi(\mathbf{q})\rangle\}$, leading to a correlated state of the form

$$|\Psi\rangle = \int f(\mathbf{q}) |\Phi(\mathbf{q})\rangle d\mathbf{q}, \quad (1.49)$$

which is the essence of the *Generator Coordinate Method* (GCM) [38, 67]. The GCM maps the microscopic many-body problem onto a *collective Schrödinger equation* (CSE)

$$\left[-\frac{\hbar^2}{2} \sum_{ij} \frac{\partial}{\partial q_i} B_{ij}(\mathbf{q}) \frac{\partial}{\partial q_j} + V(\mathbf{q}) \right] g_k(\mathbf{q}) = E_k g_k(\mathbf{q}), \quad (1.50)$$

where $B_{ij}(\mathbf{q})$ is the collective inertia tensor and $V(\mathbf{q})$ the potential energy extracted from constrained HFB. This framework naturally incorporates tunnelling through the barrier and provides access to observables such as fission lifetimes and fragment distributions.

Beyond-mean-field extensions also restore symmetries that are spontaneously broken at the mean-field level. For instance, particle-number, parity, and angular-momentum projection techniques [4, 75] are required to recover good quantum numbers and remove spurious symmetry mixing. In multi-reference DFT [3], these symmetry restorations can be combined with configuration mixing, yielding highly accurate fission barrier calculations.

Unconstrained Calculations and Symmetry Breaking

An equally important aspect of microscopic fission theory is the treatment of spatial symmetries. Historically, many calculations imposed constraints such as axial symmetry or reflection symmetry with respect to a plane to reduce the computational cost of solving the HFB equations. While such restrictions simplify the description of the nucleus, they artificially constrain the fission path and may even prevent the identification of energetically preferred configurations [8, 90], as shown in figure 1.7. Fission involves strongly deformed, triaxial, and reflection-asymmetric shapes; the correct description of barrier heights and scission configurations therefore requires breaking as many spatial symmetries as possible.

In the self-consistent mean-field framework, spontaneous symmetry breaking is a feature rather than a flaw: it allows the system to adopt a deformed intrinsic shape corresponding to a broken rotational or parity symmetry, while the symmetry of the total many-body Hamiltonian is preserved. For example, an axially deformed HFB state violates rotational invariance, but the restoration of this symmetry through angular-momentum projection

recovers the correct laboratory-frame properties. Similarly, parity breaking through octupole deformation is essential to describe asymmetric fission fragment distributions. Triaxiality, for example, has been shown to lower the inner barrier of actinides by several MeV [78, 90]. Likewise, reflection-asymmetric (octupole) degrees of freedom are necessary to reproduce mass-asymmetric fission in heavy nuclei.

Recent computational developments have made possible fully symmetry-unrestricted HFB and TDDFT calculations, in which all spatial and time-reversal symmetries can be broken if energetically favourable [78, 81]. Codes such as HFODD and Sky3D implement three-dimensional solvers capable of describing triaxial, octupole, and time-odd components of the density matrix. These advances have revealed new fission pathways, scission configurations, and fragment-spin correlations inaccessible to axially symmetric models.

In summary, microscopic theories based on DFT and its extensions offer a self-consistent foundation for the description of nuclear fission. They provide direct access to the interplay between shell effects, pairing, and deformation, which determine the shape evolution from the ground state to scission.

2 | State of the art, objectives and methods

2.1. State of the art and motivation

The need to account for nuclear deformations has been highlighted already as a central theme in chapter 1, particularly in the context of heavy nuclei and of the complex fission dynamics discussed in section 1.4. Without allowing for deformation, several key features of nuclear systems – such as the excitation spectrum when rotational bands are present – cannot be captured, and limiting the description to only a subset of shapes often proves inadequate, as seen in the case of heavy nuclei in section 1.3. Similar limitations arise in dynamical processes and nuclear reactions, where shape evolution plays an essential role.

The central issue in nuclear structure theory is that the Hamiltonian is not known exactly and must be approximated. At the same time, the problem is inherently a many-body one, which remains computationally demanding, requiring approximations to make calculations tractable. Symmetry assumptions such as spherical or axial symmetry have therefore been widely used in numerical implementations to simplify the calculations and reduce computational cost. However, these constraints become insufficient in situations where deformation is a defining aspect of the system.

With the increasing availability of computational power and the development of modern numerical techniques, the field is now in a position to move beyond these restrictive assumptions. This motivates the development of new codes capable of treating the many-body problem without imposed symmetries, allowing the full range of nuclear deformations to emerge naturally from the underlying theory.

2.2. State of the Art

The approaches to the nuclear many-body problem can be broadly divided into two families: (a) *basis expansion methods*, which represent single-particle states in truncated har-

monic oscillator bases, and (b) *coordinate-space (mesh) methods*, which discretize space directly. In the following sections, we review these two classes of methods and motivate the need for more flexible and computationally efficient unconstrained solvers.

2.2.1. Basis expansion methods

Basis expansion approaches are among the most widely used techniques for solving the HF and HFB equations. In these methods, single-particle wavefunctions are expanded on a finite HO basis, chosen for its completeness and qualitative similarity to the mean-field potential of bound nuclei, as explained in section 1.1. Codes such as `HFBTHO`, also used in this work for benchmarking our implementation in section 6.1.2, are based on this framework.

The HO basis, however efficient, introduces structural limitations. First, weakly bound and continuum-like states, crucial for nuclei near the drip lines, are poorly represented because their asymptotic behavior differs fundamentally from that of HO functions. Whereas HO states decay as e^{-r^2} , quasi-bound states decay as e^{-r} , leading to slow convergence and difficulties in describing halos, neutron skins, and quasi-resonant states [30, 85]. Second, large deformations in heavy nuclei may require many HO shells to reproduce the stretched spatial geometry, significantly increasing the computational cost. The computational complexity grows rapidly with the maximum number of oscillator shells used in the calculation, resulting in demanding memory and CPU requirements for strongly deformed configurations [56].

In summary, despite their efficiency for near-spherical and moderately deformed nuclei, basis-expansion methods become inadequate for describing nuclei near drip lines, far from stability and largely deformed.

2.2.2. Symmetry-Restricted mesh methods

A second major class of HF/HFB solvers uses a spatial mesh as the variational space. Historically, fully unconstrained three-dimensional meshes were computationally prohibitive, which motivated the introduction of *symmetry constraints* to reduce the dimensionality of the problem. By enforcing specific spatial symmetries, the number of degrees of freedom is greatly reduced, making coordinate-space calculations tractable on available hardware.

The most common choices are spherical and axial symmetry. Spherical HF/HFB solvers [26, 88] reduce the equations to a radial problem, achieving excellent computational efficiency and precision for the structure of spherical or near-spherical nuclei. Axially sym-

metric solvers [65] generalize this approach to two dimensions, allowing axial deformations while still benefitting from significant computational cost reductions.

However, the limitations of symmetry-restricted approaches are inherent to the constraints themselves, as they forbid the emergence of intrinsic shapes such as triaxial or more general octupole-deformed configurations.

2.2.3. Unconstrained coordinate-space (mesh) methods

To overcome the limitations of basis truncation and symmetry constraints, modern HF / HFB solvers have increasingly adopted coordinate-space discretizations, typically based on three-dimensional Cartesian meshes. Notable examples include **MOCCA** [73], **Sky3D** [58], and **HFBFFT** [25]. These codes solve the mean-field equations directly in coordinate space, allowing arbitrary deformations and spontaneous symmetry breaking to emerge naturally.

However, coordinate-space solvers come with their own challenges. High spatial resolution is required to accomodate sufficient numerical accuracy, leading to large three-dimensional grids, thus substantial computational cost. Even with modern resources, fully unconstrained calculations remain computationally intensive, and additional assumptions such as plane reflection symmetry are often introduced to reduce the domain size [72, 73].

Thus, while mesh-based solvers offer maximal flexibility, their computational demands motivate the search for more efficient numerical approaches.

2.2.4. Towards more efficient unconstrained methods

The limitations discussed above highlight the need for methods that combine the flexibility of coordinate-space solvers with improved computational efficiency. In this thesis, we investigate such an approach through the use of the *Generalised Conjugate Gradient* (GCG) method, presented in detail in section 4.2.3. In the HF and energy-density-functional frameworks, the core of the many-body problem reduces to solving a set of single-particle Schrödinger or Kohn-Sham eigenvalue equations, coupled self-consistently through the mean field. These equations must be solved repeatedly during the iterative HF/HFB cycle, and their efficient solution dominates the overall computational cost.

As shown in the present work, applying GCG to the HF single-particle problem provides a promising route towards efficient, symmetry-unrestricted many-body calculations while mitigating the main bottlenecks of fully coordinate-mesh methods.

2.3. Objectives

The aim of this work is to develop a new implementation of the Hartree-Fock method on an unconstrained 3D mesh, by the use of the Generalised Conjugate Gradient method. The goals addressed by this work are the following:

- assess the feasibility of the Generalised Conjugate Gradient for the solution of large-scale eigenvalue problems;
- solve the self-consistent Hartree-Fock equations on an unconstrained 3D mesh;
- verify the numerical accuracy of the new implementation against existing spherical codes;
- gauge the numerical accuracy of deformations, comparing results with well established deformed codes; and
- attempt to produce novel results that specifically require an unconstrained implementaiton of this kind, and establish the advance brought to the field by this work.

2.4. Methods

The methods used in this thesis can be grouped into two main components: the formulation of the energy density functional and the solution of the resulting self-consistent equations.

Skyrme Energy Functional The many-body nuclear problem is approached within the Hartree–Fock framework, described in section 3.1. As discussed in chapter 1, a pure HF treatment is not sufficient for a quantitative description of nuclear structure, and a more general energy density functional (EDF) formulation must be adopted. In this work, we employ the Skyrme EDF, whose construction and resulting mean-field equations are developed in section 3.3. This provides the self-consistent single-particle Hamiltonian that forms the basis for the numerical treatment.

Finite Differences and Generalised Conjugate Gradient Once the equations to solve have been derived, their numerical solution requires both a spatial discretization scheme and an efficient solver for the large-scale eigenvalue problem that arises at each iteration of the self-consistent procedure. Chapter 4 details the methods adopted in this work, starting with the finite-difference discretization of derivatives in section 4.1. The resulting discretized eigenvalue problem is then treated using the GCG method to extract

the relevant low-lying eigenstates, as described in section 4.2.3. Section 4.3 discusses implementation-specific aspects of the code, including convergence criteria, mixing strategies, and the choice of parameters required to ensure stable and efficient minimization of the energy functional.

3 | Energy functional

3.1. Hartree-Fock theory

While a phenomenological description of some nuclear structure properties can be carried out using the liquid drop model or empirical mean-field potentials like Woods-Saxon or Nilsson, as we have seen in section 1.1, this is not sufficient to accurately reproduce all experimental ground state observables, systematically throughout the chart of nuclei, in an accurate manner.

A more rigorous approach needs to take into account the fact that the mean field the nucleons interact with, is generated by the nucleons themselves. Starting from the many-body Hamiltonian of the system, we will be able to extract a single particle Hamiltonian, including an effective mean field potential generated by the effective microscopic force, through the use of the Hartree-Fock method.

We start by writing the many-body Hamiltonian of the system, which is a collection of A interacting fermions, given by

$$\hat{H} = \hat{T} + \hat{V} = \sum_i -\frac{\hbar^2}{2m} \nabla_i^2 + \sum_{i < j} v_{ij}^{(2)} + \sum_{i < j < k} v_{ijk}^{(3)} + \dots \quad (3.1)$$

The corresponding Schrödinger equation reads

$$\hat{H}\Psi = E\Psi. \quad (3.2)$$

3.1.1. Variational principle

Since \hat{H} is a many body operator, finding its eigenstates would be a rather challenging task. To our aid, comes the variational principle, from which we can show that equation (3.2) is equivalent to

$$\delta E[\Psi] = \delta \frac{\langle \Psi | E | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0. \quad (3.3)$$

The variation (3.3) can be obtained from an arbitrary variation of Ψ , which can be done independently on $\langle \Psi |$ and $|\Psi \rangle$, since Ψ is complex, yielding

$$\langle \delta\Psi | \hat{H} - E | \Psi \rangle + \langle \Psi | \hat{H} - E | \delta\Psi \rangle = 0 \quad (3.4)$$

since the variation is arbitrary, we can multiply by a phase factor $|\delta\Psi\rangle \mapsto i|\delta\Psi\rangle$ and get

$$-i\langle \delta\Psi | \hat{H} - E | \Psi \rangle + i\langle \Psi | \hat{H} - E | \delta\Psi \rangle = 0. \quad (3.5)$$

Combining equations (3.4) and (3.5), we get

$$\langle \delta\Psi | \hat{H} - E | \Psi \rangle = 0. \quad (3.6)$$

Again, since the variation is arbitrary, equation (3.6) satisfies equation (3.2).

Ground state

Since we always restrict ourselves to a certain subspace of the full Hilbert space, we can only find an approximate solution to the eigenvalue problem. Expanding this solution on the complete set of exact eigenstates of \hat{H} , we have

$$|\Psi\rangle = \sum_n a_n |\Psi_n\rangle \quad (3.7)$$

the total energy amounts to

$$E[\Psi] = \frac{\sum_{nn'} \langle a_{n'} \Psi_{n'} | \hat{H} | a_n \Psi_n \rangle}{\sum_{nn'} \langle a_{n'} \Psi_{n'} | a_n \Psi_n \rangle} = \frac{\sum_n E_n |a_n|^2}{\sum_n |a_n|^2} \geq \frac{\sum_n E_0 |a_n|^2}{\sum_n |a_n|^2} \geq E_0, \quad (3.8)$$

where E_0 is the ground state energy of the system. The orthonormality of the Hamiltonian eigenfunctions $\langle \Psi_{n'} | \Psi_n \rangle = \delta_{nn'}$ has been used. Equation (3.8) tells us that the minimum of the functional $E[\Psi]$ in any variational subspace we are considering is bound from below by the true ground state energy.

3.1.2. Hartree-Fock equations

The Hartree-Fock method is the application of the variational principle (3.6) to a system of independent particles, whose wavefunction takes the form of a Slater determinant,

which reads

$$\Psi = \frac{1}{\sqrt{A!}} \sum_{\{p\}} (-1)^p \varphi_{p(1)}(\mathbf{r}_1) \dots \varphi_{p(A)}(\mathbf{r}_A) \quad (3.9)$$

where φ_i are the single-particle orthonormal states, which serve the role of variational parameters in Hartree-Fock. The Slater determinant sums over all possible permutations of the A fermions on the single particle states, with a $-$ sign according to the parity of the permutation. The Slater determinant satisfies the permutation symmetry of fermions, so that the Pauli exclusion principle is not violated.

To ensure the orthonormality of the single-particle states, we need to add a Lagrange multiplier to the variation (3.6) of E , which ends up reading

$$\delta \left(E[\Psi] - \sum_i \lambda_i \int \varphi_i^* \varphi_i d\mathbf{r} \right) = 0. \quad (3.10)$$

The total energy of the system is given by

$$E[\Psi] = \langle \Psi | \hat{T} + \hat{V} | \Psi \rangle = \langle \Psi | \hat{T} | \Psi \rangle + \langle \Psi | \hat{V} | \Psi \rangle, \quad (3.11)$$

which can be expressed through the single-particle states $\{\varphi_i\}$, yielding

$$\langle \Psi | \hat{T} | \Psi \rangle = \sum_i^A -\frac{\hbar^2}{2m} \int \varphi_i^*(\mathbf{r}) \nabla^2 \varphi_i(\mathbf{r}) d\mathbf{r} = \sum_i \langle i | t | i \rangle \quad (3.12)$$

$$\begin{aligned} \langle \Psi | \hat{V} | \Psi \rangle &= \frac{1}{2} \sum_{ij} \int \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}') v_{ij}(\mathbf{r}, \mathbf{r}') \varphi_i(\mathbf{r}) \varphi_j(\mathbf{r}') d\mathbf{r} d\mathbf{r}' \\ &\quad - \frac{1}{2} \sum_{ij} \int \varphi_i^*(\mathbf{r}) \varphi_j^*(\mathbf{r}') v_{ij}(\mathbf{r}, \mathbf{r}') \varphi_i(\mathbf{r}') \varphi_j(\mathbf{r}) d\mathbf{r} d\mathbf{r}' \\ &= \frac{1}{2} \langle ij | \bar{v} | ij \rangle. \end{aligned} \quad (3.13)$$

If we use $\varphi_i^*(\mathbf{r})$ as the quantity to be varied in equation (3.10), we get the *Hartree-Fock equations*

$$\begin{aligned} &- \frac{\hbar^2}{2m} \nabla^2 \varphi_i \\ &+ \frac{1}{2} \sum_j^A \int \varphi_j^*(\mathbf{r}') v_{ij}(\mathbf{r}, \mathbf{r}') \varphi_j(\mathbf{r}') \varphi_i(\mathbf{r}) d\mathbf{r}' \end{aligned} \quad (3.14)$$

$$- \frac{1}{2} \sum_j^A \int \varphi_j^*(\mathbf{r}') v_{ij}(\mathbf{r}, \mathbf{r}') \varphi_j(\mathbf{r}) \varphi_i(\mathbf{r}') d\mathbf{r}' = \varepsilon_i \varphi_i \quad (3.15)$$

which can be written compactly as

$$h\varphi_i = \varepsilon_i \varphi_i, \quad (3.16)$$

where h is the single-particle Hamiltonian. Here the Lagrange multipliers λ_i have been replaced by ε_i , since they can be interpreted as the energy of the single-particle states.

The first interaction term (3.14), called Hartree term, arises from considering independent particles, each of one interacting with the mean-field produced by the others, and is also routinely found in classical physics. The second one in (3.15), called Fock term, or exchange term, takes the form of an integral operator and is present when considering quantum mechanical indistinguishable particles. For what concerns the solution of equation (3.16), the Fock term complicates the problem, as it implies solving an integro-differential equation. This can be avoided using zero-range forces like the Skyrme one [82], which is used in the present work, since it renders the exchange term as a local one.

Even if the interaction terms are local, the equation is still highly non-linear, since the mean field potential will be a function of the eigenfunctions themselves. The consequence is that the solution needs to be found *self-consistently*, that is, by solving for the set of eigenfunctions $\{\varphi_i\}$, using them to build the new mean field, and solving again, repeating the process until convergence.

3.1.3. Symmetries in Hartree-Fock

Since the objective of this work is to solve the Hartree-Fock equations without spatial symmetry assumptions, it is useful to first understand how symmetries propagate along the self-consistent calculation.

We start by defining the creation and annihilation operators of the single particle hamiltonian eigenstates, a_i^\dagger, a_i , which abide the usual anticommutation relations of fermions

$$\{a_i, a_j^\dagger\} = \delta_{ij} \quad (3.17)$$

If we expand on a different, orthonormal complete basis $\{\chi_l\}$, we can write the corresponding creation and annihilation operators c_l^\dagger, c_l as

$$\varphi_k = \sum_l D_{lk} \chi_l \quad (3.18)$$

$$a_k^\dagger = \sum_l D_{lk} c_l^\dagger \quad (3.19)$$

$$a_k = \sum_l D_{lk}^\dagger c_l \quad (3.20)$$

Since orthonormality is guaranteed for both sets, taking $\langle \varphi_j | \varphi_k \rangle$ yields

$$\delta_{jk} = \langle \varphi_j | \varphi_k \rangle = \sum_{ll'} D_{l'j}^\dagger D_{lk} \langle \chi_l | \chi_{l'} \rangle \implies DD^\dagger = 1, \quad (3.21)$$

meaning that D is a unitary transformation. We can define the density matrix as

$$\rho_{ll'} = \langle \Psi | c_{l'}^\dagger c_l | \Psi \rangle, \quad (3.22)$$

whose trace is equal to the particle number A , as per equation (3.23)

$$\text{Tr } \rho = \sum_l \langle \Psi | c_l^\dagger c_l | \Psi \rangle = \sum_{ll'} \langle \Psi | a_{l'}^\dagger a_l | \Psi \rangle = \sum_l^A \langle \Psi | \Psi \rangle = A. \quad (3.23)$$

Writing the many body hamiltonian (3.2) in the arbitrary basis of second quantization operators c_l^\dagger, c_l , we get

$$\hat{H} = \sum_{l_1 l_2} t_{l_1 l_2} c_{l_1}^\dagger c_{l_2} + \frac{1}{4} \sum_{l_1 l_2 l_3 l_4} \bar{v}_{l_1 l_2 l_3 l_4} c_{l_1}^\dagger c_{l_2}^\dagger c_{l_3} c_{l_4} \quad (3.24)$$

where $t_{l_1 l_2}$ and $\bar{v}_{l_1 l_2 l_3 l_4}$ are defined as

$$t_{l_1 l_2} = \langle - | c_{l_1} c_{l_2} t c_{l_1}^\dagger c_{l_2}^\dagger | - \rangle = \langle l_1 l_2 | t | l_1 l_2 \rangle \quad (3.25)$$

$$\bar{v}_{l_1 l_2 l_3 l_4} = \langle l_1 l_2 l_3 l_4 | v | l_1 l_2 l_3 l_4 \rangle - \langle l_1 l_2 l_4 l_3 | v | l_1 l_2 l_4 l_3 \rangle. \quad (3.26)$$

The minimization (3.10) can be restated as the variation of $\langle \Psi | \hat{H} | \Psi \rangle$, with respect to the density matrix $\rho_{ll'}$, which yields

$$h_{ll'} = \frac{\partial E[\rho]}{\partial \rho_{ll'}} = t + \sum_{kk'} \bar{v}_{lk'k'k} \rho_{kk'} = t + \Gamma_{ll'} \quad (3.27)$$

where $\Gamma_{ll'}$ is the mean field potential in the arbitrary basis. Being h diagonal in the Hartree-Fock basis, the self-consistent solution is the one for which

$$[h, \rho] = 0 \quad (3.28)$$

holds.

Symmetry propagation

When solving the Hartree-Fock equations, we start from an initial guess with a density matrix $\rho^{(0)}$. Let us suppose that this initial guess is symmetric under the action of a unitary many-body symmetry operator S , meaning

$$S\rho^{(0)}S^\dagger = \rho^{(0)}, \quad (3.29)$$

where S commutes with the many-body Hamiltonian

$$[S, \hat{H}] = 0. \quad (3.30)$$

It can be shown [69] that

$$S\Gamma[\rho]S^\dagger = \Gamma[S\rho S^\dagger], \quad (3.31)$$

the single particle Hamiltonian h will then display the same property

$$Sh[\rho]S^\dagger = h[S\rho S^\dagger]. \quad (3.32)$$

If the equality (3.29) holds, we get

$$Sh[\rho^{(0)}]S^\dagger = h[S\rho^{(0)}S^\dagger] = h[\rho^{(0)}], \quad (3.33)$$

meaning that h will be symmetric under the action of S , as well as the next iteration's density matrix $\rho^{(1)}$. The symmetry S gets propagated self-consistently until the minimum is found.

This has profound numerical implications, since the minimum energy configuration of a deformed nucleus can be reached only from a starting guesses with the same broken symmetries. It can be the case that numerical noise allows to explore the full energy surface, but if one has to take into consideration the numerical cost of a bad guess, then it's still advantageous to start from a correct one in terms of symmetries.

3.1.4. Density Functional Theory

It shall be evident shortly, in section 3.3, that a more general approach to microscopic models has to be taken in order to give a satisfactory description of nuclei and nuclear matter. The method that we will briefly outline here is called Density Functional Theory (DFT).

DFT was introduced by P Hohenberg and W Kohn in 1964 [43], by proving two theorems. The **first** Hohenberg-Kohn (HK) theorem states that the energy of a fermion system, subject to an external potential V_{ext} , can be expressed solely as a functional of the particle density ρ of the system

$$E[\rho] = F[\rho] + \int V_{\text{ext}}\rho(\mathbf{r})d\mathbf{r}, \quad (3.34)$$

where $F[\rho]$ is a universal functional given by the type of fermions considered, while V_{ext} term is the external potential to which the system is subject to; when treating atomic nuclei, the potential is generated by the nucleons themselves, so this term will be omitted in the following. The **second** HK theorem states that the ground state of the system is found by minimizing the functional (3.34) with respect to ρ .

HK theorems are fundamental but not constructive [27], since they do not provide a form for the functional F , which is intrinsic to the physics of the fermions at hand. A pragmatic approach to using DFT was outlined by Kohn and Sham in 1965 [47]. They proposed expressing the system as a set of non-interacting particles occupying auxiliary orbitals φ_i , which yield the particle density

$$\rho(\mathbf{r}) = \sum_i |\varphi_i(\mathbf{r})|^2 \quad (3.35)$$

and an energy functional of the form

$$E[\rho] = T[\rho] + E_H[\rho] + E_{\text{xc}}[\rho]. \quad (3.36)$$

where T is the kinetic energy, which reads

$$T[\rho] = -\frac{\hbar^2}{2m} \sum_i \varphi_i^*(\mathbf{r}) \nabla^2 \varphi_i(\mathbf{r}) \quad (3.37)$$

and E_H is the classical Hartree term, which in an electronic system may read

$$E_H[\rho] = \iint \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r} d\mathbf{r}' \quad (3.38)$$

while E_{xc} is an unknown exchange term. In electronic systems, the Hartree term is known (3.14) and the exchange term can be approximated thanks to the compensation of its error with the one of particles correlation neglection [57]. In nuclear physics, things are more complicated, since both terms are unknown; historically, effective interactions in HF have been used to extract an effective Hamiltonian density from which an energy density functional (EDF) can be formulated, whenever a pure interaction is not sufficient to describe nuclear systems, as we shall see in section 3.3.

3.2. Pairing in Hartree-Fock theory

In this section, we will discuss the two common approaches to include nuclear pairing in the HF theory. The aim of these few pages is to provide a brief overview of how the BCS equations are derived and understand the basics of the more general Hartree-Fock-Bogoliubov theory. The former method is the most widely implemented thanks to its low complexity [14, 26, 48], while the latter, more sophisticated and advanced, is the standard in modern codes [24, 55, 77]. We will touch on it so that the reader may appreciate in the numerical chapter the natural extension of this work to the more general Bogoliubov ansatz. The reader may refer to introductory textbooks on many-body theory, such as Ref. [69] for an in-depth treatment of nuclear pairing.

3.2.1. BCS theory

The BCS approximation, from Bardeen-Cooper-Schrieffer, is the same theory used to describe Cooper pairs in superconductors, applied to the nuclear case. The ansatz of BCS is that nucleons are paired in states whose total angular momentum is zero, so that the wavefunction of pair is $|JM\rangle = |00\rangle$ and reads

$$|00\rangle = \sum_{m_j} \langle jm_j j - m_j | 00 \rangle |jm_j\rangle |j - m_j\rangle \quad (3.39)$$

Introducing the time-reversal operator $\hat{\mathcal{T}} : t \mapsto -t$, it acts on $|jm_j\rangle$ as

$$\hat{\mathcal{T}} |jm_j\rangle = \widetilde{|jm_j\rangle} = (-1)^{j+m_j} |j - m_j\rangle, \quad (3.40)$$

and using this relation, equation (3.39) becomes

$$|00\rangle = -\frac{1}{\sqrt{2j+1}} \sum_{m_j} |jm_j\rangle \widetilde{|jm_j\rangle}. \quad (3.41)$$

The BCS ansatz amounts to replacing the Slater determinant with a more general wavefunction where pairs partially occupy time-reversal states. The BCS wavefunction reads

$$|\text{BCS}\rangle = \prod_{k>0} (u_k + v_k a_k^\dagger a_k^\dagger) |-\rangle \quad (3.42)$$

where k is a shorthand notation for $|jm\rangle$, $\tilde{k} = -k$ denotes the time-reversal state of k , and v_k and u_k are variational parameters, we shall see shortly that v_k^2 is the probability of finding a particle in state k . The product runs over positive k only. The BCS wavefunction is the creation in the vacuum of quasi-particles made of time-reversal paired particles, instead of individual ones. The normalization condition on the BCS wavefunction reads

$$1 = \langle \text{BCS} | \text{BCS} \rangle = \prod_{k>0} \langle - | (u_k + v_k a_k a_{\tilde{k}}) (u_k + v_k a_{\tilde{k}}^\dagger a_k^\dagger) | - \rangle = \prod_{k>0} (u_k^2 + v_k^2) = 1 \quad (3.43)$$

which implies, for every pair k , the normalization condition

$$u_k^2 + v_k^2 = 1. \quad (3.44)$$

Taking the expectation value of the particle number operator $\hat{N} = \sum_k a_k^\dagger a_k$ yields [9]

$$\langle \text{BCS} | \hat{N} | \text{BCS} \rangle = 2 \sum_{k>0} v_k^2, \quad (3.45)$$

where v_k^2 is the probability of finding a particle in state k , while the expectation value of the particle number dispersion reads

$$\langle \Delta \hat{N}^2 \rangle = \langle \hat{N}^2 \rangle - \langle \hat{N} \rangle^2 = 4 \sum_{k>0} v_k^2 u_k^2. \quad (3.46)$$

The consequence of this result is profound. The BCS ansatz does not assume a fixed number of particles, rather it has an expectation value that depends on how the parameters v_k^2 are set, and presents fluctuations around it.

We can now write the many body Hamiltonian of the system as in equation (3.24)

$$\hat{H} = \sum_{k_1 k_2} t_{k_1 k_2} a_{k_1}^\dagger a_{k_2} + \frac{1}{4} \sum_{k_1 k_2 k_3 k_4} \bar{v}_{k_1 k_2 k_3 k_4} a_{k_1}^\dagger a_{k_2}^\dagger a_{k_3} a_{k_4} \quad (3.47)$$

and replace it with the Routhian

$$\langle \text{BCS} | \hat{H} - \lambda \hat{N} | \text{BCS} \rangle \quad (3.48)$$

so that the expected number of particles may be fixed, under the appropriate choice of λ , by the relation

$$\frac{\partial}{\partial N} \langle \text{BCS} | \hat{H} | \text{BCS} \rangle = \lambda. \quad (3.49)$$

the Lagrange multiplier λ takes on the meaning of the Fermi energy. We can now apply the variational principle (3.6) to (3.48) using the v_k as variational quantities, which yields

$$4\tilde{\varepsilon}_k^2 u_k^2 v_k^2 = \Delta_k^2 - 4\Delta_k^2 u_k^2 v_k^2, \quad (3.50)$$

where the pairing gap Δ_k is defined as

$$\Delta_k = - \sum_{k'} \bar{v}_{k\tilde{k}k'\tilde{k}'} v_{k'} u_{k'} \quad (3.51)$$

and the quantity $\tilde{\varepsilon}_k$ is defined as

$$\tilde{\varepsilon}_k = \frac{1}{2} \left[t_{kk} + t_{\tilde{k}\tilde{k}} - 2\lambda + \sum_{k'} (\bar{v}_{k\tilde{k}k'\tilde{k}'} v_{k'} u_{k'} + \bar{v}_{\tilde{k}k'\tilde{k}k} v_{k'} u_{k'}) v_{k'}^2 \right] \quad (3.52)$$

$$= \frac{1}{2} [h_{kk} + h_{\tilde{k}\tilde{k}}] - \lambda. \quad (3.53)$$

Introducing the quasi-particle energy

$$E_k = \sqrt{\tilde{\varepsilon}_k^2 + \Delta_k^2} \quad (3.54)$$

we can combine definitions (3.51) and (3.54) with equation (3.52), under the normalization condition (3.44), to get an equation for v_k^2

$$v_k^2 = \frac{1}{2} \pm \frac{|\tilde{\varepsilon}_k|}{2E_k}. \quad (3.55)$$

Since in the Hartree-Fock limit, where the occupations v_k^2 are equal to one below the Fermi energy and zero above, and the gaps Δ_k vanish, rendering $E_k = \tilde{\varepsilon}_k$, we only select the solution

$$v_k^2 = \frac{1}{2} - \frac{\tilde{\varepsilon}_k}{2E_k}. \quad (3.56)$$

Using the normalization condition to write $u_k^2 = 1 - v_k^2$, and plugging it into the gaps

definition (3.51), we arrive to the gap equation

$$\Delta_k = - \sum_{k'} \frac{\Delta_{k'} \bar{v}_{k\tilde{k}k'\tilde{k}'}}{2E_{k'}} \quad (3.57)$$

The system of equations (3.57, 3.44, 3.55, 3.54, 3.52), together with the condition on \hat{N} – ie $\langle \hat{N} \rangle = N$ – is closed and can be solved numerically, usually through an effective pairing interaction.

3.2.2. Hartree-Fock-Bogoliubov theory

The most general ansatz to account for pairing interactions in Hartree-Fock theory is the Hartree-Fock-Bogoliubov (HFB) theory, that allows a treatment of the mean-field and pairing interactions in a unified way. The quasi-particles created on the vacuum aren't necessarily time-reversal pairs but the most general ones according to the symmetries of the system. Let us start by writing a Bogoliubov transformation from the particle basis c_i to a quasi-particle one

$$\beta_k^\dagger = \sum_l U_{lk} c_l^\dagger + V_{lk} c_l. \quad (3.58)$$

If we take the Hermitian conjugate of the relation (3.58), we get the transformation for β_k , and we are then able to write the two in matrix form

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} = \mathcal{W}^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix}, \quad (3.59)$$

where the super-matrix of matrices \mathcal{W} reads

$$\mathcal{W} = \begin{pmatrix} U & V^* \\ V & U^* \end{pmatrix}. \quad (3.60)$$

Taking the product $\mathcal{W}^\dagger \mathcal{W}$ and imposing separate fermionic commutation relations of the operators $\beta, \beta^\dagger, c, c^\dagger$, we get that \mathcal{W} is unitary, hence

$$\mathcal{W}^\dagger \mathcal{W} = \mathcal{W} \mathcal{W}^\dagger = I. \quad (3.61)$$

We can now invert equation (3.59) by multiplying both sides on the left by \mathcal{W} , which yields

$$\mathcal{W} \begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} c \\ c^\dagger \end{pmatrix}.$$

Using the Messiah-Bloch decomposition [29], we can write the unitary matrix \mathcal{W} as

$$\mathcal{W} = \begin{pmatrix} D & 0 \\ 0 & D^* \end{pmatrix} \begin{pmatrix} \bar{U} & \bar{V} \\ \bar{V} & \bar{U} \end{pmatrix} \begin{pmatrix} C & 0 \\ 0 & C^* \end{pmatrix} \quad (3.62)$$

where D and C are unitary matrices and \bar{U} and \bar{V} are real matrices, which have a particular blocked form, expressed through the coefficients u_k, v_k ; the reader may refer to appendix A.4 for the explicit representation. We can also define the matrices U, V as

$$U = D\bar{U}C, \quad V = D^*\bar{V}C. \quad (3.63)$$

Using the decomposition (3.62) we can define the *canonical basis* as

$$a_k^\dagger = \sum_l D_{lk}^\dagger c_l^\dagger, \quad (3.64)$$

a *special Bogoliubov transformation* between *paired* levels as

$$\alpha_k^\dagger = u_k a_k^\dagger - v_k a_{\bar{k}}^\dagger, \quad (3.65)$$

$$\alpha_{\bar{k}}^\dagger = u_k a_k^\dagger + v_k a_{\bar{k}}, \quad (3.66)$$

and *blocked* levels

$$\alpha_i = a_i, \quad \alpha_n^\dagger = a_n^\dagger \quad (3.67)$$

$$\alpha_i = a_i^\dagger, \quad \alpha_n = a_n, \quad (3.68)$$

where $u_k = u_{\bar{k}}$, $v_k = -v_{\bar{k}}$, and a unitary transformation of the quasi-particle operators α_k^\dagger among themselves

$$\beta_k^\dagger = \sum_{k'} C_{k'k} a_{k'}^\dagger. \quad (3.69)$$

We are now able to define the Bogoliubov ground state $|\text{HFB}\rangle$, as the one for which

$$\beta_k |\text{HFB}\rangle = 0 \quad \forall k = 1, \dots, M \quad (3.70)$$

where M is the number of single-particle states in the chosen basis. The wavefunction that satisfies this condition reads

$$|\text{HFB}\rangle = \prod_k^M \beta_k |-\rangle. \quad (3.71)$$

The *pairing tensor* is defined as

$$\kappa_{ll'} = \langle \text{HFB} | c_{l'} c_l | \text{HFB} \rangle, \quad (3.72)$$

which in matrix form reads

$$\kappa = UV^\dagger, \quad (3.73)$$

while the density matrix, defined in (3.22), in matrix form reads

$$\rho = V^* V^T. \quad (3.74)$$

We can now apply the variational principle (3.6)

$$\delta \frac{\langle \text{HFB} | \hat{H} - \lambda \hat{N} | \text{HFB} \rangle}{\langle \text{HFB} | \text{HFB} \rangle} = 0, \quad (3.75)$$

which yields the eigenvalue problem

$$\begin{pmatrix} h - \lambda & \Delta \\ -\Delta^* & -(h - \lambda)^* \end{pmatrix} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = \mathcal{H}_{\text{HFB}} \begin{pmatrix} U_k \\ V_k \end{pmatrix} = E_k \begin{pmatrix} U_k \\ V_k \end{pmatrix}, \quad (3.76)$$

here, h is the single-particle Hamiltonian, which reads

$$h_{kk'} = t_{kk'} + \Gamma_{kk'}, \quad (3.77)$$

and $\Gamma_{kk'}$ is the mean field potential, given by

$$\Gamma_{kk'} = \sum_{ll'} \bar{v}_{kl'k'l} \rho_{ll'} \quad (3.78)$$

while the pairing field Δ reads

$$\Delta_{kk'} = \sum_{ll'} \bar{v}_{kk'l'l} \kappa_{ll'}. \quad (3.79)$$

In the canonical basis, we are able to solve for the occupation numbers

$$u_k^2 = \frac{1}{2} \left(1 + \frac{h_{kk} + h_{\tilde{k}\tilde{k}}}{\sqrt{(h_{kk} + h_{\tilde{k}\tilde{k}})^2 + 4\Delta_{kk}^2}} \right) \quad (3.80)$$

where $v_k^2 = 1 - u_k^2$ is guaranteed by the unitarity of the matrices. Starting from an initial guess, we solve the eigenvalue problem (3.76), we extract the occupation numbers (3.80), use them to build the new mean field (3.78) and pairing field (3.79), and repeat the process until convergence.

HFB quasi-particle spectrum Let us assume that $\Psi = (U, V)^T$ is a solution of equation (3.76) with eigenvalue E

$$\mathcal{H}_{\text{HFB}}\Psi = E\Psi. \quad (3.81)$$

Let the particle-hole matrix \mathcal{C} be defined as

$$\mathcal{C} = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad (3.82)$$

it's trivial to show that

$$\mathcal{C}\mathcal{H}_{\text{HFB}}\mathcal{C} = -\mathcal{H}_{\text{HFB}}^*, \quad (3.83)$$

and

$$\mathcal{C} = \mathcal{C}^{-1} \implies \mathcal{C}\mathcal{H}_{\text{HFB}} = -\mathcal{H}_{\text{HFB}}^*\mathcal{C}. \quad (3.84)$$

If we take the complex conjugate of equation (3.81), we get

$$\mathcal{H}_{\text{HFB}}^*\Psi^* = E\Psi^*, \quad (3.85)$$

if we multiply both sides on the left by \mathcal{C} and use (3.84), we get

$$-\mathcal{H}_{\text{HFB}}\mathcal{C}\Psi^* = E\mathcal{C}\Psi^*, \quad (3.86)$$

$$\mathcal{H}_{\text{HFB}}\mathcal{C}\Psi^* = -E\mathcal{C}\Psi^*, \quad (3.87)$$

meaning that $\mathcal{C}\Psi^*$ is a solution of the eigenvalue problem (3.76) as well, with eigenvalue $-E$, hence for every quasi-particle energy we have a corresponding opposite-sign one; moreover, it can be proven that the HFB hamiltonian is unbounded, both from below and above [66]. This feature poses a challenge for numerical solutions of the HFB problem, as we shall see in chapter 4.

3.3. Skyrme

Now that the theoretical framework is clear, we can use the Skyrme microscopic effective interaction to do nuclear structure calculations.

3.3.1. Skyrme force

It was first proposed by Tony Skyrme in 1958 [82] as a zero range force between nucleons, comprising a two body attractive term that reads

$$\begin{aligned} v^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = & t_0 (1 + x_0 P_\sigma) \delta(\mathbf{r}) \\ & + \frac{1}{2} t_1 (1 + x_1 P_\sigma) [\mathbf{P}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{P}^2] \\ & + t_2 P_\sigma \mathbf{P}' \cdot \delta(\mathbf{r}) \mathbf{P} \\ & + i W_0 \boldsymbol{\sigma} \cdot [\mathbf{P}' \times \delta(\mathbf{r}) \mathbf{P}] \end{aligned}$$

and a three body term, that is

$$v^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = t_3 \delta(\mathbf{r}_1 - \mathbf{r}_2) \delta(\mathbf{r}_2 - \mathbf{r}_3)$$

which mimics the repulsive three-body force; without it, a collapse of the nuclear density would occur. The different operators are defined as

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad \mathbf{R} = \frac{\mathbf{r}_1 + \mathbf{r}_2}{2}, \quad (3.88)$$

which are respectively the relative position of two particles and their center of mass coordinate, assuming equal masses,

$$\mathbf{P} = \frac{-i(\nabla_1 - \nabla_2)}{2}, \quad (3.89)$$

which is the so called relative wave-number operator, corresponding to the relative momentum of the two interacting particles.

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 \quad (3.90)$$

is the total spin of the two interacting particles, and lastly

$$\mathbf{P}_\sigma = \frac{(1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)}{2} \quad (3.91)$$

represents the spin-exchange operator. Primed operators refer to the adjoint acting on the left.

It's trivial to show that the three-body term, in the case of even-even nuclei, is equivalent to a two-body, density-dependent interaction [88]

$$v^{(3)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{6} t_3 (1 + P_\sigma) \delta(\mathbf{r}) \rho(\mathbf{R}) \quad (3.92)$$

The zero-range feature is apparent in the choice of the Dirac delta $\delta(\mathbf{r})$, which allows the writing of the Fock term detailed in (3.15) as a purely local one.

Modern parametrization

The Skyrme force has evolved from the original one to accomodate new nuclei and properties, done through the addition of a few parameters, yielding the following form of the interaction [21]

$$\begin{aligned} v^{(2)}(\mathbf{r}_1, \mathbf{r}_2) &= t_0 (1 + x_0 P_\sigma) \delta(\mathbf{r}) \\ &+ \frac{1}{2} t_1 (1 + x_1 P_\sigma) [\mathbf{P}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{P}^2] \\ &+ t_2 (1 + x_2 P_\sigma) \mathbf{P}' \cdot \delta(\mathbf{r}) \mathbf{P} \\ &+ \frac{1}{6} t_3 (1 + x_3 P_\sigma) [\rho(\mathbf{R})]^\sigma \delta(\mathbf{r}) \\ &+ iW_0 \boldsymbol{\sigma} \cdot [\mathbf{P}' \times \delta(\mathbf{r}) \mathbf{P}] \\ &+ \frac{1}{6} t_3 (1 + x_3 P_\sigma) [\rho(\mathbf{R})]^\sigma \delta(\mathbf{r}) \end{aligned}$$

Here, the boundary between Hartree-Fock and DFT starts to thin out, as the exponent σ of the density makes that piece of the force a true three-body interaction only for the value $\sigma = 1$ [33]. On top of that, additional, empirical tuning of the resulting energy density needed to reach satisfactory physical accuracy, such as the case for the spin-orbit couplings [68], prompts for the following, well established proceeding: use the Skyrme interaction to obtain the Hamiltonian density

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int \mathcal{H}(\mathbf{r}) d\mathbf{r} \quad (3.93)$$

and use it as a starting point to build an energy density functional and employ DFT.

3.3.2. Energy density functional

The energy functional to be minimized is of the form [3]

$$E_{\text{HF}} = E_{\text{Kin}} + E_{\text{Skyrme}} + E_{\text{Coul}} = \int (\mathcal{E}_{\text{Kin}} + \mathcal{E}_{\text{Skyrme}} + \mathcal{E}_{\text{Coul}}) d\mathbf{r}. \quad (3.94)$$

Densities

Functional (3.94) can be expressed through a series of generalized particle densities. Let us define them and express them on the spin coordinates up (\uparrow) and down (\downarrow) for the convenience in a mesh representation.

The starting point is the density matrix, defined as

$$\rho_q(\mathbf{r}\sigma, \mathbf{r}\sigma') = \sum_{\alpha} \phi_{\alpha,\sigma}(\mathbf{r}) \phi_{\alpha,\sigma'}^*(\mathbf{r}') \quad (3.95)$$

where the index α goes through all single particle states of the particles of type q (protons, neutrons) and the index σ refers to the spin coordinate. The particle density is defined as

$$\begin{aligned} \rho_q(\mathbf{r}) := \rho_q(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}=\mathbf{r}'} &:= \sum_{\sigma} \rho(\mathbf{r}\sigma, \mathbf{r}'\sigma) \Big|_{\mathbf{r}=\mathbf{r}'} = \sum_{\alpha} \phi_{\uparrow}(\mathbf{r}) \phi_{\uparrow}^*(\mathbf{r}') + \phi_{\downarrow}(\mathbf{r}) \phi_{\downarrow}^*(\mathbf{r}') \Big|_{\mathbf{r}=\mathbf{r}'} \\ &= \sum_{\alpha} |\phi_{\uparrow}(\mathbf{r})|^2 + |\phi_{\downarrow}(\mathbf{r})|^2. \end{aligned} \quad (3.96)$$

The kinetic density reads

$$\begin{aligned} \tau_q(\mathbf{r}) := \sum_{\alpha} \nabla' \cdot \nabla \rho_q(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}'=\mathbf{r}} &= \sum_{\sigma, \alpha} \nabla \phi_{\sigma}(\mathbf{r}) \cdot \nabla \phi_{\sigma}^*(\mathbf{r}') \Big|_{\mathbf{r}'=\mathbf{r}} = \sum_{\sigma, \alpha} |\nabla \phi_{\sigma}(\mathbf{r})|^2 \\ &= \sum_{\alpha} |\nabla \phi_{\uparrow}(\mathbf{r})|^2 + |\nabla \phi_{\downarrow}(\mathbf{r})|^2. \end{aligned} \quad (3.97)$$

The spin density reads

$$s_q(\mathbf{r}, \mathbf{r}') := \sum_{\sigma\sigma', i} \rho_q(\mathbf{r}\sigma, \mathbf{r}'\sigma') \langle \sigma' | \hat{\boldsymbol{\sigma}} | \sigma \rangle = \sum_{\alpha} \begin{bmatrix} \phi_{\uparrow}^*(\mathbf{r}') & \phi_{\downarrow}^*(\mathbf{r}') \end{bmatrix} \hat{\boldsymbol{\sigma}} \begin{bmatrix} \phi_{\uparrow}(\mathbf{r}) \\ \phi_{\downarrow}(\mathbf{r}) \end{bmatrix} \quad (3.98)$$

and lastly, the spin-orbit density tensor reads

$$\begin{aligned}
J_{q,\mu\nu} &:= \frac{1}{2i}(\partial_\mu - \partial'_\mu)s_{q,\nu}(\mathbf{r}, \mathbf{r}') \Big|_{\mathbf{r}'=\mathbf{r}} \\
&= \frac{1}{2i} \left(\begin{bmatrix} \phi_\uparrow^*(\mathbf{r}') & \phi_\downarrow^*(\mathbf{r}') \end{bmatrix} \partial_\mu \hat{\sigma}_\nu \begin{bmatrix} \phi_\uparrow(\mathbf{r}) \\ \phi_\downarrow(\mathbf{r}) \end{bmatrix} - \begin{bmatrix} \phi_\uparrow(\mathbf{r}) & \phi_\downarrow(\mathbf{r}) \end{bmatrix} \partial'_\mu \hat{\sigma}_\nu \begin{bmatrix} \phi_\uparrow^*(\mathbf{r}') \\ \phi_\downarrow^*(\mathbf{r}') \end{bmatrix} \right)_{\mathbf{r}'=\mathbf{r}} \\
&= \sum_\alpha \text{Im} \left\{ \begin{bmatrix} \phi_\uparrow^*(\mathbf{r}) & \phi_\downarrow^*(\mathbf{r}) \end{bmatrix} \partial_\mu \hat{\sigma}_\nu \begin{bmatrix} \phi_\uparrow(\mathbf{r}) \\ \phi_\downarrow(\mathbf{r}) \end{bmatrix} \right\}
\end{aligned} \tag{3.99}$$

which also defines the spin-orbit current vector \mathbf{J} that reads

$$J_{q,\kappa}(\mathbf{r}) = \sum_{\mu\nu} \epsilon_{\kappa\mu\nu} J_{q,\mu\nu}(\mathbf{r}). \tag{3.100}$$

Kinetic functional

The kinetic term can be expressed as

$$\mathcal{E}_{\text{Kin}} = \frac{\hbar^2}{2m}\tau \tag{3.101}$$

which is found integrating by parts (3.37).

Skyrme functional

Since this work only deals with even-even nuclei, only time-even densities, which are the ones previously defined, are non-vanishing, due to the ground state being time-reversal invariant [3]. This reduces the Skyrme functional to the following form [84]

$$\mathcal{E}_{\text{Skyrme}} = \sum_{t=0,1} \left\{ C_t^\rho [\rho_0] \rho_t^2 + C_t^{\Delta\rho} \rho_t \nabla^2 \rho_t + C_t^{\nabla \cdot J} \rho_t \nabla \cdot \mathbf{J}_t + C_t^\tau \rho_t \tau_t \right\} \tag{3.102}$$

where

$$C_0^\rho = +\frac{3}{8}t_0 + \frac{3}{48}t_3\rho_0^\sigma \quad (3.103)$$

$$C_1^\rho = -\frac{1}{8}t_0(1+2x_0) - \frac{1}{48}t_3(1+x_3)\rho_0^\sigma \quad (3.104)$$

$$C_0^\tau = +\frac{3}{16}t_1 + \frac{1}{16}t_2(5+4x_2) \quad (3.105)$$

$$C_1^\tau = -\frac{1}{16}t_1(1+2x_1) + \frac{1}{16}t_2(1+2x_2) \quad (3.106)$$

$$C_0^{\Delta\rho} = -\frac{9}{64}t_1 + \frac{1}{64}t_2(5+4x_2) \quad (3.107)$$

$$C_1^{\Delta\rho} = +\frac{3}{64}t_1(1+2x_1) + \frac{1}{64}t_2(1+2x_2) \quad (3.108)$$

$$C_0^{\nabla\cdot J} = -\frac{3}{4}W_0 \quad (3.109)$$

$$C_1^{\nabla\cdot J} = -\frac{1}{4}W_0. \quad (3.110)$$

Here, $t = 0, 1$ refers to the isoscalar and isovector components of the densities, that is

$$\rho_0 = \rho_p + \rho_n$$

$$\rho_1 = \rho_p - \rho_n$$

and the same holds for all generalised densities. We can now derive the Kohn-Sham equations, by minimizing the functional under the constraint

$$\langle \varphi_i | \varphi_j \rangle = \delta_{ij}. \quad (3.111)$$

The resulting Kohn-Sham equations are of the form

$$\left[-\nabla \left(\frac{\hbar^2}{2m_q^*(\mathbf{r})} \nabla \right) + U_q(\mathbf{r}) + \delta_{q,\text{proton}} U_C(\mathbf{r}) - i\mathbf{B}_q(\mathbf{r}) \cdot (\nabla \times \boldsymbol{\sigma}) \right] \varphi_\alpha = \varepsilon_\alpha \varphi_\alpha \quad (3.112)$$

where an effective mass field arises, which is defined as

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = \frac{\delta \mathcal{E}}{\delta \tau_q} \quad (3.113)$$

a mean field potential, which reads

$$U_q(\mathbf{r}) = \frac{\delta \mathcal{E}}{\delta \rho_q} \quad (3.114)$$

and a spin-orbit field, given by

$$\mathbf{B}_q(\mathbf{r}) = \frac{\delta \mathcal{E}}{\delta \mathbf{J}_q}. \quad (3.115)$$

The coulomb field U_C , which is present only in the single particle equation for protons, doesn't come from the Skyrme interaction, rather from the Coulomb part of the whole functional. It will be properly derived in section 3.4.

Following the rules for functional derivatives, outlined in the appendix A.3 we get

$$\begin{aligned} \frac{\hbar^2}{2m_q^*(\mathbf{r})} = & + \frac{\hbar^2}{2m} \\ & + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho(\mathbf{r}) \\ & - \frac{1}{8}[t_1(1+2x_1) + t_2(1+2x_2)]\rho_q(\mathbf{r}) \end{aligned} \quad (3.116)$$

$$\begin{aligned} U_q(\mathbf{r}) = & + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho \\ & + \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\rho_q \\ & + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau \\ & + \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\tau_q \\ & + \frac{1}{16}[t_2(2+x_2) - 3t_1(2+x_1)]\nabla^2\rho \\ & + \frac{1}{16}[3t_1(2x_1+1) + t_2(2x_2+1)]\nabla^2\rho_q \end{aligned} \quad (3.117)$$

$$\begin{aligned} \mathbf{B}_q(\mathbf{r}) = & + \frac{1}{2}W_0[\nabla\rho + \nabla\rho_q] \\ & - \frac{1}{8}(t_1x_1 + t_2x_2)\mathbf{J} + \frac{1}{8}(t_1 - t_2)\mathbf{J}_q. \end{aligned} \quad (3.118)$$

Unless otherwise specified, unlabelled densities denote isoscalar quantities (sum of neutron and proton).

3.3.3. Functionals

The set of parameters $(t_0, t_1, t_2, t_3, x_0, x_1, x_2, \sigma, W_0)$ in the Skyrme functional (3.102) is not fixed and may vary for different parametrizations. These parameters are fitted on experimental data so that the EDF may produce accurate results.

The first parametrization was given by D Vautherin and D M Brink [88], known as S I, was fitted on double magic nuclei and nuclear matter data. This was sufficient for their calculations but not enough to describe other nuclei. Fitting these parameters on

further data over the years led to the introduction of other parameter sets such as S I, S II, S III [21]. These were good functionals to reproduce ground states and certain aspects of nuclear structure, but they lacked the ability to account with good accuracy for deformation properties and fission barriers. The first modern functional to address this issue has been the SkM* [2].

Nowadays functionals such as the SLy family [22], try to be as broad as possible, taking into account results from ab-initio theories, exotic nuclei, drip lines, nuclei far from stability and so on.

3.4. Coulomb interaction

Unlike the Skyrme interaction, the Coulomb force is finite-range, giving rise to an unwanted integral operator in the single-particle Hamiltonian. A well known and widely used device is the Slater approximation [39], which gives a local exchange interaction. In this approximation, the Coulomb energy reads

$$E_{\text{Coul}} = \int \mathcal{E}_{\text{Coul}}(\mathbf{r}) d\mathbf{r}$$

where the energy density is given by

$$\mathcal{E}_{\text{Coul}}(\mathbf{r}) = \frac{e^2}{2} \left[\int \frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - \frac{3}{2} \left(\frac{3}{\pi} \right)^{\frac{1}{3}} \rho_p^{4/3}(\mathbf{r}) \right]. \quad (3.119)$$

which results in the Coulomb potential field

$$U_C(\mathbf{r}) = \frac{\delta \mathcal{E}_{\text{Coul}}}{\delta \rho_p} = \frac{e^2}{2} \left[\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 \mathbf{r}' - 2 \left(\frac{3}{\pi} \right)^{\frac{1}{3}} \rho_p^{1/3}(\mathbf{r}) \right] \quad (3.120)$$

where the first term is the direct Coulomb interaction, which simply is the Coulomb energy generated by the proton density, while the second term is the exchange Coulomb interaction, which is local and depends on the proton density through a power factor of 1/3. From a computational standpoint, the exchange part is trivial, while the direct one is more involved. One could compute the integral, but the complexity on a 3D mesh grows as $\mathcal{O}(N^6)$, where N is the total number of points on the mesh, rendering it unfeasible for fine calculations.

An alternative approach is to solve the Poisson equation (from now on, V_c refers to the direct part only)

$$\nabla^2 V_c = 4\pi e^2 \rho_p. \quad (3.121)$$

Given the proton density, we can impose Dirichlet boundary conditions, which can be extracted from a quadrupole expansion of the charge density [45]

$$V_c(\mathbf{r}) = 4\pi e^2 \sum_{\lambda=0}^2 \sum_{\mu=-\lambda}^{\lambda} \frac{\langle Q_{\lambda\mu} \rangle Y_{\lambda\mu}}{r^{1+\lambda}} \text{ on } \partial\Omega \quad (3.122)$$

where $\langle Q_{\lambda\mu} \rangle$ is defined as

$$\langle Q_{\lambda\mu} \rangle = \int r^\lambda Y_{\lambda\mu}^*(\mathbf{r}) \rho_p(\mathbf{r}) d^3\mathbf{r} \quad (3.123)$$

Since we expect a charge density confined to the nuclear shape, higher order terms in the expansion can be neglected, provided that the box is sufficiently large.

In a reference frame where the nucleus center of mass is at the origin, the expansion reduces to

$$V_c(\mathbf{r}) = \frac{Ze^2}{r} + e^2 \sum_{\mu=-2}^2 \frac{\langle Q_{2\mu} \rangle Y_{2\mu}}{r^3} \text{ on } \partial\Omega. \quad (3.124)$$

The reader can refer to appendix A.1 for the definition and numerical evaluation of the spherical harmonics $Y_{\lambda\mu}$.

3.5. Energy calculation

One, if not the most important physical quantity we want to compute is the total energy of the system.

Integrated energy

The obvious way would be to evaluate the functional for a given density. We will call this *integrated energy*.

$$E_{\text{int}} = E[\rho, \tau, J_{\mu\nu}] = \int \mathcal{E} d\mathbf{r}$$

Hartree-Fock energy

An alternative approach can be used, as in a stationary point $\delta E = 0$, the single particle eigenvalue equation (3.112) stands true, summarized as

$$(t + U)\varphi_k = \varepsilon_k \varphi_k \quad (3.125)$$

We can multiply (3.125) on the left by φ_k^* and integrate to get

$$\int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\mathbf{r} + \int \varphi_k^* U \varphi_k d\mathbf{r} = \int \varphi_k^* \varepsilon_k \varphi_k d\mathbf{r} \quad (3.126)$$

The integral on the right hand side of (3.126) evaluates to ε_k due to the orthonormality constraint. If we sum over all states k we get

$$\sum_k \left\{ \int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\mathbf{r} + \int \varphi_k^* U \varphi_k d\mathbf{r} \right\} = \sum_k \varepsilon_k \quad (3.127)$$

$$\sum_k t_k + \int \rho U = \sum_k \varepsilon_k \quad (3.128)$$

Since U is calculated as the functional derivative with respect to the density ρ (3.114), assuming that the functional has a power dependence from ρ of the form $\mathcal{E}_{\text{Skyrme}} = A\rho^{\sigma+1}$ as in our case, we get the *rearrangement energy*

$$\rho U = \rho \frac{\delta \mathcal{E}_{\text{Skyrme}}}{\delta \rho} = \rho(1+\sigma)A\rho^\sigma = (1+\sigma)A\rho^{\sigma+1} = \mathcal{E}_{\text{Skyrme}} + \sigma \mathcal{E}_{\text{Skyrme}} = \mathcal{E}_{\text{Skyrme}} - \mathcal{E}_{\text{rea}} \quad (3.129)$$

If we explicit ρU in equation (3.128) using (3.129), we get to

$$\sum_k t_k + \int (\mathcal{E}_{\text{Skyrme}} - \mathcal{E}_{\text{rea}}) d\mathbf{r} = \sum_k \varepsilon_k$$

Isolating the Skyrme energy density

$$\int \mathcal{E}_{\text{Skyrme}} d\mathbf{r} = \sum_k (\varepsilon_k - t_k) + \int \mathcal{E}_{\text{rea}} d\mathbf{r} \quad (3.130)$$

and given the total energy of the system from (3.11)

$$E = \sum_k t_k + \frac{1}{2} \int \mathcal{E}_{\text{Skyrme}} d\mathbf{r} \quad (3.131)$$

substituting (3.130) in (3.131) yields

$$E_{\text{HF}} = \frac{1}{2} \sum_k (\varepsilon_k + t_k) + \int \mathcal{E}_{\text{rea}} d\mathbf{r} = \frac{1}{2} \left(T + \sum_k \varepsilon_k \right) + E_{\text{rea}} \quad (3.132)$$

which is called *Hartree-Fock energy*.

Sidenote The actual functional, including the Coulomb exchange term, has different ρ terms, which can be summarized as

$$\mathcal{E}_{\text{Skyrme}} = \sum_j A_j \rho^{\sigma_j + 1} \implies E_{\text{rea}} = - \sum_j \sigma_j A_j \rho^{\sigma_j + 1}$$

This means that only terms with a $\sigma_j \neq 0, -1$ actually contribute to the rearrangement energy.

Since equation (3.132) is valid only for $\delta E = 0$, it's useful to check its equivalence with the integrated energy at convergence, so one can be sure to actually be in a stationary point.

4 | Numerical methods

This chapter is devoted to describing the practical implementation of the nuclear Hartree-Fock method of this work. In section 4.1, the two partial differential equations (PDEs) of interest, the Kohn-Sham equation and the Poisson equation, are numerically approximated through finite differences. In section 4.2.2, a breakdown of numerical solvers for the large-scale eigenvalue problem posed by the KS equation is presented, to pedagogically illustrate the rationale and implementation of the GCG algorithm. Finally, in section 4.3, the self-consistent calculation is presented, along with the implementation of spatial constraints and the optimization of the numerical parameters of GCG.

4.1. Finite differences

The framework used to numerically solve the relevant PDEs of the problem, is the one of finite differences. The core idea is to discretize the domain on a 3D mesh, use Taylor expansions to approximate differential operators and then solve the resulting system of linear equations.

4.1.1. 3D mesh

The first step of the process is representing the different fields in a numerical, discretized fashion. Generally speaking, we deal at most with 2-rank tensors, which depend on three space coordinates and one spin coordinate.

Discretizing the 3D cartesian space with a 3-index mesh, choosing a box whose size along x, y, z is respectively $[-a_x, a_x]$, $[-a_y, a_y]$, $[-a_z, a_z]$, and a number of points n_x, n_y, n_z , the resulting lattice will be given by

$$V = \{(-a_x + ih_x, -a_y + ih_y, -a_z + ih_z)\} = \{(x_i, y_j, z_k)\}$$

Where the indices and step sizes are

$$\begin{aligned} i &= 0, \dots, n_x - 1 & h_x &= \frac{2a_x}{n_x - 1} \\ j &= 0, \dots, n_y - 1 & h_y &= \frac{2a_y}{n_y - 1} \\ k &= 0, \dots, n_z - 1 & h_z &= \frac{2a_z}{n_z - 1} \end{aligned}$$

The following implementation assumes $a = a_x = a_y = a_z = a$ and $n = n_x = n_y = n_z = n$, without losing generality.

Including the spin degree of freedom, we can finally represent the fields in a numerical way through

$$\varphi(\mathbf{r}, \sigma) \mapsto \varphi(x_i, y_j, z_k, s) = \varphi_{ijk s} \quad (4.1)$$

Differential operators discretization

By using Taylor series, it's possible to write approximations to derivatives [93], in any point of the lattice, of any (reasonable) order of accuracy, involving only near neighbouring points. In the present work, 5-points derivatives are used, meaning Taylor expansions are written for $\varphi(x \pm h)$ and $\varphi(x \pm 2h)$ to compute the differential operators. Formulae for first and second derivates are given in appendix A.2.

From the theory background of chapter 3, we discern two main kinds of PDEs: the Schrödinger-like KS equation, and the Poisson equation.

4.1.2. Schrödinger equation

Starting from the Schrödinger equation (3.112), reported here for clarity

$$\left[-\nabla \left(\frac{\hbar^2}{2m_q^*(\mathbf{r})} \nabla \right) + U_q(\mathbf{r}) + \delta_{q,\text{proton}} U_C(\mathbf{r}) - i\mathbf{B}_q(\mathbf{r}) \cdot (\nabla \times \boldsymbol{\sigma}) \right] \varphi = \varepsilon \varphi$$

it can be compactly written as

$$f(\nabla^2 \varphi, \nabla \varphi, \varphi, \mathbf{r}, s) = \varepsilon \varphi. \quad (4.2)$$

If f is linear in φ , it is possible to rewrite it as a linear combination of the values of φ on the mesh, after which we can use linear algebra methods to solve the problem.

Linearity Breaking down each part of the equation, the kinetic term

$$\nabla \left(\frac{\hbar^2}{2m_q^*(\mathbf{r})} \nabla \right) \varphi = \frac{\hbar^2}{2m_q^*(\mathbf{r})} \nabla^2 \varphi + \nabla \left(\frac{\hbar^2}{2m_q^*(\mathbf{r})} \right) \cdot \nabla \varphi \quad (4.3)$$

is evidently linear in φ .

The spin-orbit term of (3.112), which we write as

$$\begin{aligned} \hat{h}_{SO} &= -i\mathbf{B}_q(\mathbf{r}) \cdot (\nabla \times \boldsymbol{\sigma}) \\ &= -i[\mathbf{B}_{q,x}(\mathbf{r})(\sigma_z \partial_y - \sigma_y \partial_z) + \mathbf{B}_{q,y}(\mathbf{r})(\sigma_x \partial_z - \sigma_z \partial_x) + \mathbf{B}_{q,z}(\mathbf{r})(\sigma_y \partial_x - \sigma_x \partial_y)] \end{aligned}$$

is also linear in φ .

Finally, the mean field terms U_q, U_c

$$(U_q + \delta_{q,\text{proton}} U_c) \varphi$$

are just multiplicative, hence linear.

Given that the whole equation is linear in φ , we can evaluate it on the chosen mesh, using finite differences to approximate the differential operators, yielding a linear eigenvalue problem of the form

$$\sum_{\alpha=1}^N A_{\alpha\beta} \varphi_\beta = E \varphi_\alpha \quad (4.4)$$

where the shorthand notation $N = 2 \cdot N_x \cdot N_y \cdot N_z$ is used to denote the size of the matrix A , which is $N \times N$.

Boundary conditions

We expect the nucleus to be a localized object, leading to vanishing Dirichlet boundary conditions for the Schrödinger equation. Near the boundaries, the derivatives will involve points outside the box and setting these points to zero, is equivalent to solving

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & A & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \varphi_{-2} \\ \varphi_{-1} \\ \varphi \\ \varphi_N \\ \varphi_{N+1} \end{bmatrix} = E \begin{bmatrix} \varphi_{-2} \\ \varphi_{-1} \\ \varphi \\ \varphi_N \\ \varphi_{N+1} \end{bmatrix} \quad (4.5)$$

From this system of equations, we get for points outside the boundary:

$$\begin{cases} \varphi_{-2} = 0 \\ \varphi_{-1} = 0 \\ \dots \end{cases} \quad (4.6)$$

Meaning that φ outside the box will automatically be set to zero if the A matrix is built assuming those points to be zero when computing its coefficients.

4.1.3. Poisson equation

The other fundamental PDE we need to solve is the Poisson equation encountered in section 3.4. Dropping the c and p subscripts, it reads

$$\nabla^2 V = 4\pi e^2 \rho$$

It's simpler than the Schrödinger equation, as it only involves a Laplacian and it's not an eigenvalue problem. The right side is given, and the solution is found by inverting the coefficients' matrix.

Boundary conditions

Unlike the Schrödinger equation, we do not expect the solution to rapidly decay near the boundaries; as reported in section 3.4, we have fixed, non-vanishing boundary conditions, which we have to properly impose on the system.

We can choose a direction, say x , and look at the discretized equation at the boundaries $x = \pm a$. Since the indices j, k won't vary, we can omit them, and ignore the other derivates in the following equations.

$$\begin{aligned} \nabla^2 V &= \partial_{xx} V + \partial_{yy} V + \partial_{zz} V \\ &= \frac{-V_{i-2} + 16V_{i-1} - 30V_i + 16V_{i+1} - V_{i+2}}{12h^2} + \dots = 4\pi e^2 \rho_i \end{aligned} \quad (4.7)$$

Near a boundary, say $i = 0$, the formula calls for points outside the box, known as *ghost points*. Since they are not part of the linear system, but they are known, we can bring them on the right side of equation (4.7).

$$\frac{-30V_0 + 16V_1 - V_2}{12h^2} = 4\pi e^2 \rho_0 + \frac{V_{-2} - 16V_{-1}}{12h^2} = \tilde{\rho}_0 \quad (4.8)$$

The same procedure must be applied to all equations involving ghost points, e.g. for $i = 1$

$$\frac{+16V_0 - 30V_1 + 16V_2 - V_3}{12h^2} = 4\pi e^2 \rho_1 + \frac{V_{-1}}{12h^2} = \tilde{\rho}_1. \quad (4.9)$$

The proper system to solve will then be

$$AV = \tilde{\rho} \quad (4.10)$$

Where A is constructed as previously specified. Solving with $\tilde{\rho}$ on the right hand side will force the solution to obey boundary conditions.

On higher order approximations and performance

Higher and higher order approximations for derivatives involve more points that are further away. This increases accuracy by reducing the finite differences error, but it also decreases the matrix sparseness.

4.2. Eigenvalue problem

This section is devoted to the approximate solution of the eigenvalue problem, needed for the Schrödinger equation (3.112).

Eigenvalue problems are ubiquitous in physics and engineering, and while solving one for a small matrix is trivial, it still requires roughly $O(n^3)$ operations [37] to do so. More often than not, real computational applications result in large-scale matrices, which are completely out of question for exact eigenvalues calculations, thus requiring the use of approximate algorithms.

We will begin by describing common building blocks of iterative eigensolvers in section 4.2.1, namely:

- the approximate solutions of linear systems by the use of the Conjugate Gradient method;
- matrix preconditioning to speed up convergence;
- the Rayleigh-Ritz procedure to find good approximations to the eigenpairs in a certain subspace; and
- the shift-and-invert method, to select the desired portion of the eigenvalue spectrum.

After describing these building blocks, some of the most commonly used eigensolvers are described in section 4.2.2, focusing on the core ideas and stating their limitations, to

finally address the Generalised Conjugate Gradient method, whose implementation in the present work is detailed in section 4.2.3.

4.2.1. Conjugate Gradient and numerical techniques

Conjugate Gradient method

Solving linear systems of the form

$$Ax = b \quad (4.11)$$

is crucial in many eigensolvers. The Conjugate Gradient (CG) is perhaps the most famous iterative solver in this sense, especially in connection with sparse matrices, as we will see in a moment. CG applies to cases where A is a real, $n \times n$, positive-definite, symmetric matrix, and x and b are n -dimensional vectors.

Many generalizations to this method exist, which relax the requirements on the matrix, like BiCGSTAB, CGRES and so on [74]. We will describe the working principle of CG, but the same applies to all the others, with slight variations.

Steepest descent method The quadratic form $f(x)$ derived from the system (4.11) is

$$f(x) = \frac{1}{2}x^T Ax - b^T x \quad (4.12)$$

If A is symmetric, positive-definite, the shape of $f(x)$ is convex and has a global minimum for

$$\nabla_x f(x) = Ax_m - b = 0 \implies Ax_m = b, \quad (4.13)$$

hence the extremum of the quadratic form is the also the solution of the linear system (4.11).

We can employ the well-known gradient descent technique [80] to find such point: starting from a guess x_0 , we compute the direction d_i where f decreases the most (the residual r_i), compute the step size that gives the largest decrease, and update x_i at each iteration accordingly, repeating until convergence.

$$d_i = r_i = b - Ax_i \quad (4.14)$$

$$x_{i+1} = x_i + \alpha_i r_i \quad (4.15)$$

$$\text{with } \alpha_i \text{ such that } \frac{df}{d\alpha_i} = 0 \implies \alpha_i = \frac{r_i^T r_i}{r_i^T A r_i} \quad (4.16)$$

This is a powerful but highly inefficient procedure. We are not ensuring that the search direction doesn't end up with components in subspaces that were explored already.

It can be proven [80] that the norm of the error $e_i = x_i - x_m$ is minimal at each iteration if the search directions d_i are chosen to be A -orthogonal to the next error, i.e. $d_i^T A e_{i+1} = 0$. This makes the algorithm converge at the exact solution in n steps, but most importantly it allows to truncate the iterations without a large error on the approximation x_i .

In this case, the algorithm is called Conjugate Gradient Method and is formulated as

$$\alpha_i = \frac{r_i^T r_i}{d_i^T A d_i} \quad (4.17)$$

$$x_{i+1} = x_i + \alpha_i d_i \quad (4.18)$$

$$r_{i+1} = r_i - \alpha_i A d_i \quad (4.19)$$

$$\beta_{i+1} = \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i} \quad (4.20)$$

$$d_{i+1} = r_{i+1} + \beta_{i+1} d_i \quad (4.21)$$

where iterations are truncated if the norm of the residual r_i is smaller than a certain threshold. It can be proven that the orthonormalization of the new search direction, with respect to all the previous ones, can be done only through the rescaling factor β_{i+1} [80]. CG converges to the exact solution in n steps, moreover, it represents a great method for sparse matrices, because it can be proven to be of complexity $O(m)$, where m is the number of non-zero elements in A [80]. In figure 4.1, a visual representation of the conjugation of search directions and the subsequent exact solution is shown for a two-dimensional problem.

Complex matrices Algorithm (4.17) and the CG method in general can be used for complex matrices, under the condition that A is Hermitian and positive-definite when using the complex inner product, meaning that

$$A = A^\dagger \text{ and } x^\dagger A x > 0. \quad (4.22)$$

Preconditioning

The CG method convergence is known to be limited by the modulus of the condition number of A , $\kappa(A)$, given by [80]

$$\kappa(A) = \frac{\lambda_{\max}(A)}{\lambda_{\min}(A)} \quad (4.23)$$

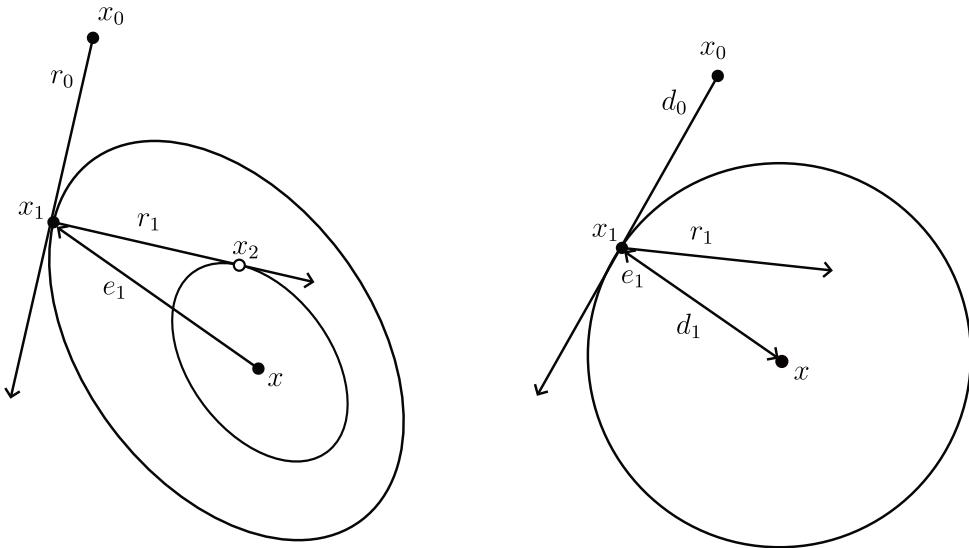


Figure 4.1: Comparison between the steepest descent method, on the left, and the conjugate gradient method, on the right, for a two-dimensional matrix. Ellipses represent contour lines of the quadratic form $f(x) = x^T Ax - b^T x$, in the ‘stretched’ space Ax on the right. As shown in the figure, the conjugation of the search directions eliminates components of the error e_i , until the exact convergence in n (2) steps.

where λ_{\max} and λ_{\min} are respectively the largest and smallest eigenvalues of A in magnitude. If we were able to find a good *preconditioner* M , symmetric and positive-definite, such that $\kappa(M^{-1}A) \ll \kappa(A)$, and M^{-1} is easy to compute, then the algorithm would converge much faster, by solving $M^{-1}Ax = M^{-1}b$, since x is also the solution of $Ax = b$.

$$x = (M^{-1}A)^{-1}M^{-1}b = A^{-1}MM^{-1}b = A^{-1}b. \quad (4.24)$$

Without delving into the details of the preconditioner implementation, detailed in [80], note that, in general, $M^{-1}A$ is neither positive-definite nor symmetric, which requires a Cholesky decomposition [50] $M = EE^T$ to be used, so that the problem may be restated with a symmetric positive-definite matrix $E^{-1}AE^{-T}$.

The catch with preconditioning is that M has no unique recipe. Preconditioners are widely spread across numerical analysis, so many methods have been explored and implemented [64].

Rayleigh-Ritz procedure

A common denominator of all these algorithms is the search of good approximations for the correct eigenvectors in a certain subspace. The method is called Rayleigh-Ritz (RR) procedure [74], and is here outlined.

Let us suppose to have a matrix A of size $n \times n$, with entries in \mathbf{C} and a collection of vectors k organized in a matrix K , where K is of size $n \times k$. Generally speaking, n is large, while k is much smaller.

The best approximation of the true eigenvectors of A in the subspace \mathcal{K} spanned by the vectors in K can be computed by solving the small scale eigenvalue problem

$$K^\dagger A K C = C \Lambda. \quad (4.25)$$

Here matrices $K^\dagger A K$ and C are of size $k \times k$. Computing $K C$ gives a matrix of size $n \times k$, whose column vectors are the best approximations of the true eigenvectors of A in the subspace \mathcal{K} , with their corresponding eigenvalues in the entries of the diagonal matrix Λ .

Shift and Invert

The power iteration is the technique on which Krylov subspace search methods are based [37]. By repeatedly applying matrix A to a vector x , x gets skewed towards the eigenvector whose eigenvalue is of largest magnitude λ_n .

Let us assume A is a hermitian matrix, thus diagonalizable. This means we can write an arbitrary vector $x^{(0)}$ as a linear combination of the eigenvectors $\{v_i\}$ of A .

$$x^{(0)} = \sum_i^n \alpha_i v_i \quad (4.26)$$

If we apply A to $x^{(0)}$ k times, we get

$$x^{(k)} = A^k x^{(0)} = \sum_i^n \alpha_i A^k v_i = \sum_i^n \alpha_i \lambda_i^k v_i \quad (4.27)$$

It can be proven that the ratio of the j -th component of $x_j^{(k)}$ and $x_j^{(k-1)}$ converges to λ_n

$$\lim_{k \rightarrow \infty} \frac{x_j^{(k)}}{x_j^{(k-1)}} = \lambda_n \quad (4.28)$$

which means, that for large enough k , we have the relation

$$A x^{(k)} \approx \lambda_n x^{(k)} \quad (4.29)$$

So $x^{(k)}$ is an approximation of the eigenvector v_n of A whose eigenvalue is λ_n .

Smallest eigenvalue If instead of the largest eigenvalue, we were interested in the smallest one – in magnitude – λ_0 , then we would need to apply the inverse matrix A^{-1} to $x^{(k)}$, which would change the ratio (4.28) to

$$\lim_{k \rightarrow \infty} \frac{x_j^{(k)}}{x_j^{(k-1)}} = \lambda_0 \quad (4.30)$$

Let us assume for a moment that we're solving a nuclear single-particle Hamiltonian, where we have a certain number of bound states of negative energy and a much larger number of unbound states with positive energy. In this case, the inverse power iteration would converge to the states whose energy is closer to zero, avoiding the interesting ones on the bottom of the spectrum.

The solution is, before inverting, to shift the matrix by a quantity σ that is very close to the lowest eigenvalue we want to compute, call it λ_σ (eigenvector v_σ). Now, the eigenvalue of lowest magnitude of $(A - \sigma I)$ is $\lambda_\sigma - \sigma$ and by applying $(A - \sigma I)^{-1}$ to $x^{(k)}$, we will get the approximation to the eigenvector v_σ . This is the procedure implemented in step 8 of algorithm 4.3.

4.2.2. Iterative eigensolvers

Now that the main techniques used by iterative eigensolvers have been laid out, we can look at three general methods, which are the most commonly used ones.

Jacobi-Davidson

The Jacobi-Davidson method is a type of algorithm where at each iteration, the approximation to an eigenpair of matrix A , is improved by correcting the eigenvector through the solution of a certain linear system, as we shall see shortly.

Given an approximation (u, θ) of an eigenpair of matrix A , where u is the approximate eigenvector and θ is the approximate eigenvalue, if the residual

$$r = Au - \theta u \quad (4.31)$$

is ≈ 0 , then the eigenpair converged. Otherwise, we want to find a correction t such that

$$r = A(u + t) - (\theta + \delta\theta)(u + t) = 0 \quad (4.32)$$

Linearizing this equation in t gives

$$(A - \theta I)t = -r \quad (4.33)$$

To avoid singularity of the equation near convergence, since u approximately spans a subspace of the system's kernel $\ker(A - \theta I)$, and enrich the subspace search with a useful orthogonal correction, we project the problem onto the orthogonal subspace of u , which finally gives

$$(I - uu^\dagger)(A - \theta I)(I - uu^\dagger)t = -r \quad (4.34)$$

Although simple, this method is computationally efficient only by using preconditioning,

Algorithm 4.1 Jacobi-Davidson method

- 1: Choose normalised initial vectors $\{u_k\}$, set $V = [u_1, \dots, u_k]$
 - 2: **repeat**
 - 3: Compute eigenpair: $T = V^\dagger AV$, solve $Ty = \theta y$
 - 4: Set $u = Vy$, residual $r = Au - \theta u$
 - 5: **if** $\|r_k\| < \varepsilon \forall k$ **then**
 - 6: **return** (θ, u)
 - 7: **end if**
 - 8: Solve approximately $(I - u_k u_k^\dagger)(A - \theta I)(I - u_k u_k^\dagger)t_k = -r_k$ using preconditioned iterative solver, ensuring $t_k \perp u_k$
 - 9: Normalize: $v_k = t_k / \|t_k\|$
 - 10: Expand subspace, setting $V = [V, v]$
 - 11: **until** convergence for $k = 1, \dots, \text{nev}$
-

which is known to be unstable in many cases [74].

Lanczos

Lanczos algorithm [51] is probably the most used iterative eigensolver for hermitian matrices. It's a Krylov subspace search method, meaning the Rayleigh-Ritz procedure is done on a subspace formed as

$$\mathcal{K} = \{v_1, Av_1, A^2v_1, \dots, A^{k-1}v_1\} \quad (4.35)$$

which exploits the power iteration. After orthogonalizing the new approximation to the previous one and diagonalizing the small scale problem, we end up with the new best approximations to the eigenvectors of A . Lanczos is extremely efficient, memory- and CPU-wise for extremal eigenvalues, but this limits its applicability, as one may be interested in the inner portion of the eigenvalue spectrum, such in the case of Hartree-Fock-Bogoliubov

Algorithm 4.2 Lanczos Method

```

1: Choose normalised initial vector  $v_1$ , set  $\beta_0 = 0$ ,  $m$  = subspace size.
2: repeat
3:   for  $j = 1, 2, \dots, m$  do
4:      $w \leftarrow Av_j - \beta_{j-1}v_{j-1}$ 
5:      $\alpha_j \leftarrow v_j^*w$ 
6:      $w \leftarrow w - \alpha_jv_j$ 
7:      $\beta_j \leftarrow \|w\|$ 
8:     if  $\beta_j = 0$  then
9:       break
10:    end if
11:     $v_{j+1} \leftarrow w/\beta_j$ 
12:  end for
13:  Form tridiagonal matrix  $T_m = \text{tridiag}(\beta_{1:m-1}, \alpha_{1:m}, \beta_{1:m-1})$ 
14:  Compute eigen-decomposition  $T_m y_k = \theta_k y_k$ , for  $k = 1, \dots, \text{nev}$ 
15:  Form Ritz approximations  $x_k = V_m y_k$ , where  $V_m = [v_1, \dots, v_m]$ 
16:  Compute residual norms  $r_k = \|Ax_k - \theta_k x_k\|$  for all  $k$ 
17: until convergence for  $k = 1, \dots, \text{nev}$ 

```

(HFB).

A shift-and-invert strategy would be unfeasible in the case of large scale problems, since all Lanczos steps need to be performed exactly to avoid instabilities, a well known problem in the Arnoldi generalization [74].

LOBPCG

The last algorithm of this short list is LOBPCG, it's the newest and most sophisticated one of the three.

Introduced by A. V. Knyazev in 1991 [46], it's a block, preconditioned conjugate gradient method, explicitly targeted at solving large-scale eigenvalue problems, and it has been used in modern solutions of the Schrödinger/KS equation in recent years [52, 54, 62, 92]. We won't go into the details of LOBPCG, since GCG shares with it many aspects, like blocking and search directions calculation.

LOBPCG works very well for large scale problems, but it has limitations. On the one hand, it's not possible to arbitrarily select the portion of the matrix spectrum to calculate, which is required for problems where variational collapse happens, like in HFB or the Dirac equation, which manifests particle/antiparticle solutions [52]. To solve this, an additional filtering step is required [52, 54], which introduces a computational cost in the algorithm. Lastly, LOBPCG may fail when poor conditioning is present or when high precision on the eigenvalues is required [53].

4.2.3. Generalised Conjugate Gradient

The Generalised Conjugate Gradient is an iterative eigensolver designed with the aim of improving LOBPCG, it is a blocked algorithm, which uses the inverse power method and previous search directions to generate the search subspace. GCG is proven to be faster and more stable than LOBPCG [53].

The search subspace is built as

$$V = [X, P, W], \quad (4.36)$$

where X , of dimensions $n \times k$ is the matrix containing the approximations, to the eigenvectors of matrix A , P , of dimensions $n \times k$ is the matrix containing the previous search directions, and W , of dimension $n \times a$ is the matrix containing the eigenvectors on which the inverse power method is applied approximately using the CG.

A slightly different implementation of the algorithm is employed in the present work, detailed in algorithm 4.3, to improve applicability to HF calculations and reduce the computational cost.

Eigenvalue problem The original algorithm aims at solving the general eigenvalue problem $AX = \lambda BX$. Since in our case $B = I$, it is omitted from the procedure, reducing the computational cost of the algorithm, in particular, the one of the search direction block P . After orthonormalization of V , the columns of X are orthonormal as well and the calculation of P is given by

$$P = X_{\text{new}} - X(X^\dagger X_{\text{new}}) \quad (4.37)$$

which is the projection of X_{new} onto the orthogonal complement of X , used in step 12 of algorithm 4.3.

Complex matrix The algorithm has been generalised to the complex case, where the matrix is complex Hermitian and, as such, the transposition operation is replaced by the conjugate transpose.

Blocking The algorithm is designed to allow blocking of the eigenvectors, such that $X = [X_c, X_a, X_r]$, where X_c are the converged eigenvectors, X_a are the active eigenvectors on which we perform the inverse power iteration, with $\text{col}(X_a)$ being a fixed number, and X_r are the remaining eigenvectors, which are to be inserted in X_a as soon as some of its columns converge. This allows to save some computations by avoiding the expensive inverse power on pairs that have already converged. Since in a self-consistent calculation

the matrix changes rapidly at each HF iteration, it is the case that the maximum number of iterations is reached before convergence of all eigenpairs, so we must work at all times on the remaining un converged eigenvectors. For this reason, we only implement the $X = [X_c, X_a]$ scheme, where the only distinction we make is between converged eigenvectors X_c and un converged ones X_a .

Orthogonalization The original paper [53] suggests an improved orthogonalization procedure; being beyond the scope of this work, the simpler Gram-Schmidt [10] orthogonalization is used in the present work.

Shift update The shift update is either fixed, in case of known spectrum, eg for HFB `shift = 0`, or adaptive [53], so that the inverse power step can find the lowest eigenvalues, using the update formula

$$\text{shift} = (\lambda_{\text{nev}} - 100\lambda_1)/99 \quad (4.38)$$

where λ_{nev} is the biggest eigenvalue of the RR procedure and λ_1 is the smallest of the active eigenpairs.

Preconditioning The use of a preconditioner is beyond the scope of this work, a simple diagonal preconditioner is used.

Algorithm 4.3 Generalised Conjugate Gradient algorithm

- 1: **Input:** Matrix A of dimensions $n \times n$, number of desired eigenpairs `nev`, X_{guess} initial guess of dimensions $n \times k$, with $= k \geq \text{nev}$, `max_iter` maximum iterations
 - 2: Initialize block $X = [X_a] \leftarrow X_{\text{guess}}$ and X_c as an empty block
 - 3: Initialize blocks P and W as empty blocks
 - 4: Solve the Rayleigh Ritz problem $X^\dagger A X C = C \Lambda$
 - 5: Update $X = XC$
 - 6: Initialize `shift`, Initialize `iter` = 0
 - 7: **while** $\text{col}(X_c) < \text{nev}$ and $\text{iter} < \text{max_iter}$ **do**
 - 8: Solve approximately $(A + \text{shift} \cdot I)W = X_a \Lambda$ with some CG steps, initial value X_a to generate W as an approximation to $W = (A + \text{shift} \cdot I)^{-1} X_a \Lambda$
 - 9: Orthogonalize $V = [X, P, W]$, of dimensions $n \times (k + k + a)$
 - 10: Solve the Rayleigh Ritz problem $V^\dagger (A + \text{shift} \cdot I) V C = C \Lambda$
 - 11: Update X_{new} with the first `nev` columns of VC and $\Lambda_{\text{new}} = \Lambda - \text{shift} \cdot I$
 - 12: Compute $P = X_{\text{new}} - X(X^\dagger X_{\text{new}})$
 - 13: Compute the residual $R = AX_{\text{new}} - \Lambda X_{\text{new}}$
 - 14: Check convergence on k -th column norm of R , if $\|R_k\| < \text{tol}$, move $X_{a,k}$ to X_c .
 - 15: Update `shift` using formula (4.38) and $\text{iter} \leftarrow \text{iter} + 1$
 - 16: **end while**
 - 17: **Output:** Approximate eigenpairs (Λ, X)
-

4.3. Code implementation details

In this last section regarding numerical methods, some important features about the actual code implementation of the HF method are discussed. Mainly, the implementation of the Augmented Lagrangian Method to enforce spatial constraints on the HF solution, the pseudocode of the entire self-consistent procedure, and the choice of optimal parameters for the functional minimization.

4.3.1. Constraints

The purpose of spatial constraints is to find the minimum of the energy functional under the condition that the expectation value of a given operator \mathcal{Q} equals a prescribed target value q_0 . Constrained calculations are a fundamental tool to assess the stability of the ground-state minimum and to investigate dynamical properties of the nucleus, such as fission barriers [13].

Constraints can be formulated as an equality-constrained optimization problem (ECP), formulated as

$$\min_{|\Psi\rangle} E \quad (4.39)$$

$$\text{constrained to } \langle \Psi | \mathcal{Q} | \Psi \rangle = \langle \mathcal{Q} \rangle = q_0 \quad (4.40)$$

Which yields the Lagrangian

$$E' = E + \lambda(\langle \mathcal{Q} \rangle - q_0) \quad (4.41)$$

where λ is a Lagrange multiplier determined by the condition $\langle \mathcal{Q} \rangle = q_0$. After finding the minimum of E' , it's trivial to show that for a given λ , we get [34]

$$\frac{dE}{d\langle \mathcal{Q} \rangle} = -\lambda. \quad (4.42)$$

From a numerical standpoint, λ needs to be tuned at each iteration to reach the desired value of q_0 . This method was the one used in early constrained Hartree-Fock calculations [28].

Although this method is simple, it often fails. Moreover, for the same value of λ , many, possibly infinite values of $\langle \mathcal{Q} \rangle$ can be obtained, for which we are only allowed to get the one with the most stable solution.

A different method is provided by the Quadratic Penalty Method (QPM). Briefly speaking, instead of a Lagrange multiplier, we add a quadratic contribution to the functional, such that

$$E' = E + \frac{c}{2}(\langle \mathcal{Q} \rangle - q_0)^2. \quad (4.43)$$

This is a straightforward method; intuitively one penalizes (hence the name), any solution for which $\langle \mathcal{Q} \rangle \neq q_0$ by increasing its energy. However, the success of such procedure is heavily influenced by the choice of c , often leading to instabilities for large values.

What happens is that for small values of c , the penalty may be insufficient to reach the target q_0 , while for bigger values, the penalty may be so strong that the self-consistent calculation oscillates and fails.

Augmented Lagrangian Method

A modern, robust approach, used by HF/HFB codes [23, 71] is given in the form of the Augmented Lagrangian Method (ALM) [83]. Its main idea is to combine the precision of the ECP with the accuracy of the QPM.

Without delving into cumbersome mathematical details, we'll see how the algorithm is practically implemented in the code.

Given the functional

$$E' = E + \lambda(q - q_0) + \frac{c}{2}(q - q_0)^2 \quad (4.44)$$

where $q = \langle \mathcal{Q} \rangle$, the resulting mean field potential will be given by

$$U' = U + \lambda\mathcal{Q} + c(q - q_0)\mathcal{Q} \quad (4.45)$$

$$= U + c(q - q_0(\lambda))\mathcal{Q} \quad (4.46)$$

where $q_0(\lambda)$ is updated at each iteration with the formula

$$q_0(\lambda) = q_0 - \frac{\lambda}{c} \quad (4.47)$$

$$\lambda^{(i+1)} = \lambda^{(i)} + \mu c(q - q_0) \quad (4.48)$$

Here, a slight deviation from the original ALM is present. Since the original work [83] doesn't provide guidance regarding what is considered an *iteration*, we employ the strategy [23] of using a damping factor $\mu \in [0, 1]$, so λ can be updated at each HF iteration for fast convergence, without large oscillations or instabilities of any kind.

This method is what powers the deformation curves that are shown in chapter 6, allowing to explore the energy surface with arbitrary precision in reaching the value of q_0 at convergence, provided that enough HF iterations are performed.

Note that, since $\lambda^{(0)} = 0$, for $\mu = 0$ ALM reduces to the standard QPM.

4.3.2. Details on the implementation of the code

The whole Hartree-Fock framework presented up to this point, has been implemented using the C++ language [86] and the Eigen linear algebra library [40], which implements linear algebra operations through low level routines such as LAPACK and BLAS. In figure 4.2, the schematics of the program structure is reported.

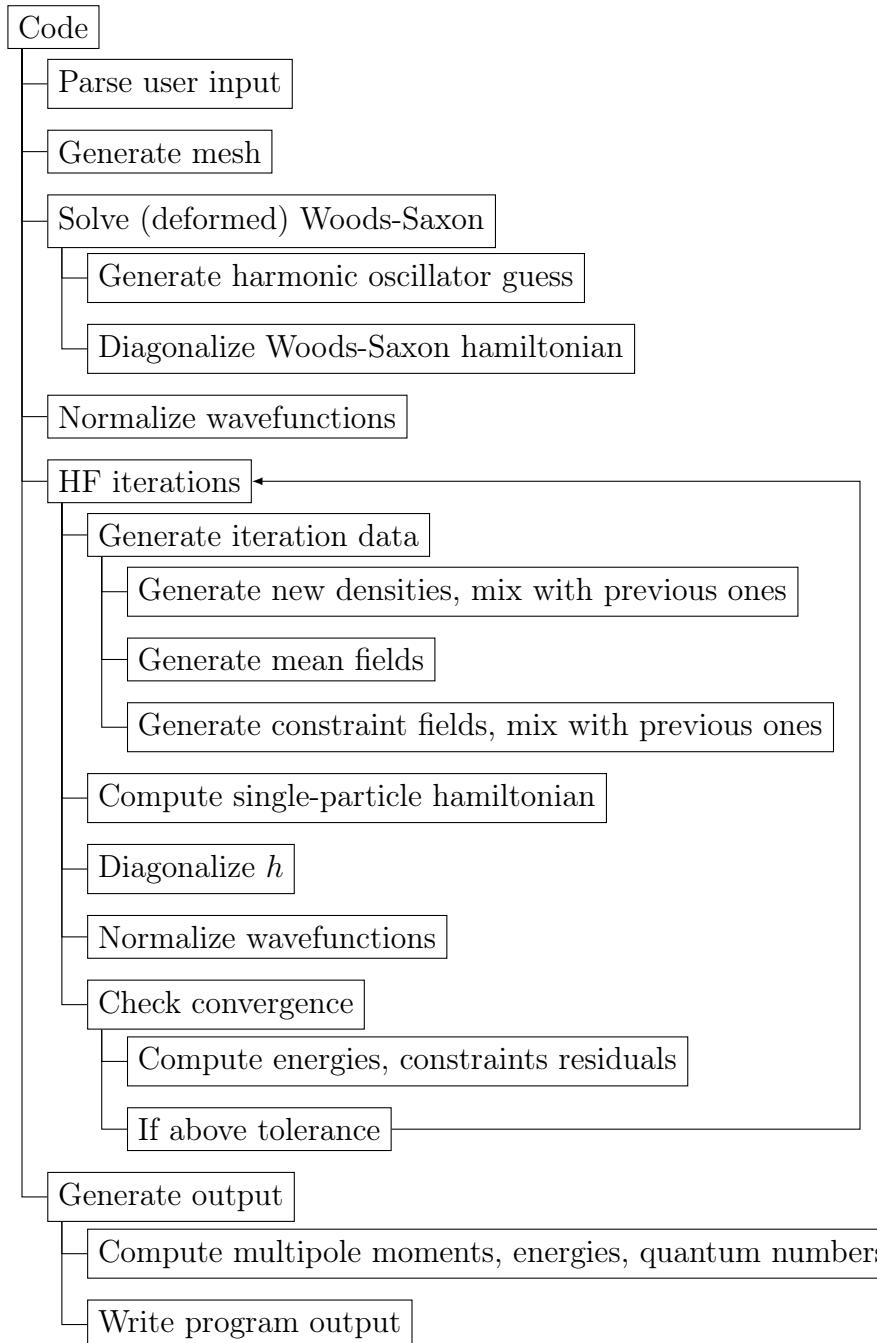


Figure 4.2: Pseudocode of the Hartree-Fock program.

4.3.3. Optimal parameters choice

Inside the ‘Diagonalize h ’ step in figure 4.2, the execution of the GCG algorithm is performed, using the current iteration’s single-particle Hamiltonian as the matrix to diagonalize and the previous iteration’s orbitals as the initial guess. This is the main computational bottleneck of the code, where a correct choice of the execution parameters can drastically reduce execution times. The parameters that need to be chosen carefully are essentially the inverse power step tolerance and the number of maximum GCG iterations.

Inverse power step tolerance

The first parameter to be tuned is the tolerance on the CG step which approximately solves the system

$$(A + \text{shift} \cdot I)W = X_a\Lambda \quad (4.49)$$

in algorithm 4.3, where A is actually the single-particle Hamiltonian h . When the CG residual $(A + \text{shift} \cdot I)W - X_a\Lambda$ is smaller than the tolerance, the procedure stops and outputs the W block.

In figure 4.3, the relative absolute error of the total energy is calculated against a reference benchmark value (details in the results chapter 5), for different values of the CG tolerance. It’s clear that at least a tolerance of 10^{-3} is needed for good convergence, while tolerances $\geq 10^{-4}$ stop offering increasing returns, rendering a choice between 10^{-4} and 10^{-5} an optimal one.

Inner GCG iterations

The number of inner GCG maximum iterations, here named ‘inverse power steps’ to avoid confusion, is slightly more nuanced than the CG tolerance. The algorithm converges to the true eigenpairs as the power steps are performed, so one could think that a higher number of steps would bring to HF convergence faster, since the precision on the eigenvalues increases, but this is not the case.

In figures 4.4 and 4.5, the convergence of the HF calculation is plotted for different number of steps, respectively, for the spherical nucleus ^{16}O and the deformed nucleus ^{24}Mg . It’s evident that in both cases, a steps number greater than 3 leads to oscillating behaviour near convergence, without accelerating it, while in the case of the spherical nucleus, just one step is enough to quickly, and reliably reach convergence. In any case, it’s clear that delaying the inverse power steps to later HF iterations is safer in terms of stability.

This counter intuitive behavior is likely due to the fact that at each HF iteration the hamiltonian changes and a great number of steps leads to solutions too biased towards

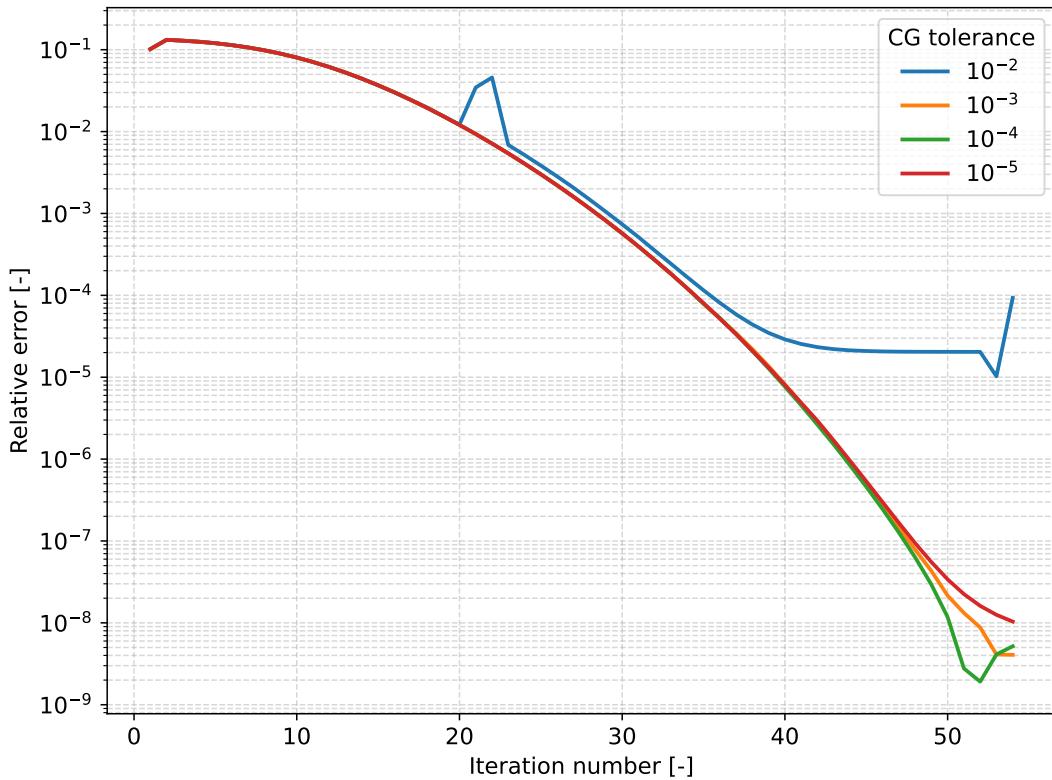


Figure 4.3: HF calculation convergence with varying CG tolerance for ^{16}O , box $[-9, 9]$ fm, step size 0.3 fm.

the current matrix eigenpairs, at the expense of the next iteration; however, in the case of deformed nuclei, due to sharp shape changes at the start of the calculation, just one step may not be enough to sustain the pace at which the Hamiltonian changes, hence the quicker convergence with more steps.

4.3.4. Numerical stability

As a final remark, the numerical stability of the solver is reported in figure 4.6. The map is produced for a spherical calculation of ^{16}O , with varying box and mesh sizes.

It's possible to observe that for a box whose side is at least ≈ 2.5 times the nuclear radius, the solver numerical stability is loosely dependent on the box extension, but rather on the step size. This is not surprising, as the points separation in space h dictates the precision of the discretized derivatives, as mentioned in section 4.1.

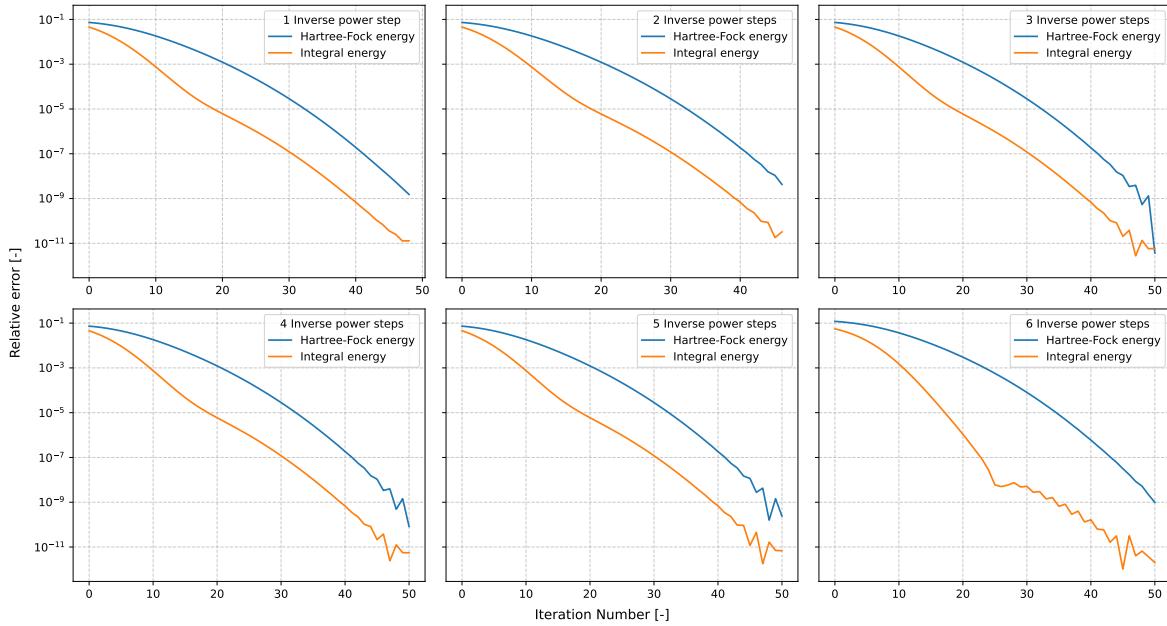


Figure 4.4: HF calculation convergence with varying number of inverse power steps for ^{16}O , box $[-9, 9]$ fm, step size 0.3 fm.

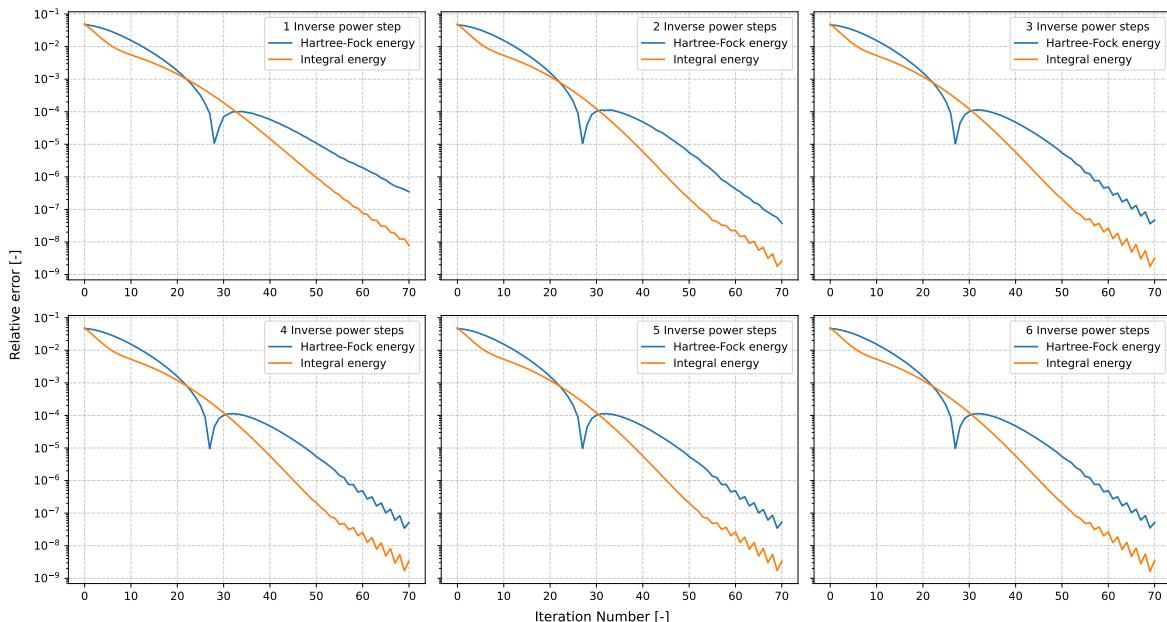


Figure 4.5: HF calculation convergence with varying number of inverse power steps for the deformed nucleus ^{24}Mg , box $[-10, 10]$ fm, step size 0.33 fm.

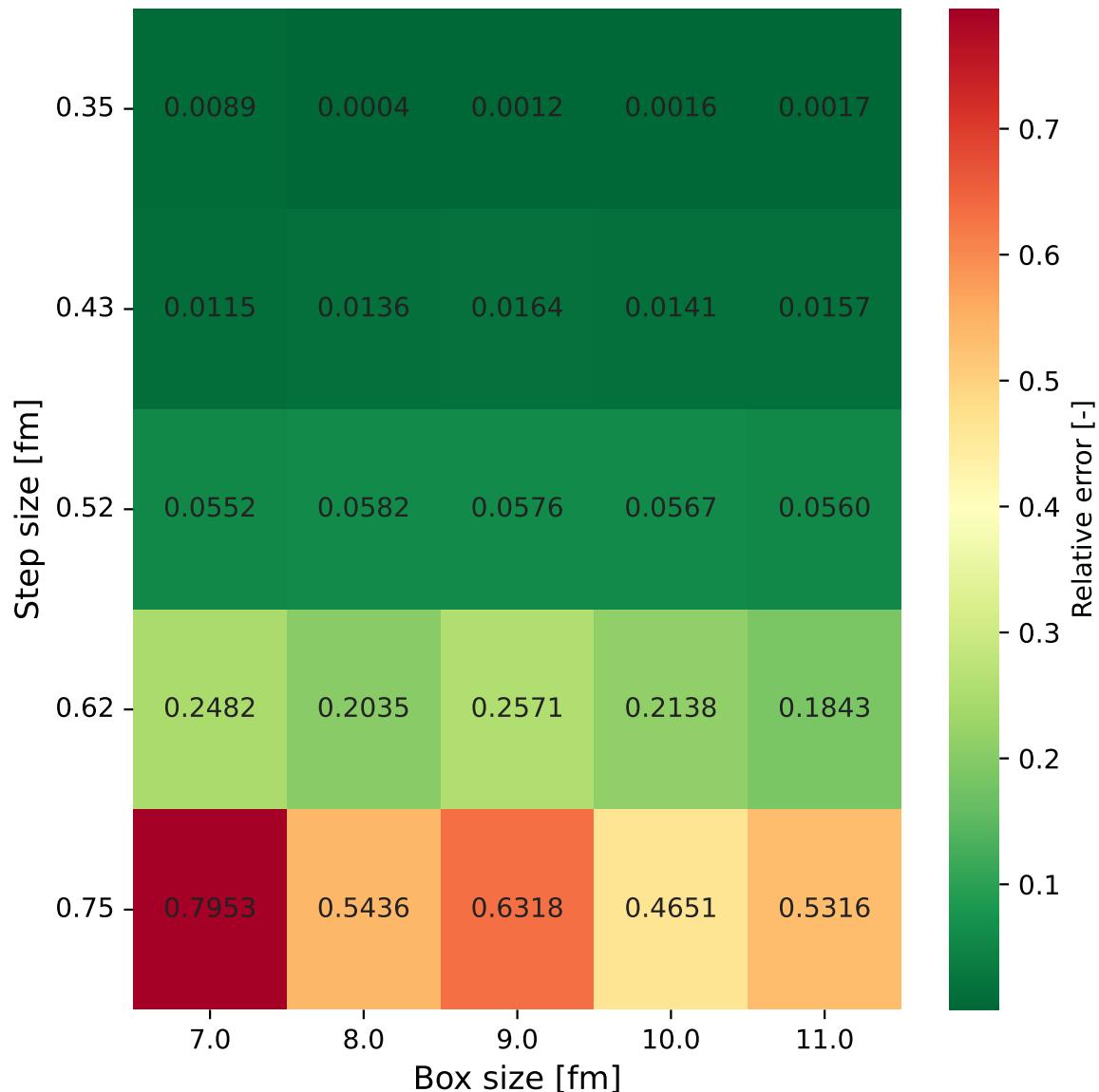


Figure 4.6: Numerical stability map of the HF solver for ^{16}O for different box and step sizes. Relative error is taken against a benchmark reference value.