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Abstract

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Abstract in lingua italiana

Qui va l'Abstract in lingua italiana della tesi seguito dalla lista di parole chiave.

Parole chiave: qui, vanno, le parole chiave, della tesi

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1.1. Hartree-Fock theory

An empirical description of nuclear structure can be carried out using phenomenological models, as reported in section (REF).
A more rigorous approach needs to take into account the fact that the mean field which the nucleons interact with, is generated by the nucleons themselves, due to some microscopic interaction. Starting from the many-body Hamiltonian of the system, we will be able to extract a single particle hamiltonian, where the nucleon is subject to a mean field potential generated by the effective microscopic force.
The many-body hamiltonian of the system, made of A fermions, given by

$$\hat{H} = \hat{T} + \hat{V} = \sum_i -\frac{\hbar^2}{2m}\nabla_i^2 + \sum_{i<j} v_{ij}^{(2)} + \sum_{i<j<k} v_{ijk}^{(3)} \tag{1.1}$$

which acts on the slater determinant given by

$$\Psi = \frac{1}{\sqrt{A!}} \sum_{\{p\}} (-1)^p \varphi_{p(1)}(\boldsymbol{r}_1) \dots \varphi_{p(A)}(\boldsymbol{r}_A) \tag{1.2}$$

where φ_i are single-particle states. 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.

1.1.1. Hartree-Fock equations

It is possible to show [17] that the ground state of the many-body system, found by minimizing the functional

$$E[\Psi] = \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{1.3}$$

Is found in the basis of eigenstates of the single-particle hamiltonian, found by setting to 0 the functional variation of $E[\Psi]$ in φ_i^* with the orthonormality constraint.

$$\frac{\delta}{\delta\varphi_i^*}\left(E[\Psi] - \lambda \int \varphi_j^* \varphi_i d\boldsymbol{r}\right) = 0 \tag{1.4}$$

Doing this yields the *Hartree-Fock equations*

$$-\frac{\hbar^2}{2m}\nabla^2\varphi_i + \sum_j^A \int \varphi_j^*(\boldsymbol{r}')v_{ij}(\boldsymbol{r},\boldsymbol{r}')\varphi_j(\boldsymbol{r}')\varphi_i(\boldsymbol{r})d\boldsymbol{r}' - \sum_j^A \int \varphi_j^*(\boldsymbol{r}')v_{ij}(\boldsymbol{r},\boldsymbol{r}')\varphi_j(\boldsymbol{r})\varphi_i(\boldsymbol{r}')d\boldsymbol{r}' = \varepsilon_i\varphi_i \tag{1.5}$$

Here, a couple of observations are in order.
The first interaction term, called Hartree term, arises from considering independent particles, and is also routinely found in classical physics. The second one, called Fock term, or exchange term is non-local and is given by the quantum mechanical nature of the system. From the standpoint of the solution of the eigenvalue problem, the Fock term is very problematic, and is usually avoided using finite-range interaction like the Gogny force [18], or contact forces like the Skyrme one [21], used in the present work. They render 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 various eigenstates. The consequece is that the equation will be solved *self-consistently*, that is, by solving for the set of orbitals $\{\varphi_i\}$, using them to build the new mean field, and solving again, repeating the process until convergence.

1.1.2. Symmetries

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

$$\{a_i, a_j^\dagger\} = \delta_{ij} \tag{1.6}$$

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

$$\varphi_k = \sum_l D_{lk}\chi_l \tag{1.7}$$

$$a_k^\dagger = \sum_l D_{lk}c_l^\dagger \tag{1.8}$$

$$a_k = \sum_l D_{lk}^\dagger c_l \tag{1.9}$$

Since orthonormality is guaranteed for both sets, taking

$$\delta_{jk} = \langle\varphi_j|\varphi_k\rangle = \sum_{ll'} D_{l'j}^\dagger D_{lk} \langle\chi_l|\chi_l'\rangle \implies DD^\dagger = 1 \tag{1.10}$$

Symmetry propagation

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1.1.3. Density Functional Theory

It shall be evident shortly, in section 1.2, that a more general approach to microscopic models has to be taken, in order to give a satisfactory description of the nuclear world. The framework that we'll briefly outline here is called Density Functional Theory (DFT). DFT was introduced by P. Hohenberg and W. Kohn in 1964 [9], by proving two theorems. The **first** 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.

$$E[\rho] = F[\rho] + \int V_{\text{ext}}\rho(\boldsymbol{r})d\mathbf{r} \tag{1.11}$$

While the **second** one states that the ground state of the system is found by minimizing its variation with respect to ρ.
HK theorems are fundamental but not constructive [3], since they do not provide a form for the functional F, which is intrinsic to the physics of the fermions at hand. COMPLETARE

1.2. Skyrme

Now that the theoretical framework is clear, we can investigate a plausible nucleonic interaction, which in the present work, takes the form of the Skyrme force.

1.2.1. Skyrme force

It was first proposed by Tony Skyrme in 1958 [21] as a zero range force between nucleons, and has been used successfully as the building block of theoretical nuclear structure. It comprises a two body attractive term that reads

$$\begin{aligned} v^{(2)}(\mathbf{r}_1,\mathbf{r}_2) = {} & t_0\,(1+x_0P_\sigma)\,\delta(\mathbf{r}) \\ & + \frac{1}{2}t_1\,(1+x_1P_\sigma)\left[\mathbf{P}'^2\delta(\mathbf{r}) + \delta(\mathbf{r})\mathbf{P}^2\right] \\ & + t_2P_\sigma\mathbf{P}'\cdot\delta(\mathbf{r})\mathbf{P} \\ & + iW_0\boldsymbol{\sigma}\cdot[\mathbf{P}'\times\delta(\mathbf{r})\mathbf{P}] \end{aligned}$$

And a three body interaction, that is

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

which mimics the repulsive three-body force; without it, a collapse of the nuclear density would occur.
It's trivial to show that the three-body term is equivalent to a two-body, density-dependent interaction: [25]

$$v^{(3)}(\boldsymbol{r}_1,\boldsymbol{r}_2) = \frac{1}{6}t_3(1+P_\sigma)\delta(\boldsymbol{r})\rho(\boldsymbol{R}) \tag{1.12}$$

The different operators here are defined as

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \quad \mathbf{R} = \frac{\mathbf{r}_1+\mathbf{r}_2}{2} \tag{1.13}$$

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

$$\mathbf{P} = \frac{-i(\nabla_1-\nabla_2)}{2} \tag{1.14}$$

which is the so called relative wave-number operator.

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 \tag{1.15}$$

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

$$\mathbf{P}_\sigma = \frac{(1+\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)}{2} \tag{1.16}$$

which represents the spin-exchange operator. Primed operators refer to the adjoint acting on the left.
The zero-range characteristic takes the form of a Dirac delta $\delta(\mathbf{r})$, which allows the writing of the Fock term detailed in (REF) as a purely local one.
Taking the expectation value of the many body hamiltonian, in the Hilbert space of Slater determinants, yields an energy density which can be expressed as a function of $\rho_q, \tau_q, \boldsymbol{J}_q$ [25].

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int \mathcal{H}(\boldsymbol{r}) d\mathbf{r} \tag{1.17}$$

Modern parametrization

The Skyrme force has evolved from the original one to accomodate new nuclei, done through the addition of a few parameters, yielding the following form of the interaction [1]

$$\begin{aligned} v^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = & \, t_0 \left(1 + x_0 P_\sigma\right) \delta(\mathbf{r}) \\ & + \frac{1}{2} t_1 \left(1 + x_1 P_\sigma\right) \left[\mathbf{P}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{P}^2\right] \\ & + t_2 \left(1 + x_2 P_\sigma\right) \mathbf{P}' \cdot \delta(\mathbf{r}) \mathbf{P} \\ & + \frac{1}{6} t_3 \left(1 + x_3 P_\sigma\right) \left[\rho(\mathbf{R})\right]^\sigma \delta(\mathbf{r}) \\ & + i W_0 \boldsymbol{\sigma} \cdot \left[\mathbf{P}' \times \delta(\mathbf{r}) \mathbf{P}\right] \\ & + \frac{1}{6} t_3 \left(1 + x_3 P_\sigma\right) \left[\rho(\mathbf{R})\right]^\sigma \delta(\mathbf{r}) \end{aligned}$$

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 $\sigma = 1$ [5].
On top of that, additional, empirical tweaking of the resulting energy density needed to reach satisfactory physical accuracy, such as the case for the spin-orbit couplings [16], prompts for the following, well established proceeding: use the Skyrme interaction as a starting guide for building the energy functional to employ Density Functional Theory.

1.2.2. Skyrme functional

The energy functional we want to minimize is rather complex, due to the rich phenomenology of nuclear interactions and numerical nuances.
The complete energy functional is

$$E_{\mathrm{HF}} = E_{\mathrm{Skyrme}} + E_{\mathrm{Coul}} + E_{\mathrm{Kin}} \tag{1.18}$$

We'll begin by looking at the Skyrme and kinetic parts, while later on give a treatment for the Coulomb one.

$$\langle H \rangle = \langle \Psi | \, H \, | \Psi \rangle = \int (\mathcal{E}_{\text{Skyrme}} + \mathcal{E}_{\text{Kin}}) d\mathbf{r} = \int \mathcal{E} d\mathbf{r} \tag{1.19}$$

Since the Skyrme interaction is time-reversal invariant (as well as the kinetic operator), this means that the total Hamiltonian must be time-even. Different additive contributions must be time-even as well, even if the densities from which they are calculated are not. Unless we reduce to the even-even nucleus case, where total angular momentum is defined at $J = 0$, giving vanishing time-odd densities. This allows us to write the functional in a simpler form as [24]

$$\mathcal{E}_{\text{Kin}} = \frac{\hbar^2}{2m}\tau \tag{1.20}$$

$$\mathcal{E}_{\text{Skyrme}} = \sum_{t=0,1} \left\{ C_t^{\rho}[\rho_0]\rho_t^2 + C_t^{\Delta\rho}\rho_t \nabla^2 \rho_t + C_t^{\nabla \cdot J}\rho_t \nabla \cdot \mathbf{J}_t + C_t^{\tau}\rho_t\tau_t \right\} \tag{1.21}$$

Here, $t = 0, 1$ refers to the isoscalar and isovector components of the densities, e.g.

$$\rho_0 = \rho_p + \rho_n$$
$$\rho_1 = \rho_p - \rho_n$$

Where

$$C_0^{\rho} = +\frac{3}{8}t_0 + \frac{3}{48}t_3\rho_0^{\sigma} \tag{1.22}$$

$$C_1^{\rho} = -\frac{1}{8}t_0(1 + 2x_0) - \frac{1}{48}t_3(1 + x_3)\rho_0^{\sigma} \tag{1.23}$$

$$C_0^{\tau} = +\frac{3}{16}t_1 + \frac{1}{16}t_2(5 + 4x_2) \tag{1.24}$$

$$C_1^{\tau} = -\frac{1}{16}t_1(1 + 2x_1) + \frac{1}{16}t_2(1 + 2x_2) \tag{1.25}$$

$$C_0^{\Delta\rho} = -\frac{9}{64}t_1 + \frac{1}{64}t_2(5 + 4x_2) \tag{1.26}$$

$$C_1^{\Delta\rho} = +\frac{3}{64}t_1(1 + 2x_1) + \frac{1}{64}t_2(1 + 2x_2) \tag{1.27}$$

$$C_0^{\nabla \cdot J} = -\frac{3}{4}W_0 \tag{1.28}$$

$$C_1^{\nabla \cdot J} = -\frac{1}{4}W_0 \tag{1.29}$$

As outlined in previous chapters (REF), we can now derive the Kohn-Sham equations, by constraining orthonormality and enforcing the variation of the functional to be zero.

What we end up with is

$$\left[-\nabla\left(\frac{\hbar^2}{2m_q^*(\mathbf{r})}\nabla\right) + U_q(\mathbf{r}) + \delta_{\mathrm{q,proton}}U_C(\mathbf{r}) - i\mathbf{B}_q(\mathbf{r})\cdot(\nabla\times\boldsymbol{\sigma})\right]\varphi_\alpha = \varepsilon_\alpha\varphi_\alpha \tag{1.30}$$

The index $q = n, p$ refers respectively to the neutron and proton quantities.
Where the different terms are given by

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = \frac{\delta\mathcal{E}}{\delta\tau_q} \tag{1.31}$$

$$U_q(\mathbf{r}) = \frac{\delta\mathcal{E}}{\delta\rho_q} \tag{1.32}$$

$$\mathbf{B}_q(\mathbf{r}) = \frac{\delta\mathcal{E}}{\delta\mathbf{J_q}} \tag{1.33}$$

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 1.3.
Following the rules for functional derivatives, outlined in the appendix (REF) we get

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = + \frac{\hbar^2}{2m} \tag{1.34}$$

$$+ \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho(\mathbf{r}) \tag{1.35}$$

$$- \frac{1}{8}[t_1(1+2x_1) + t_2(1+2x_2)]\rho_q(\mathbf{r}) \tag{1.36}$$

$$\tag{1.37}$$

$$U_q(\mathbf{r}) = + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho \tag{1.38}$$

$$+ \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\rho_q \tag{1.39}$$

$$+ \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau \tag{1.40}$$

$$+ \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\tau_q \tag{1.41}$$

$$+ \frac{1}{16}[t_2(2+x_2) - 3t_1(2+x_1)]\nabla^2\rho \tag{1.42}$$

$$+ \frac{1}{16}[3t_1(2x_1+1) + t_2(2x_2+1)]\nabla^2\rho_q \tag{1.43}$$

$$\tag{1.44}$$

$$\mathbf{B}_q(\mathbf{r}) = + \frac{1}{2}W_0[\nabla\rho + \nabla\rho_q] \tag{1.45}$$

$$- \frac{1}{8}(t_1x_1 + t_2x_2)\mathbf{J} + \frac{1}{8}(t_1 - t_2)\mathbf{J}_q \tag{1.46}$$

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

1.3. Coulomb interaction

Unlike the Skyrme interaction, the Coulomb force is not local, giving rise to an unwanted integral operator in the Hamiltonian. A well known and widely used device is the Slater approximation [8], which gives a local exchange interaction.
In this approximation, the Coulomb energy reads

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

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

Which gives

$$U_C(\mathbf{r}) = \frac{\delta \mathcal{E}_{\text{Coul}}}{\delta \rho_p} = \frac{e^2}{2}\left[\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} d^3\mathbf{r}' - 2\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \rho_p^{1/3}(\mathbf{r})\right] \tag{1.47}$$

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 is $\mathcal{O}(N^6)$, rendering it unusable for fine meshes.
An alternative approach is to solve the poisson equation (from now on, V_c refers to the direct part only)

$$\nabla^2 V_c = 4\pi e^2 \rho_p \tag{1.48}$$

Given the proton density, we can impose Dirichlet boundary conditions, which can be extracted from a quadrupole expansion of the charge density [10]

$$V_c(\mathbf{r}) = 4\pi e^2 \sum_{\lambda=0}^{2} \sum_{\mu=-\lambda}^{\lambda} \frac{\langle Q_{\lambda\mu} \rangle Y_{\lambda\mu}}{r^{1+\lambda}} \text{ on } \partial\Omega \tag{1.49}$$

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

$$\langle Q_{\lambda\mu} \rangle = \int r^\lambda Y^*_{\lambda\mu}(\mathbf{r}) \rho_p(\mathbf{r}) d^3\mathbf{r} \tag{1.50}$$

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

$$V_c(\mathbf{r}) = \frac{Ze^2}{r} + e^2 \sum_{\mu=-2}^{2} \frac{\langle Q_{2\mu} \rangle Y_{2\mu}}{r^3} \text{ on } \partial\Omega \tag{1.51}$$

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

1.4. 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 1.30 stands true, summarized as

$$(\hat{t} + U)\varphi_k = \varepsilon_k \varphi_k \tag{1.52}$$

We can multiply 1.52 on the left by φ_k^* and integrate to get

$$\int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\boldsymbol{r} + \int \varphi_k^* U \varphi_k d\boldsymbol{r} = \int \varphi_l^* \varepsilon_k \varphi_k d\boldsymbol{r} \tag{1.53}$$

The integral on the right hand side of 1.53 evaluates to ε_k due to the orthonormality constraint. If we sum over all states k we get

$$\sum_k \left\{ \int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\boldsymbol{r} + \int \varphi_k^* U \varphi_k d\boldsymbol{r} \right\} = \sum_k \varepsilon_k \tag{1.54}$$

$$\sum_k t_k + \int \rho U = \sum_k \varepsilon_k \tag{1.55}$$

Since U is calculated as 1.32, 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*

$$\rho U = \rho\frac{\delta\mathcal{E}_{\text{Skyrme}}}{\delta\rho} = \rho(\sigma+1)A\rho^{\sigma} = (\sigma+1)A\rho^{\sigma+1} = \mathcal{E}_{\text{Skyrme}} + \sigma\mathcal{E}_{\text{Skyrme}} = \mathcal{E}_{\text{Skyrme}} - \mathcal{E}_{\text{rea}} \tag{1.56}$$

If we explicit ρU in equation 1.55 using 1.56, we get to

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

Isolating the Skyrme energy density

$$\int \mathcal{E}_{\text{Skyrme}}d\boldsymbol{r} = \sum_k(\varepsilon_k - t_k) + \int \mathcal{E}_{\text{rea}}d\boldsymbol{r} \tag{1.57}$$

and given the total energy of the system from 1.19

$$E = \sum_k t_k + \frac{1}{2}\int \mathcal{E}_{\text{Skyrme}}d\boldsymbol{r} \tag{1.58}$$

substituting 1.57 in 1.58 yields

$$E_{\text{HF}} = \frac{1}{2}\sum_k(\varepsilon_k + t_k) + \int \mathcal{E}_{\text{rea}}d\boldsymbol{r} = \frac{1}{2}\left(T + \sum_k \varepsilon_k\right) + E_{\text{rea}} \tag{1.59}$$

which will be called *Hartree-Fock energy* throughout this text.

Sidenote: The actual functional has a plethora of 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 1.59 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.

2 | Numerical methods

In this chapter, we will tackle the practical implementation of the Hartree-Fock method and the numerical details of the code.

2.1. Finite differences

One, if not the easiest way to numerically represent and solve differential equations, is through finite differences. The core idea is to find a suitable 3D mesh for the problem at hand, use an approximation for derivatives on said mesh, and ultimately using the language of linear algebra to formulate and solve the resulting system of equations.

2.1.1. 3D mesh

The first task on the agenda, is finding a suitable representation of the various fields for a computer. Generally speaking, we deal at most with 2-rank tensors, which vary in space and spin.
Discretizing the 3D cartesian space with a 3-index mesh, choosing a box which size on 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 size are

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

For ease of notation, we will assume $a = a_x = a_y = a_z = a$ and $N = N_x = N_y = N_z = N$, without losing generality.

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

$$\psi(\boldsymbol{r}, \sigma) \mapsto \psi(x_i, y_j, z_k, s) = \psi_{ijks} \tag{2.1}$$

Discretizing differential operators

By using Taylor series, it's possible to write approximations to derivatives [27], in any point of the lattice, of any (reasonable) order of accuracy, involving only near neighbouring points. In the present work, 5-points derivates are used, meaning Taylor expansions are written for $\psi(x \pm h)$ and $\psi(x \pm 2h)$ to compute the differential operators. Formulae for first and second derivates in this framework are given in appendix A.2.

2.1.2. Schrödinger equation

As outlined in (REF), one of the two PDEs we want to solve is the single particle Schrödinger equation 1.30.
It can be summarized as

$$f(\nabla^2\psi, \nabla\psi, \psi, \boldsymbol{r}, s) = E\psi \tag{2.2}$$

If f is linear in ψ, it would be possible to employ the powerful numerical methods of linear algebra to solve the problem. Breaking down each part of the equation, the kinetic term

$$\nabla\left(\frac{\hbar^2}{2m_q^*(\mathbf{r})}\nabla\right)\psi = \frac{\hbar^2}{2m_q^*(\mathbf{r})}\nabla^2\psi + \nabla\left(\frac{\hbar^2}{2m_q^*(\mathbf{r})}\right)\nabla\psi \tag{2.3}$$

Is evidently linear in ψ.
The spin-orbit coupling, which most generally reads

$$\begin{aligned}\hat{h}_{\mathrm{SO}} &= \boldsymbol{f}(\boldsymbol{r}) \cdot (\nabla \times \boldsymbol{\sigma}) \\ &= f_x(\boldsymbol{r})(\sigma_z\partial_y - \sigma_y\partial_z) + f_y(\boldsymbol{r})(\sigma_x\partial_z - \sigma_z\partial_x) + f_z(\boldsymbol{r})(\sigma_y\partial_x - \sigma_x\partial_y)\end{aligned}$$

where $\hat{h}_{\mathrm{SO}}$ acts linearly on the spinor ψ_{ijk}. Finally, the mean field terms U_q, U_c are just multiplicative, hence linear in ψ.

$$U\psi$$

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

$$\sum_{n}^{N_x \cdot N_y \cdot N_z \cdot 2} A_{mn}\psi_n = E\psi_m \tag{2.4}$$

Boundary conditions

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

$$\begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & A & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \psi_{-2} \\ \psi_{-1} \\ \psi \\ \psi_N \\ \psi_{N+1} \end{bmatrix} = E \begin{bmatrix} \psi_{-2} \\ \psi_{-1} \\ \psi \\ \psi_N \\ \psi_{N+1} \end{bmatrix} \tag{2.5}$$

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

$$\begin{cases} \psi_{-2} = 0 \\ \psi_{-1} = 0 \\ \dots \end{cases} \tag{2.6}$$

Meaning that ψ outside the box will automatically be set to zero if the A matrix is built assuming those points to be zero.

2.1.3. Poisson equation

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

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

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

Boundary conditions

Unlike the Schrödinger equation, we do not expect the solution to rapidly decay near the boundaries; as reported in section 1.3, we have fixed, non-null boundary conditions, which we have to properly impose on the system.
We can choose a direction, say x, and look at the equation at the boundaries $x = \pm a$. Since the indeces j, k won't vary, we can omit them, and ignore the other derivates in the

following equations.

$$\nabla^2 V = \partial_{xx}V + \partial_{yy}V + \partial_{zz}V = \frac{-V_{i-2} + 16V_{i-1} - 30V_i + 16V_{i+1} - V_{i+2}}{12h^2} + \cdots = 4\pi e^2 \rho_i \tag{2.7}$$

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 2.7.

$$\frac{-30V_0 + 16V_1 - V_2}{12h^2} = 4\pi e^2 \rho_0 + \frac{V_{-2} - 16V_{-1}}{12h^2} = \tilde{\rho}_0 \tag{2.8}$$

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

$$\frac{+16V_0 - 30V_1 + 16V_2 - V_3}{12h^2} = 4\pi e^2 \rho_1 + \frac{V_{-1}}{12h^2} = \tilde{\rho}_1 \tag{2.9}$$

The proper system to solve will then be

$$AV = \tilde{\rho} \tag{2.10}$$

Where A is constructed as previously specified. $\tilde{\rho}$ will force the solution to abide boundary conditions.

On higher order approximations and performance

Higher and higher order approximations for derivatives involve points that are further and further away. This increases accuracy, but it also decreases matrix sparseness.
Algorithms like Conjugate Gradient, as we'll see in the next section, and linear algebra computing libraries, benefit from matrix sparseness. The implication is that performance *vs* accuracy is a tradeoff that isn't univocal to every problem.
In the present work, the golden choice has been 5-point stencils; but it's not definitive, as the lattice points rapidly cap depending on the system's memory.
As an example, take a seemingly harmless grid, made of 50 points in each direction. The resulting matrix will be $50 \times 50 \times 50 \times 2 = 2.5 \times 10^5$ both in columns and rows. It may be the case in the future, that higher order derivatives will be needed, to compensate for the limitation brought by the $\mathcal{O}(h^n)$ polynomial accuracy of the method in the step size.

2.2. Iterative eigensolvers

This section is devoted to approximate, iterative eigensolvers, exploring the idea behind the Conjugate Gradient (CG) algorithm and its use in the General Conjugate Gradient (GCG).
Eigenproblems are ubiquitous in physics and engineering, and while solving one for a small matrix is trivial, it still requires roughly $O(n^3)$ [7] operations to do so. More often than not, real computational applications result in large-scale matrices, which are completely out of the question for exact eigenvalues calculation.
The workaround, is to use approximate algorithms. To keep things simple, we'll skim through the basics of the most modern and used ones, address their limitations, and move on to a new one, the General Conjugate Gradient (GCG).

2.2.1. Techniques

Iterative eigensolvers often share some common numerical techniques, like the Rayleigh-Ritz procedure, shift-and-invert, and approximate linear systems solvers. We will begin by describing these recurring techniques, then look at commonly used algorithms and finally move on to the solver used in this work, the GCG.

Conjugate Gradient and numerical techniques

Solving linear systems of the form

$$Ax = b \tag{2.11}$$

is crucial in many eigensolvers. The Conjugate Gradient (CG) is perhaps the most famous iterative solver in this sense, especially in regards to sparse matrices, as we'll see in a moment. CG applies to cases where A is an $n \times n$, positive-definite, symmetric matrix, and x and b are n-dimensional vectors. Many generalizations to this methods exist, which relax the requirements on the matrix, like BiCGSTAB, CGNR, MINRES, and so on. We'll describe the working principle of CG, but the same applies to all the others, with slight variations.
The quadratic form $f(x)$ associated to system 2.11 is

$$f(x) = \frac{1}{2}x^T Ax - b^T x \tag{2.12}$$

If A is symmetric, positive-definite,

Preconditioning

Rayleigh-Ritz procedure

A common denominator of all these algorithms is the search of good approximations for the correct eigenvectors in a certain subspace $\mathcal{K}$. The method is called Rayleigh-Ritz (RR) procedure [20], and is here outlined.
Suppose to have a matrix A of size $n \times n$, with entries in $\mathbf{C}$ and a collection of vectors k which form a subspace $\mathcal{K} \subset \mathbf{C}^n$, where $\mathcal{K}$ is an $n \times k$ matrix. Generally speaking, n is large, while k is much smaller.
The best approximation of the true eigenvectors of A in $\mathcal{K}$ can be computed by solving the small scale eigenvalue problem

$$\mathcal{K}^\dagger A \mathcal{K} X = X\lambda \tag{2.13}$$

Resulting in a matrix X of size $k \times k$. Computing $\mathcal{K}X$ gives a matrix of size $n \times k$, whose column vectors are the best approximations of the eigenvectors of A in $\mathcal{K}$, with their corresponding eigenvalues λ.

Shift and Invert

2.2.2. Iterative eigensolvers

Jacobi-Davidson

The Jacobi-Davidson method [22] performes the RR procedure on a subspace which is enriched at each iteration by a correction to the previous eigenvectors.
Given an approximation (u, θ) of an eigenpair of matrix A, if the residual

$$r = Au - \theta u \tag{2.14}$$

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

$$r = A(u + t) - (\theta + \delta\theta)(u + t) = 0 \tag{2.15}$$

Linearizing this equation in t gives

$$(A - \theta I)t = -r \tag{2.16}$$

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

$$(I - uu^\dagger)(A - \theta I)(I - uu^\dagger)t = -r \tag{2.17}$$

Algorithm 2.1 Jacobi-Davidson method for $Ax = \lambda x$

1: Choose normalized initial vectors $\{u_k\}$, set $V = [u_1, \ldots, u_k]$
2: **repeat**
3: Compute Ritz pair: $T = V^*AV$, 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 $(I - u_k u_k^*)(A - \theta I)(I - u_k u_k^*)t_k = -r_k$ 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 $k = 1, \ldots,$ nev

Although simple, this method is computationally efficient only by using preconditioning, which is known to be unstable [20].

Lanczos

Lanczos algorithm [12] is probably the most used iterative eigensolver in regards to hermitian matrices. It's a Krylov subspace search method, meaning the Rayleigh-Ritz procedure is done on a subspace formed as

$$\mathcal{K} = \{v_1, Av_1, A^2v_1, \ldots, A^{k-1}v_1\} \tag{2.18}$$

By iteratively applying A to the search vector, orthogonalizing it to the previous one and diagonalizing the small scale problem.

Algorithm 2.2 Lanczos Method for Computing nev Lowest Eigenpairs of Hermitian A

Choose normalized initial vector v_1, set $\beta_0 = 0$, $m =$ subspace size.
repeat
  for $j = 1, 2, \ldots, m$ **do**
    $w \leftarrow Av_j - \beta_{j-1}v_{j-1}$
    $\alpha_j \leftarrow v_j^* w$
    $w \leftarrow w - \alpha_j v_j$
    $\beta_j \leftarrow \|w\|$
    if $\beta_j = 0$ **then**
      break
    end if
    $v_{j+1} \leftarrow w/\beta_j$
  end for
  Form tridiagonal matrix $T_m = \text{tridiag}(\beta_{1:m-1}, \alpha_{1:m}, \beta_{1:m-1})$
  Compute eigen-decomposition $T_m y_k = \theta_k y_k$, for $k = 1, \ldots, \text{nev}$
  Form Ritz approximations $x_k = V_m y_k$, where $V_m = [v_1, \ldots, v_m]$
  Compute residual norms $r_k = \|Ax_k - \theta_k x_k\|$ for all k
until convergence for $k = 1, \ldots, \text{nev}$

Lanczos is extremely efficient memory and computationally wise for extremal eigenvalues, but this limits its applicability to unbound discretized operators, where unwanted eigenvalues may dominate the Krylov subspace, and most importantly, for applications where the inner part of the spectrum is of interest, as in the case of Hartree-Fock-Bogoliubov. 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 [20].

LOBPCG

The last algorithm of this short list is LOBPCG, it's the newest and most sofisticated one of the three.
Introduced by A. V. Knyazev in 1991 [11], it's a block, preconditioned conjugate gradient method, explicitly targeted at solving large-scale eigenvalue problems, and it's been used in modern solutions of the Schrödinger/KS equation in recent years [13–15, 26]. In this algorithm, the Rayleigh-Ritz procedure is done on a subspace formed as

$$V = [X, W, P] \tag{2.19}$$

Where X is the current best eigenvectors approximation, P is the block of previous search directions, and W is a block formed by preconditioning P.
We won't go into the details of LOBPCG, since GCG shares with it many aspects, like blocking and search directions calculation.

2.2.3. General Conjugate Gradient

2.3. Code implementation details

2.3.1. Constraints

The HF ground state is a great starting point to get theoretical results regarding many nuclear properties; however, for a plethora of applications, calculating the state of the nuclear system under certain constraints becomes necessary.
Effectively, a need to explore the energy surface arises. This means minimizing the energy functional, under a series of constraints of the type $\langle \mathcal{Q} \rangle = q_0$, where q_0 is the desired expectation value of the operator $\mathcal{Q}$.
This is an equality-constrained optimization problem (ECP), formulated as

$$\min_{|\Psi\rangle} E \tag{2.20}$$

$$\text{constrainted to } \langle \Psi | \mathcal{Q} | \Psi \rangle = \langle \mathcal{Q} \rangle = q_0 \tag{2.21}$$

Which yields the Lagrangian

$$E' = E + \lambda(\langle \mathcal{Q} \rangle - q_0) \tag{2.22}$$

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 [6]

$$\frac{\mathrm{d}E}{\mathrm{d}\langle \mathcal{Q} \rangle} = -\lambda \tag{2.23}$$

If λ is properly adjusted, a certain value for q_0 can be obtained. From a numerical standpoint, λ needs to be tuned at each iteration to reach the desired value. This method was the one used in early constrained Hartree-Fock calculations [4].
Although the method is simple, it's often the case that it 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

$$E' = E + \frac{c}{2}(\langle \mathcal{Q} \rangle - q_0)^2. \tag{2.24}$$

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 large values, the penalty may be so big that the self consistent calculation oscillates and fails.

Augmented Lagrangian Method

A modern, robust approach, used by HF/HFB codes [2, 19] is given in the form of the Augmented Lagrangian Method (ALM) [23]. 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

$$E' = E + \lambda(q - q_0) + \frac{c}{2}(q - q_0)^2 \tag{2.25}$$

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

$$U' = U + \lambda \mathcal{Q} + c(q - q_0)\mathcal{Q} \tag{2.26}$$

$$= U + c(q - q_0(\lambda))\mathcal{Q} \tag{2.27}$$

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

$$q_0(\lambda) = q_0 - \frac{\lambda}{c} \tag{2.28}$$

$$\lambda^{(i+1)} = \lambda^{(i)} + \mu c(q - q_0) \tag{2.29}$$

Here, a slight deviation from the original ALM is present. Since the original work [23] doesn't provide guidance regarding what is considered an *iteration*, we employ the strategy [2] 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 section (REF), 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.

2.3.2. Self consistent procedure pseudocode

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A | Appendix

A.1. Spherical harmonics

Spherical harmonics, of order λ, μ, are defined as

$$Y_{\lambda\mu}(\theta, \phi) = (-1)^{\mu} \sqrt{\frac{2\lambda + 1}{4\pi} \frac{(\lambda - \mu)!}{(\lambda + \mu)!}} P_{\lambda}^{\mu}(\cos\theta)\, e^{i\mu\phi}. \tag{A.1}$$

Being able to provide the expression for arbitrary μ, λ through an algorithm is important in the current framework, to solve the Poisson equation and investigate nuclear properties. The major challenge is to generate the associated Legendre polynomials P_{λ}^{μ}. They can be expressed in the form (for positive μ)

$$P_{\lambda}^{\mu}(x) = (1 - x^2)^{\mu/2} \frac{\mathrm{d}^{\mu} P_{\lambda}(x)}{\mathrm{d}x^{\mu}}, \tag{A.2}$$

where $x = \cos\theta$ and

$$P_{\lambda}(x) = \frac{1}{2^{\lambda}\lambda!} \frac{\mathrm{d}^{\lambda}(x^2 - 1)^{\lambda}}{\mathrm{d}x^{\lambda}}. \tag{A.3}$$

To compute the arbitrary λ, μ associated Legendre polynomial we can employ a recursive approach, setting $\lambda = \mu$

$$P_{\mu}^{\mu}(x) = (2\mu - 1)!!\, (1 - x^2)^{\mu/2}, \tag{A.4}$$

where $(2\mu - 1)!! = 1 \cdot 3 \cdot 5 \ldots (2\mu - 1)$ denotes the double factorial. Once $P_{\mu}^{\mu}(x)$ is known, the next element with $\lambda = \mu + 1$ reads

$$P_{\mu+1}^{\mu}(x) = x(2\mu + 1) P_{\mu}^{\mu}(x). \tag{A.5}$$

All higher orders are then generated using the standard upward recurrence relation in λ:

$$(\lambda - \mu + 1)\, P_{\lambda+1}^{\mu}(x) = (2\lambda + 1)\, x\, P_{\lambda}^{\mu}(x) - (\lambda + \mu)\, P_{\lambda-1}^{\mu}(x), \tag{A.6}$$

valid for all $\lambda \geq \mu + 1$.

A.1.1. Algorithm

1. Compute the base case P_{μ}^{μ} from the closed-form formula.
2. If $\mu = \lambda$ the procedure ends, otherwise
3. Evaluate $P_{\mu+1}^{\mu}$, if $\lambda = \mu + 1$ the procedure ends, otherwise
4. Apply the recurrence relation $P_{\lambda+1}^{\mu}$ until the desired degree is reached

This ought to be applied only for $\mu \geq 0$. For $\mu < 0$ the procedure is carried out using $-\mu$ and in the end using the relation

$$Y_{\lambda-\mu} = (-1)^{\mu} Y_{\lambda\mu}^{*} \tag{A.7}$$

A.2. 5-point derivatives

The first and second derivatives of a function $\psi(x)$ in $x = x_i$, using 5-points formulae, read

$$\psi'(x_i) = \frac{\psi_{i-2} - 8\psi_{i-1} + 8\psi_{i+1} - \psi_{i+2}}{12h} \tag{A.8}$$

$$\psi''(x_i) = \frac{-\psi_{i-2} + 16\psi_{i-1} - 30\psi_i + 16\psi_{i+1} - \psi_{i+2}}{12h^2} \tag{A.9}$$

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Variable	Description	SI unit
$\boldsymbol{u}$	solid displacement	m
$\boldsymbol{u}_f$	fluid displacement	m

Acknowledgements

Here you might want to acknowledge someone.