Notes

Contents

1 Conjugate Gradient Method

1.1 Overview

The conjugate gradient method (cgm) is an algorithm used to solve a linear system of the form

$$Ax = b \tag{1}$$

Where A is a symmetric ($A^T = A$) positive definite ($x^T Ax > 0$) $n \times n$ matrix, $x,\ b$ vectors.
The algorithm is iterative, starting from a guess solution x_0 and taking a step towards the solution at each cycle.
The search directions are calculated from the residual term, defined as $r_i = b - Ax_i$.
It is possible to prove that by choosing the step direction to be A-orthogonal to all the previous ones, the solution converges the fastest (i.e. the error term $\|e_i\| = \|x_i - x\|$ is minimized).

1.2 Steepest descent

A simpler algorithm is the steepest descent.
The idea is to take a step in the direction of the residual so that the quadratic form is minimized.

$$x_{i+1} = x_i + \alpha_i r_i \tag{2}$$

$$\alpha_i \text{ such that } \frac{df(x_{i+1})}{d\alpha_i} = 0 \implies \alpha_i = \frac{r_i^T r_i}{r_i^T A r_i} \tag{3}$$

This method is inefficient as x_i often finds itself oscillating around the solution, since the search directions explore non-disjoint subspaces.

1.3 The algorithm

A better alternative is to set the search direction to be A-orthogonal to the error at the next iteration. If this is the case, it can be proven that the components of the error term are reduced to zero at each iteration, implying a convergence to the exact solution in n steps.

$$d_i^T A e_{i+1} = 0 \implies \frac{df(x_{i+1})}{d\alpha_i} = -r_{i+1}^T d_i = 0 \tag{4}$$

$$\alpha_i = \frac{r_i^T d_i}{d_i^T A d_i} \tag{5}$$

By definition, the residual is orthogonal to the previous search directions, we also have $r_i^T r_j = \gamma ij$. Since

$$r_{i+1} = -A(e_{i+1}) = -A(e_i + \alpha_i d_i) = r_i - \alpha_i A d_i \tag{6}$$

1.3.1 Procedure

The cgm algorithm can be summed up as follows:
Start with a guess solution x_0.
Let the first direction be the residual in x_0

$$d_0 = r_0 = b - Ax_0 \tag{7}$$

Now, at each iteration, we can compute

$$\alpha_i = \frac{r_i^T r_i}{d_i^T A d_i}$$
$$x_{i+1} = x_i + \alpha_i d_i$$
$$r_{i+1} = r_i - \alpha_i A d_i$$
$$\beta_{i+1} = \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i}$$
$$d_{i+1} = r_{i+1} + \beta_{i+1} d_i$$

1.4 Preconditioning

The rate of convergance of cgm depends on the conditioning of the matrix A, defined as $\kappa(A) = \frac{\max \lambda_i}{\min \lambda_i}$, where λ_i are the eigenvalues of the matrix.
The closer $\kappa(A)$ is to 1, the faster the convergence of the method.
Given a certain matrix M, symmetric, positive definite and easily invertible and such that $M^{-1}A$ has better conditioning than A, which is to say M well approximates A, we can hope to solve the problem

$$M^{-1}Ax = M^{-1}b \tag{8}$$

much faster than the original problem, where the two solutions will be the same.
The problem is that $M^{-1}A$ is not necessarily symmetric or positive definite.
The fact that $\exists E$ such that $M = EE^T$ and $E^{-1}AE^{-T}$ is symmetric and positive definite, we can solve the problem.

$$E^{-1}AE^{-T}x = E^{-1}b \tag{9}$$

By using some clever substitutions, we can go back to the original problem with the aid of the preconditioner, giving the following algorithm

$$\begin{aligned} r_0 &= b - Ax_0 \\ d_0 &= M^{-1} r_0 \\ \alpha_i &= \frac{r_i^T M^{-1} r_i}{d_i^T A d_i} \\ x_{i+1} &= x_i + \alpha_i d_i \\ r_{i+1} &= r_i - \alpha_i A d_i \\ \beta_{i+1} &= \frac{r_{i+1}^T M^{-1} r_{i+1}}{r_i^T M^{-1} r_i} \\ d_{i+1} &= M^{-1} r_{i+1} + \beta_{i+1} d_i \end{aligned}$$

2 Finding the smallest eigenvalue

Finding the smallest/biggest eigenvalue-eigenvector pair of a matrix amounts to evaluating the unconstrained minimum/maximum of the Reyleigh quotient

$$\lambda(x) = \frac{x^T A x}{x^T x} \tag{10}$$

Or, more generally

$$Ax = B\omega x \implies \lambda(x) = \frac{x^T A x}{x^T B x} \tag{11}$$

λ is not a quadratic form, hence the cgm needs to be modified to use it.

2.1 Useful multivariable relations

Given $f(x) = x^T A x$ and taking the derivative of f in the direction of v

$$f(x + hv) = (x + hv)^T A (x + hv) = f(x) + hv^T Ax + hx^T Av + o(h) \tag{12}$$

$$\frac{\mathrm{d}f}{\mathrm{d}v} = \lim_{h \to 0} \frac{f(x + hv) - f(x)}{h} = v^T Ax + x^T Av = v^T Ax + v^T A^T x \tag{13}$$

We can now evaluate the gradient of f in x

$$\nabla_x f(x) = \frac{\mathrm{d}f}{\mathrm{d}v} = (A + A^T)x \tag{14}$$

We can now take the gradient of the Rayleigh quotient

$$\nabla\lambda(x) = \frac{(A + A^T)xx^T Bx - (B + B^T)xx^T Ax}{(x^T Bx)^2} \tag{15}$$

Using the fact that A and B are symemtric

$$\nabla\lambda(x) = 2\frac{Axx^T Bx - Bxx^T Ax}{(x^T Bx)^2} = 2\frac{Ax - \lambda(x)Bx}{x^T Bx} \tag{16}$$

2.2 Non linear conjugate gradient

Using a non quadratic form as function to be minimized, the things that will change will be

- The step size α_i will be different, we may now have multiple zeros regarding the orthogonality of the gradient and search direction.
- The factor β to compute conjugated directions no longer has equivalent forms.
- The residual needs to be computed each time as $-\nabla f(x_i)$

Let's take a look at each problem and find a workaround.

2.2.1 Step size

We ought to find the step size for which λ is minimized at each iteration. Being non linear (and non quadratic), an approximation must be done.
We can Taylor expand the function around x_i, in the direction αd_i, and find the minimum of the polynomial.
Regarding the Rayleigh quotient, it amounts to finding the positive roots of the following polynomial:

$$
\begin{aligned}
a\alpha_i^2 + b\alpha_i + c = 0 \\
a = (d_i^T A d_i)(x_i^T B d_i) - (x_i^T A d_i)(d_i^T B d_i) \\
b = (d_i^T A d_i)(x_i^T B x_i) - (x_i^T A x_i)(d_i^T B d_i) \\
c = (x_i^T A d_i)(x_i^T B x_i) - (x_i^T A x_i)(x_i^T B d_i)
\end{aligned}
$$

Being the search direction always descending, we can simply select the positive root.

2.2.2 Factor β

The choice for β is neither trivial nor unique, different formulations lead to distinct convergence properties and applicabilities.
Two possible choices are

$$
\beta_{i+1}^{\text{FR}} = \frac{r_{i+1}^T r_{i+1}}{r_i^T r_i} \quad \text{or} \quad \beta_{i+1}^{\text{PR}} = \max\left\{ \frac{r_{i+1}^T (r_{i+1} - r_i)}{r_i^T r_i}, 0 \right\} \tag{17}
$$

The max operation will restart the method if β is negative in the Polak Ribière, guaranteeing convergence.

2.2.3 Algorithm

The algorithm for minimizing the Rayleigh quotient can now be formulated as follows.
Choose an initial guess x_0.
Set the first search direction as the residual in x_0: $d_0 = r_0 = -g(x_0)$.

At each iteration, we can compute

$$\begin{aligned} \alpha_i \text{ such that } f(x+\alpha_i d_i) \text{ minimized} \\ x_{i+1} = x_i + \alpha_i d_i \\ r_{i+1} = -g(x_{i+1}) \\ \beta_{i+1} \text{ from one of the possible choices} \\ d_{i+1} = r_{i+1} + \beta_{i+1} d_i \end{aligned}$$

Since $\lambda(x)$ is not a quadratic form, the algorithm won't converge in n steps, so that we will need to check for convergence at each iteration.

2.2.4 Stopping

As suggested in [painless conjugate gradient], a possible stopping criterion can be to check whether

$$\|g(x_i)\| < \epsilon \|g(x_0)\| \tag{18}$$

3 Finite Differences

We can employ discretization methods such as finite differences to approximate the solution of a differential equation.

3.1 Second order ODEs

The taylor expansion of a function $\psi(x \pm h)$ around a point x is given by

$$\psi(x \pm h) = \psi(x) \pm h\psi'(x) + \frac{h^2}{2!}\psi''(x) + \dots \tag{19}$$

3.1.1 First and second derivative

By subtracting $\psi(x+h)$ and $\psi(x-h)$, we get an approximation for the first derivative

$$\psi'(x) \approx \frac{\psi(x+h) - \psi(x-h)}{2h} \tag{20}$$

By adding them, we can get an approximation for the second derivative

$$\psi''(x) \approx \frac{\psi(x+h) - 2\psi(x) + \psi(x-h)}{h^2} \tag{21}$$

3.2 Discretization

Given an eigenvalue boundary problem, formulated as

$$\psi''(x) = f(x, \psi, \psi', E) \quad \forall x \in [a, b] \tag{22}$$

We can build a lattice of n points

$$X = \{x_i = a + ih \; \forall i = 0, \dots, n-1\} \tag{23}$$

Writing $\psi(x_i) = \psi_i$, and the equation $\psi_i'' = f(x_i, \psi_i, \psi_i', E)\ \forall i$ we get a linear system of the form

$$A\underline{\psi} = E\underline{\psi} \tag{24}$$

Finding the eigenvalues and eigenvectors of A amounts to finding the solutions ψ and the corrisponding eigenvalues E of the eigenvalue problem 22.

3.3 1D Harmonic oscillator

In quantum mechanics, one often finds necessary to solve the reduced Schrödinger equation

$$\hat{H}\psi = (\hat{T} + \hat{V})\psi = E\psi \tag{25}$$

Where $\hat{H}$ is the Hamiltonian, a differential operator, and E the energy associated to a state ψ.
A simple but rather useful example is the harmonic oscillator, where the potential is given by

$$V(x) = \frac{1}{2}m\omega^2(x - x_0)^2 \tag{26}$$

3.3.1 Harmonic oscillator and equilibrium

The power of the harmonic oscillator comes from the fact that a system at equilibrium will roughly have its particles in the minium of the potential energy.
From a single particle point of view, we can say that the potential to which it's subjected is a function of its position x, which at equilibrium can be expanded as

$$V(x) = V(x_0) + \left.\frac{\mathrm{d}V}{\mathrm{d}x}\right|_{x_0}(x - x_0) + \frac{1}{2}\left.\frac{\mathrm{d}^2V}{\mathrm{d}x^2}\right|_{x_0}(x - x_0)^2 \tag{27}$$

Since the first derivative is zero at equilibrium, and the potential additive constant can be ignored, we can write

$$V(x) = \frac{1}{2}m\omega^2(x - x_0)^2 \tag{28}$$

Where

$$m\omega^2 = \left.\frac{\mathrm{d}^2V}{\mathrm{d}x^2}\right|_{x_0} \tag{29}$$

3.4 Matrix solution

Given the Hamiltonian

$$\hat{H} = \frac{-\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2x^2 \tag{30}$$

We can combine 22 and 21, using a step size h to get

$$\frac{(\frac{C}{2}m\omega^2x_i^2h^2 - 2)\psi_j + \psi_{j-1} + \psi_{j+1}}{h^2C} = E\psi_j \tag{31}$$

Where $C = -2m/\hbar^2$.
The left hand side of 31 gives the entries of matrix A, for which the smallest eigenvalue can be found by minimizing the Rayleigh quotient with the non linear cgm.

3.4.1 Harmonic oscillator applied to nuclei

A numerical solution to the harmonic oscillator is now given for the applied case of a nucleon in the nucleus.
The value of ω can be calculated from the empirical density of nuclei, which can be written as a function of $\sqrt{\langle r^2 \rangle}$, analytically known in the case of an harmonic oscillator.

$$\hbar\omega = \frac{41}{A^{1/3}}\text{MeV} \tag{32}$$

This may seem tautological but the aim is to verify the validity of the numerical solution while seeing the method in action for a real case.
The mass of the particle is assumed to be 939 MeV.
A calculation was performed on a grid of 1000 points, in an interval $[-a, a]$ such that $a = 10$ fm.
The resulting wavefunction is shown in figure 1.
Assuming a mass number of $A = 16$, the eigenvalue (energy) associated to the graound state is 8.143 MeV.
Since the computation was done in one dimension, a factor of 3 is needed to compare it to a real nucleus.
Assuming the nucleon to be bound through a potential well of $\approx$ 40 MeV, the separation energy will be $\approx$ 40 - 8.143 $\cdot$ 3 = 15.571 MeV.

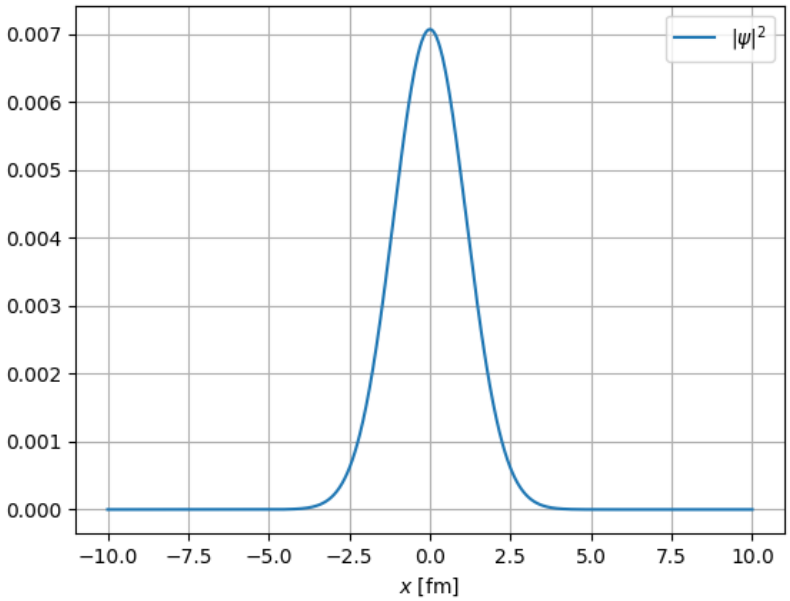

Figure 1: Ground state wavefunction of the harmonic oscillator. The solution starts roughly vanishes for $|x| > 3$ fm, as expected for a nucleus of this size.

3.5 Second order PDEs

The method of finite differences can be extended to second order PDEs.
For the moment, we will consider only a 2 dimensional problem, without losing generality.
Given the boundary eigenvalue problem

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = f(\psi, \frac{\partial\psi}{\partial x}, \frac{\partial\psi}{\partial y}, x, y, E) \tag{33}$$

We can build a lattice of N_x, N_y points as follows

$$X = \{x_i = a_x + ih_x \ \forall i = 0, \dots, N_x - 1\},\ Y = \{y_j = a_y + jh_y \ \forall j = 0, \dots, N_y - 1\} \tag{34}$$

By applying the finite differences method on x we get

$$\frac{\partial^2\psi_i}{\partial y^2} + \frac{\psi_{i+1}(y) - 2\psi_i(y) + \psi_{i-1}(y)}{h_x^2} = f(\psi_i(y), \frac{\delta\psi_i}{\delta x}, \frac{\partial\psi_i}{\partial y}, x_i, y, E) \tag{35}$$

Where the δ denotes the first partial derivative in the finite differences approximation.
We can now apply again the finite differences approximation to the y coordinate, which yields

$$\frac{\psi_{i,j+1} + \psi_{i,j-1} - 2\psi_{i,j}}{h_y^2} + \frac{\psi_{i+1,j} + \psi_{i-1,j} - 2\psi_{i,j}}{h_x^2} = f(\psi_{i,j}, x_i, y_j, \frac{\delta\psi_{ij}}{\delta x}, \frac{\delta\psi_{ij}}{\delta y}, E) \tag{36}$$

Rearranging the terms, it's possible to obtain the following system of equations:

$$\sum_{i'j'} A_{i,j,i',j'}\psi_{i'j'} = E\psi_{i,j} \tag{37}$$

Where $A_{i,j,i',j'}$ is a hypermatrix of size $N_x \times N_y \times N_x \times N_y$.
The next task will be to find a way to express 37 as a linear system of equations, by finding a choice of index that encapsulates the relation for all pairs (i, j), with the constraint that the resulting matrix is symmetric.
Formally

$$F : (i, j) \mapsto \gamma \text{ such that } \alpha = F(i, j),\ \beta = F(i', j') \implies A_{\alpha\beta} = A_{\beta\alpha} \tag{38}$$

This is guaranteed if the factors $A_{i,j,i',j'}$ are symmetric under the exchange $i \leftrightarrow i'$ and $j \leftrightarrow j'$ and the map F is bijective.

$$A_{F(i,j),F(i',j')} = A_{i,j,i',j'} = A_{i',j',i,j} = A_{F(i',j'),F(i,j)} \tag{39}$$

3.5.1 Indeces parametrization

A possible map $(i, j) \mapsto \gamma$ is

$$F(i, j) = \gamma = i + N_x j \tag{40}$$

Using this map, the entries of ψ_μ will be organized as

$$\psi = (\psi_{(0,0)}, \psi_{(1,0)}, \dots, \psi_{(N_x-1,0)}, \psi_{(0,1)}, \dots, \psi_{(N_x-1,N_y-1)}) \tag{41}$$

And the problem will be reduced to

$$\sum_{\beta=0}^{N_xN_y} A_{\alpha\beta}\psi_\beta = E\psi_\alpha \tag{42}$$

3.6 Spin

In the case of this work, dealing with non relativisitic quantum mechanics, we treat spin as an additional degree of freedom of our single particle system.
Recalling the commutators that define the spin operator in 3 dimensions:

$$[S_i, S_j] = i\hbar\epsilon_{ijk}S_k \tag{43}$$

Where ϵ_{ijk} is the Levi-Civita symbol.
Spin comes into action by means of Spin Orbit interaction through the operator $\hat{\mathbf{L}} \cdot \hat{\mathbf{S}}$.
$\hat{\mathbf{L}}$ acts on the Hilbert space of position by $\hat{\mathbf{L}} = (\mathbf{r} \times \mathbf{p}) = -i\hbar(\mathbf{r} \times \nabla)$.
While $\hat{\mathbf{S}}$ acts on the Hilbert space of spin, a representation of SU(2) where the basis vectors are its projection on the z axis.
We can then rewrite by the pauli matrices $\hat{\mathbf{S}} = i\frac{\hbar}{2}\boldsymbol{\sigma}$, where

$$\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z) = \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) \tag{44}$$

3.6.1 Spin and finite differences

Working in 3D, together with spin, the lattice on which we want to solve our eigenvalue problem is given by sets of points $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$ as done previously, while the spin, discrete by nature, can be represented by

$$\mathcal{S} = \{-\hbar/2, \hbar/2\} \tag{45}$$

Since we're adding a "fourth" dimension to the problem, the transformations that maps all the different indeces to a single one will be

$$F(i, j, k, s) = s + 2(i + N_x(j + N_y k)) \tag{46}$$

Where 2 comes from the size of the spin representation.

3.7 Parametrization and discretization of the spin orbit interaction

In the case of the Woods Saxon potential, the spin orbit is phenomenologically parametrized as

$$\hat{H}_{\mathrm{SO}} = v_{\mathrm{LS}}(\mathbf{r})\mathbf{L} \cdot \mathbf{S} \tag{47}$$

Where

$$v_{\mathrm{LS}}(\mathbf{r}) = v_{\mathrm{LS}}^{(0)} \left(\frac{r_0}{\hbar}\right)^2 \frac{1}{r} \left[\frac{\mathrm{d}}{\mathrm{d}r} \frac{1}{1 + e^{\frac{r-R}{a}}}\right] \tag{48}$$

We can develop the product

$$\mathbf{L} \cdot \mathbf{S} = -i\frac{\hbar^2}{2}\left(\sigma_x\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) + \sigma_y\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) + \sigma_z\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\right) \tag{49}$$

Using finite differences, thanks to the approximation in equation 20, we are able to write the first partial derivatives in terms of ψ

$$\frac{\partial\psi}{\partial x} = \frac{\psi_{i+1,j,k} - \psi_{i-1,j,k}}{2h_x}; \quad \frac{\partial\psi}{\partial y} = \frac{\psi_{i,j+1,k} - \psi_{i,j-1,k}}{2h_y}; \qquad \frac{\partial\psi}{\partial z} = \frac{\psi_{i,j,k+1} - \psi_{i,j,k-1}}{2h_z}$$

Table 1: Woods-Saxon proton single particle energies in ^{40}Ca

Shell	Degeneracy	WS Energy (MeV)	WS Energy ref. (MeV)
$1s_{1/2}$	2	-29.983	-29.982
$1p_{3/2}$	4	-21.257	-21.255
$1p_{1/2}$	2	-18.576	-18.573
$1d_{5/2}$	6	-11.877	-11.871
$2s_{1/2}$	4	-7.907	-7.900
$1d_{3/2}$	8	-6.496	-6.489

It's obious that the matrix elements describing the spin orbit interaction will be off-diagonal, since they are non local.
The matrix elements of H_{SO} will then be defined by

$$\hat{H}_{\mathrm{SO}} \to -v_{\mathrm{LS}}(r)\frac{i\hbar^2}{2}\left[\sigma_x\left(y_j\frac{\psi_{ijk+1}-\psi_{ijk-1}}{2h_z}-z_k\frac{\psi_{ij+1,jk}-\psi_{ij-1k}}{2h_y}\right)+\dots\right] \tag{50}$$

Where the expression above acts on a 2×1 spin vector.
The discretized $\hat{H}$, a matrix $2N_xN_yN_z\times 2N_xN_yN_z$ will then be the sum $T+V+H_{\mathrm{SO}}$ of the kinetic energy, the potential energy and the spin orbit interaction.

3.8 Shell model

3.8.1 Coulomb interaction

Protons are positively charged, which means that beside the strong force we have to take into account the Coulomb interaction.
Keeping in theme with a mean field approach, we can approximate the Coulomb potential generated by the protons as the one of a uniform sphere, of charge Z, with radius R.

$$v_{\mathrm{C}}(r)=\frac{Ze^2}{4\pi\varepsilon_0}\begin{cases}\frac{3-(r/R)^2}{2R} & r\le R\\ \frac{1}{r} & r>R\end{cases} \tag{51}$$

3.9 Shell model calculation

The final Hamiltonian for our mean field phenomenological nuclear model will be

$$H_p=H_{\mathrm{WS}}+H_{\mathrm{SO}}+H_{\mathrm{C}} \tag{52}$$

for protons, while

$$H_n=H_{\mathrm{WS}}+H_{\mathrm{SO}} \tag{53}$$

for neutrons.
Applying the theory explained so far, we get the following results

Table 2: Woods-Saxon neutron single particle energies in ^{40}Ca

Shell	Degeneracy	WS Energy (MeV)	WS Energy ref. (MeV)
$1s_{1/2}$	2	-38.843	-38.842
$1p_{3/2}$	6	-29.543	-29.541
$1p_{1/2}$	2	-26.944	-26.942
$1d_{5/2}$	6	-19.618	-19.614
$2s_{1/2}$	4	-15.689	-15.684
$1d_{3/2}$	6	-14.315	-14.310

Table 3: Woods-Saxon proton single particle energies in ^{16}O

Shell	Degeneracy	WS Energy (MeV)	WS Energy ref. (MeV)
$1s_{1/2}$	2	-26.446	-26.445
$1p_{3/2}$	6	-14.453	-14.451
$1p_{1/2}$	2	-9.330	-9.328
$1d_{5/2}$	6	-2.734	-2.731
$2s_{1/2}$	2	-0.722	-0.709
$1d_{3/2}$	4	4.026	4.088

Table 4: Woods-Saxon neutron single particle energies in ^{16}O

Shell	Degeneracy	WS Energy (MeV)	WS Energy ref. (MeV)
$1s_{1/2}$	2	-31.091	-31.095
$1p_{3/2}$	6	-18.614	-18.612
$1p_{1/2}$	2	-13.467	-13.466
$1d_{5/2}$	6	-6.361	-6.359
$2s_{1/2}$	2	-3.977	-3.970
$1d_{3/2}$	4	1.092	1.098

3.10 General Conjugate Gradient

Now that we are able to solve for the minimum eigenvalue of a matrix, we would like to extend our analysis to the smallest **nev** eigenpairs.
A minimization of the Rayleigh quotient could be used in principle, but searching for a solution x which is a matrix $n \times$ nev needs to be done ensuring orthogonality of the columns.
This can be numerically expensive and unstable.
An alternative, efficient solution is to use the generalized conjugate gradient method.
It's a subspace projection method, where the search directions are calculated at each iteration by performing a Rayleigh Ritz procedure on the orthogonalized block $V = [X, P, W]$.

Algorithm 1 GCG Algorithm

Input: Matrices A, B, number of desired eigenpairs `nev`
Initialize block X with `nev` orthonormal vectors
Initialize blocks P and W with `nev` null vectors
Solve the Rayleigh Ritz problem $X^T AXC = X^T BXC\Lambda$ with `nev` eigenpairs
Update $X = XC$
while not converged **do**
    Solve approximately $AW = BX\Lambda$ with some CGM steps
    B-Orthogonalize $V = [X, P, W]$
    Solve the Rayleigh Ritz problem $V^T AVC = C\Lambda$
    Update $X_{\text{new}} = VC$
    Compute the residual $R = AX_{\text{new}} - B\Lambda X$
    If $\|R\| < \epsilon$ then converged
    Otherwise, compute $P = X_{\text{new}} \setminus X$
end while
Output: Approximate eigenpairs (Λ, X)

Given the search subspace X, the Rayleigh-Ritz procedure gives us the best approximation Λ, C to the eigenpair of the large scale problem.
Thus, we need a larger basis to explore better solutions, which comes in the form of W and P
The block **W** is calculated from the inverse power method: Applying A^{-1} to a vector we get an enhancement of the correct components.
The block **P** is calculated from the last search direction. This ensures after orthonormalization of the V matrix that the new approximation X is orthogonal to it, as in the simple CGM.
This procedure enhances stability and convergence speed by somewhat preventing the exploration of previously investigated subspaces.

4 Deformed Woods Saxon

We can now introduce deformations in the nuclear structure by modifying the effective Woods Saxon potential.
More specifically, we can introduce a functional dependence of the nuclear surface R on the direction of the position vector.
In the case of an axially symmetric, quadrupole deformation, R will be given by

$$R(\theta) = R_0[1 + \beta_2 Y_{20}(\theta)] \tag{54}$$

Where $Y_{20}(\theta)$ is the spherical harmonic $l = 0,\ m = 2$, and β_2 characterizes the degree of deviation from sphericity, and θ is the angle between the z-axis and the position vector.

$$Y_{20}(\theta) = \sqrt{\frac{5}{16\pi}}(3\cos^2(\theta) - 1) \quad \cos\theta = \frac{z}{\sqrt{x^2 + y^2 + z^2}}$$

- $\beta_2 > 0$ characterizes a prolate nucleus.
- $\beta_2 < 0$ characterizes an oblate nucleus.

- $\beta_2 = 0$ reduces to the previous spherical case.

And the corresponding Woods Saxon potential is given by

$$V_{\mathrm{WS}}(r) = \frac{-V_0}{1 + \exp\left(\frac{r - R(\theta)}{a}\right)} \tag{55}$$

On top of it, we need to adjust the spin orbit potential.
In the deformed case, the general form should be used

$$V_{\mathrm{SO}}(r) = V_{\mathrm{SO}} \nabla V_{\mathrm{WS}} \cdot (\boldsymbol{\sigma} \times \boldsymbol{p}) \tag{56}$$

Where

$$\nabla V_{\mathrm{WS}} = \frac{V_0/a}{\left[1 + \exp\left(\frac{r - R(\theta)}{a}\right)\right]^2} \exp\left(\frac{r - R(\theta)}{a}\right)(\nabla r - \nabla R) \tag{57}$$

$$\nabla r = \begin{pmatrix} x/r \\ y/r \\ z/r \end{pmatrix} \quad \nabla R = R_0 \beta_2 \frac{\mathrm{d}Y_{20}}{\mathrm{d}\theta} \nabla\theta \tag{58}$$

$$\nabla\theta = \frac{1}{r^2 \sin\theta} \begin{pmatrix} \frac{-xz}{\sqrt{x^2+y^2+z^2}} \\ \frac{-yz}{\sqrt{x^2+y^2+z^2}} \\ \frac{x^2+y^2}{\sqrt{x^2+y^2+z^2}} \end{pmatrix} \quad \frac{\mathrm{d}Y_{20}}{\mathrm{d}\theta} = -6\sqrt{\frac{5}{16\pi}} \sin\theta \cos\theta \tag{59}$$

5 The Hartree-Fock method

A many body system, like the nucleus, is made of indistinguishible particles from the standpoint of quantum mechanics.
Suppose to have a nucleus, with A nucleons, where the mass difference between neutrons and protons is neglected.
The state of the system will be described by a wavefunction $\Psi(\mathbf{r_1}, \dots, \mathbf{r_A})$.
The HF approximation states that the wavefunction can be approximated as a product of single particle states:

$$\Psi(\mathbf{r_1}, \dots, \mathbf{r_A}) = \prod_{i=1}^{A} \phi_i(\mathbf{r_i}) \tag{60}$$

Since we are dealing with fermions, the correct state must be antisymmetric with respect to a particle exchange, forcing the use of a slater determinant:

$$\Psi(\mathbf{r_1}, \dots, \mathbf{r_A}) = \frac{1}{\sqrt{A!}} \det \begin{pmatrix} \phi_1(\mathbf{r_1}) & \dots & \phi_A(\mathbf{r_A}) \\ \dots & \ddots & \dots \\ \phi_1(\mathbf{r_A}) & \dots & \phi_A(\mathbf{r_1}) \end{pmatrix} = \sum_p (-1)^p \phi_{p(1)}(\mathbf{r_1}) \dots \phi_{p(A)}(\mathbf{r_A}) \tag{61}$$

Where the sum is performed over all possible permutations of the particles.
Using the variational principle, we can determine the ground state by minimizing the energy functional

$$E[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle \tag{62}$$

With the constraint that the single particle states be orthogonal to each other.

$$\delta E = \delta(\langle \Psi | \hat{H} | \Psi \rangle - \sum_A \varepsilon_i \langle \phi_i | \phi_i \rangle) = 0 \tag{63}$$

This variation, along with the constraint, gives rise to a single particle Schrodinger-like equation:

$$-\frac{\hbar^2}{2m} \nabla_i^2 \phi_i(\mathbf{r}) + \sum_{j=1}^{A} \int d^3r' \ \phi_j^*(\mathbf{r'}) v(\mathbf{r}, \mathbf{r'}) \phi_j(\mathbf{r'}) \phi_i(\mathbf{r}) - \sum_{j=1}^{A} \int d^3r' \ \phi_j^*(\mathbf{r'}) v(\mathbf{r}, \mathbf{r'}) \phi_j(\mathbf{r}) \phi_i(\mathbf{r'}) = \varepsilon_i \phi_i(\mathbf{r}). \tag{64}$$

One can choose a proper potential $v(\mathbf{r_1}, \mathbf{r_2})$, a trial set of wavefunctions, and solve for (ϕ_i, ε_i).
Since the equation changes for the new solutions, one can use an iterative procedure to solve the self consistent problem.

5.1 Formal treatment

Often there is the need of expanding the coordinate space representation of the single particle hamiltonian solution on an arbitrary basis.

$$\phi_k = \sum_i D_{ik} \chi_i \tag{65}$$

Defining the corresponding creation/annihilation operators $c_l^\dagger, c_l$ for $\{\chi_l\}$ and $a_l^\dagger, a_l$ for $\{\phi_k\}$, the transformation between the two will be

$$a_k^\dagger = \sum_l D_{lk} c_l^\dagger \tag{66}$$

Since we're dealing with otrhonormal, complete basis sets, it's trivial to show that the transformation matrix D is unitary.
This also implies that the c/a operators commute and obey separate anticommutation relations.

5.2 Skyrme interaction

In nuclear physics, the interaction between two nucleons has a very complex functional form. This requires choosing an interaction potential which enables us to simplify the equations and solve the problem.
One of such potentials is the Skyrme interaction, whose formulation is based on the physical principle of a short range interaction among nucleons, consequence of the exchange of massive bosons as the force mediators.
It is made up of two parts, a two body interaction and a three body interaction.

$$V = \sum_{i<j} v_{ij}^{(2)} + \sum_{i<j<k} v_{ijk}^{(3)}$$

The standard modern parametrization for $v^{(2)}$ is (Chabanat 1998)

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

Where

$$\begin{aligned} \mathbf{r} &= \mathbf{r}_1 - \mathbf{r}_2 \\ \mathbf{R} &= \frac{\mathbf{r}_1 + \mathbf{r}_2}{2} \\ \mathbf{P} &= -i(\nabla_1 - \nabla_2)/2 \\ \boldsymbol{\sigma} &= \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2 \\ \mathbf{P}_\sigma &= (1 + \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2)/2 \end{aligned}$$

Primed operators refer to the complex conjugate acting on the left.
This formulation respects all symmetries required of a non relativistic nuclear interaction (Galilean boost, particle exchange, translation, rotation, parity, time inversion and translation).

5.2.1 Three body interaction

The three body term of the Skyrme force is encapsulated by the term

$$\frac{1}{6} t_3 \left(1 + x_3 P_\sigma\right) \left[\rho(\mathbf{R})\right]^\sigma \delta(\mathbf{r})$$

Here, σ in the exponent is a free parameter of the force.

5.2.2 Energy functional

Evaluating the energy functional 62, we get

$$\langle \Psi | \, H \, | \Psi \rangle = \int H(\mathbf{r}) d^3 r \tag{67}$$

$$\mathcal{H}(\mathbf{r}) = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{coul}} \tag{68}$$

5.3 Density matrix and associated quantities

$\mathcal{H}$ depends on $\mathbf{r}$ through a series of known and physically relevant quantities.
Starting from the density matrix, defined as

$$\rho_q(\mathbf{r}\sigma, \mathbf{r}\sigma') = \sum_\alpha \phi_{\alpha,\sigma}(\mathbf{r}) \phi^*_{\alpha,\sigma'}(\mathbf{r}') \tag{69}$$

The index α goes through all single particle states of the particles of type q (Protons, Neutrons), while the index σ refers to the spin coordinate (Up, Down).

$$\rho_q(\mathbf{r}, \mathbf{r}') = \sum_\sigma \rho(\mathbf{r}\sigma, \mathbf{r}'\sigma) = \sum_\alpha \phi_\uparrow(\mathbf{r}) \phi^*_\uparrow(\mathbf{r}') + \phi_\downarrow(\mathbf{r}) \phi^*_\downarrow(\mathbf{r}') \tag{70}$$

$$\rho_q(\mathbf{r}) = \rho_q(\mathbf{r}, \mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}} = \sum_\alpha |\phi_\uparrow(\mathbf{r})|^2 + |\phi_\downarrow(\mathbf{r})|^2 \tag{71}$$

$$\tau_q(\mathbf{r}) = \sum_\alpha \nabla' \cdot \nabla \rho_q(\mathbf{r}, \mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}} \tag{72}$$

$$= \sum_{\sigma,\alpha} \nabla \phi_\sigma(\mathbf{r}) \cdot \nabla \phi^*_\sigma(\mathbf{r}')\Big|_{\mathbf{r}=\mathbf{r}'} = \sum_{\sigma,\alpha} |\nabla \phi_\sigma(\mathbf{r})|^2 \tag{73}$$

$$= \sum_\alpha |\nabla \phi_\uparrow(\mathbf{r})|^2 + |\nabla \phi_\downarrow(\mathbf{r})|^2 \tag{74}$$

$$s_q(\mathbf{r}, \mathbf{r}') = \sum_{\sigma\sigma',i} \rho_q(\mathbf{r}\sigma, \mathbf{r}'\sigma') \langle \sigma' | \, \hat{\boldsymbol{\sigma}} \, | \sigma \rangle = \sum_\alpha \begin{bmatrix} \phi^*_\uparrow(\mathbf{r}') & \phi^*_\downarrow(\mathbf{r}') \end{bmatrix} \hat{\boldsymbol{\sigma}} \begin{bmatrix} \phi_\uparrow(\mathbf{r}) \\ \phi_\downarrow(\mathbf{r}) \end{bmatrix} \tag{75}$$

$$J_{q,\mu\nu} = \frac{1}{2i}(\partial_\mu - \partial'_\mu) s_{q,\nu}(\mathbf{r}, \mathbf{r}')\Big|_{\mathbf{r}'=\mathbf{r}} \tag{76}$$

$$= \frac{1}{2i}\left(\begin{bmatrix} \phi^*_\uparrow(\boldsymbol{r}') & \phi^*_\downarrow(\boldsymbol{r}') \end{bmatrix} \partial_\mu \hat{\sigma}_\nu \begin{bmatrix} \phi_\uparrow(\mathbf{r}) \\ \phi_\downarrow(\mathbf{r}) \end{bmatrix} - \begin{bmatrix} \phi_\uparrow(\boldsymbol{r}) & \phi_\downarrow(\boldsymbol{r}) \end{bmatrix} \partial'_\mu \hat{\sigma}_\nu \begin{bmatrix} \phi^*_\uparrow(\mathbf{r}') \\ \phi^*_\downarrow(\mathbf{r}') \end{bmatrix} \right)_{\mathbf{r}'=\mathbf{r}} \tag{77}$$

$$= \sum_\alpha \text{Im} \left\{ \begin{bmatrix} \phi^*_\uparrow(\boldsymbol{r}) & \phi^*_\downarrow(\boldsymbol{r}) \end{bmatrix} \partial_\mu \hat{\sigma}_\nu \begin{bmatrix} \phi_\uparrow(\mathbf{r}) \\ \phi_\downarrow(\mathbf{r}) \end{bmatrix} \right\} \tag{78}$$

Where α goes through all single particle states, the index is omitted on ϕ for brevity.
Taking the variation of $E[\Psi]$ with respect to ϕ^*_i we get a single particle equation

$$\left(-\nabla \frac{\hbar^2}{2m^*(\mathbf{r})} \nabla + U_q(\mathbf{r}) + \delta_{q,\text{proton}} V_c(\mathbf{r}) + \frac{1}{i} \mathbf{W}_q \cdot (\nabla \times \boldsymbol{\sigma}) \right) \phi_\alpha = \varepsilon_\alpha \phi_\alpha \tag{79}$$

We will now see how to properly treat each term of the equation.

5.4 Functional

For $\boldsymbol{s} = 0$ (even-even nuclei), the functional reduces to the following terms

5.4.1 t0 t3 Interaction

The t_0 part of the functional is given by

$$\mathcal{H}_0 = \frac{1}{2}t_0[(1+\frac{x_0}{2})\rho^2 - (x_0+\frac{1}{2})(\rho_p^2+\rho_n^2)]$$

Taking the variation with respect to ρ_q, we get

$$\frac{\delta H_0}{\delta \rho_q} = \frac{1}{2}t_0[(2+x_0)\rho - (2x_0+1)\rho_q] \tag{80}$$

Which in the case where $\rho_n = \rho_p = \rho_q$, $x_0 = 0$ gives

$$\frac{\delta H_0}{\delta \rho_q} = \frac{1}{2}t_0(2\rho - \rho_q)$$

The t_3 part of the functional is given by

$$\mathcal{H}_3 = \frac{1}{24}t_3\rho^\sigma[(2+x_3)\rho^2 - (2x_3+1)(\rho_p^2+\rho_n^2)]$$

Taking the variation with respect to ρ_q, we get

$$\frac{\delta H_3}{\delta \rho_q} = \frac{1}{24}t_3[(2+x_3)(\sigma+2)\rho^{\sigma+1} - (2x_3+1)(\sigma\rho^{\sigma-1}(\rho_n^2+\rho_p^2)+2\rho^\sigma\rho_q)] \tag{81}$$

$$= \frac{1}{24}t_3\rho^\sigma[(2+x_3)(\sigma+2)\rho - (2x_3+1)(\sigma\rho^{-1}(\rho_n^2+\rho_p^2)+2\rho_q)] \tag{82}$$

$$= \frac{1}{12}t_3\rho^\sigma[(1+\frac{x_3}{2})(\sigma+2)\rho - (x_3+\frac{1}{2})(\sigma\rho^{-1}(\rho_n^2+\rho_p^2)+2\rho_q)] \tag{83}$$

In the case where $\rho_n = \rho_p = \rho_q$, $x_3 = 0,\ \sigma = 1$, we get

$$\frac{\delta H_3}{\delta \rho_q} = \frac{1}{24}t_3\rho[6\rho - 3\rho_q] = \frac{t_3}{4}(\rho^2 - \rho_q^2)$$

Assuming only t_0 and t_3 to be non zero parameters, we get the following single particle equation

$$\Big(-\frac{\hbar^2}{2m}\nabla^2 + \frac{\delta\mathcal{H}_0}{\delta\rho_q} + \frac{\delta\mathcal{H}_3}{\delta\rho_q}\Big)\phi_\alpha = \varepsilon_\alpha\phi_\alpha \tag{84}$$

5.5 Full interaction, neglecting Coulomb, S.O. and S.G. terms

We can add further terms, which will also depend on $\tau_q, \nabla\rho_q$.
The part giving rise to an effective mass develops as

$$\mathcal{H}_{\text{eff}} = +\frac{1}{8}[t_1(2+x_1)+t_2(2+x_2)]\rho\tau \tag{85}$$

$$+\frac{1}{8}[t_2(1+2x_2)-t_1(1+2x_1)]\rho_q\tau_q \tag{86}$$

$$\frac{\delta\mathcal{H}_{\text{eff}}}{\delta\rho_q} = +\frac{1}{8}[t_1(2+x_1)+t_2(2+x_2)]\tau \tag{87}$$

$$+\frac{1}{8}[t_2(1+2x_2)-t_1(1+2x_1)]\tau_q \tag{88}$$

$$\frac{\delta\mathcal{H}_{\text{eff}}}{\delta\tau_q} = +\frac{1}{8}[t_1(2+x_1)+t_2(2+x_2)]\rho \tag{89}$$

$$+\frac{1}{8}[t_2(1+2x_2)-t_1(1+2x_1)]\rho_q \tag{90}$$

While the finite range term

$$\mathcal{H}_{\text{fin}} = +\frac{1}{32}[3t_1(2+x_1)-t_2(2+x_2)]|\nabla\rho|^2 \tag{91}$$

$$-\frac{1}{32}[3t_1(2x_1+1)+t_2(2x_2+1)](|\nabla\rho_p|^2+|\nabla\rho_n|^2) \tag{92}$$

Having in mind the relation

$$\mathcal{F}[\rho] = |\nabla\rho|^2 \implies \frac{\delta\mathcal{F}}{\delta\rho} = -2\nabla^2\rho$$

Gives

$$\frac{\delta\mathcal{H}_{\text{fin}}}{\delta\rho_q} = +\frac{1}{16}[t_2(2+x_2)-3t_1(2+x_1)]\nabla^2\rho \tag{93}$$

$$+\frac{1}{16}[3t_1(2x_1+1)+t_2(2x_2+1)](\nabla^2\rho_q) \tag{94}$$

The final single particle equation will now have effective mass terms and further ones in the mean field

$$\Big(-\nabla\frac{\hbar^2}{2m^*(\mathbf{r})}\nabla+\frac{\delta(\mathcal{H}_0+\mathcal{H}_3+\mathcal{H}_{\text{eff}}+\mathcal{H}_{\text{fin}})}{\delta\rho_q}\Big)\phi_\alpha = \varepsilon_\alpha\phi_\alpha \tag{95}$$

Where

$$\frac{\hbar^2}{2m^*(\mathbf{r})} = \frac{\hbar^2}{2m}+\frac{\delta\mathcal{H}_{\text{eff}}}{\delta\tau_q}$$

5.6 Spin Orbit interaction

The spin orbit interaction arises by including

$$\mathcal{H}_{\text{so}} = \frac{1}{2}W_0[\mathbf{J}\cdot\nabla\rho+\mathbf{J}_p\cdot\nabla\rho_p+\mathbf{J}_n\cdot\nabla\rho_n] \tag{96}$$

Which adds a contribution to the mean field

$$\frac{\delta \mathcal{H}_{\text{so}}}{\delta \rho_q} = -\frac{1}{2} W_0 [\nabla \cdot \mathbf{J} + \nabla \cdot \mathbf{J}_q] \tag{97}$$

And a contribution to the spin orbit interaction

$$\mathbf{W}_q(\mathbf{r}) = \frac{1}{2} W_0 [\nabla \rho + \nabla \rho_q] \tag{98}$$

5.6.1 Kinetic term

Regarding the kinetic component, we end up with an effective mass, such that

$$\frac{\hbar^2}{2m^*(\mathbf{r})} = \frac{\hbar^2}{2m} + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho(\mathbf{r}) - \frac{1}{8}[t_1(1+2x_1) + t_2(1+2x_2)]\rho_q(\mathbf{r}) = \mu(\mathbf{r})$$

This allows us to write

$$\nabla\left(\frac{\hbar^2}{2m^*(\mathbf{r})}\nabla\phi\right) = \nabla\mu(\mathbf{r}) \cdot \nabla\phi + \mu(\mathbf{r})\nabla^2\phi \tag{99}$$

Where both $\nabla\cdot, \nabla^2$ can be readily evaluated in the previously illustrated finite difference scheme as matrix coefficients.

5.7 Total energy calculation

There are two main ways of computing the total energy of the system.
The obious one, which we already encountered, is to evaluate the integral of the energy density.

$$E[\Psi] = \langle \Psi | \hat{H} | \Psi \rangle = \int \mathcal{H}(\mathbf{r}) d^3\mathbf{r}$$

On the other hand, at a local minimum, following equation 63, we get

$$\langle \Psi | \hat{H} | \Psi \rangle = \sum_\alpha \varepsilon_\alpha \tag{100}$$

5.8 Coulomb interaction

In the Slater approximation, the Coulomb interaction energy contribution to the energy density reads

$$\mathcal{H}_{\text{coul}} = \frac{e^2}{2}\left[\iint \frac{\rho_p(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}d^3\mathbf{r}' - \frac{3}{2}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\int \rho_p^{4/3}(\mathbf{r})d^3\mathbf{r}\right] \tag{101}$$

Which gives

$$V_{c,D+E}(\mathbf{r}) = \frac{e^2}{2}\left[\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}d^3\mathbf{r}' - 2\left(\frac{3}{\pi}\right)^{\frac{1}{3}}\rho_p^{1/3}(\mathbf{r})\right] \tag{102}$$

From a computational standpoint, the exchange part is trivial, while the direct one is more involved. One could compute the integral, but the complexity is $\mathcal{O}(N^6)$, rendering it impractical for 3d meshes.
An alternative approach is to solve the poisson equation (from now on, V_c refers to the direct part only)

$$\nabla^2 V_c = 4\pi e^2 \rho_p \tag{103}$$

On the considered mesh, using the already defined finite differences approach.
The boundary conditions are of Dirichlet type, which can be extracted from a quadrupole expansion of the charge density

$$V_c(\mathbf{r}) = 4\pi e^2 \sum_{\lambda=0}^{2}\sum_{\mu=-\lambda}^{\lambda} \frac{\langle Q_{\lambda\mu}\rangle\, Y_{\lambda\mu}}{r^{1+\lambda}} \text{ on } \partial V \tag{104}$$

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

$$\langle Q_{\lambda\mu}\rangle = \int r^\lambda Y^*_{\lambda\mu}(\mathbf{r})\rho_p(\mathbf{r})d^3\mathbf{r} \tag{105}$$

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 the frequent case of a nucleus in a parity eigenstate, the charge density is even, leading to

$$V_c(\mathbf{r}) = \frac{Ze^2}{r} + e^2\frac{\langle Q_{20}\rangle\, Y_{20}(\mathbf{r}) + \langle Q_{22}\rangle \operatorname{Re} Y_{22}(\mathbf{r})}{r^3} \text{ on } \partial V \tag{106}$$

5.8.1 Imposing the boundary conditions

The high order discretization stencil of the laplacian, like in our case, involves points with a distance up to ± 2, this means that the quadrupole expanded potential must be calculated on a box bigger than the one used.
Without losing generality, we can look at how boundary conditions are set in 1D. The 3D case follows trivially.
The linear system of equations will look like

$$\begin{bmatrix} c_{0,0} & \cdots & c_{0,N-1} \\ \vdots & \ddots & \vdots \\ c_{N-1,0} & \cdots & c_{N-1,N-1} \end{bmatrix}\begin{bmatrix} V_0 \\ \vdots \\ V_{N-1} \end{bmatrix} = 4\pi e^2 \begin{bmatrix} \rho_0 \\ \vdots \\ \rho_{N-1} \end{bmatrix}$$

Near a boundary, say $i = 0$, the stencil has the form

$$c_{0,-2}V_{-2} + c_{0,-1}V_{0,-1} + c_{0,0}V_0 + c_{0,1}V_1 + c_{0,2}V_2 = 4\pi e^2\rho_0 \tag{107}$$

The C matrix only accounts for points inside the box, namely $i = 0, 1, 2$ we can take advantage of this and bring the "missing" terms on the right side of the equation, calculated from the multipole expansion.

$$c_{0,0}V_0 + c_{0,1}V_1 + c_{0,2}V_2 = 4\pi e^2\rho_0 - c_{0,-2}V_{-2} - c_{0,-1}V_{-1}$$

This forces the linear system to always abide by the boundary conditions.
This same procedure must be applied to every equation involving points outside the box, e.g. for $i = 1$

$$c_{1,0}V_0 + c_{1,1}V_1 + c_{1,2}V_2 + c_{1,3}V_3 = 4\pi e^2\rho_1 - c_{1,-1}V_{-1}$$

Finally, we can compute the potential vector using the simple conjugate gradient.

6 Spherical harmonics

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

$$Y_{\lambda\mu}(\theta, \phi) = (-1)^\mu \sqrt{\frac{2\lambda+1}{4\pi}\frac{(\lambda-\mu)!}{(\lambda+\mu)!}}\, P_\lambda^\mu(\cos\theta)\, e^{i\mu\phi}. \tag{108}$$

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)

$$P_\lambda^\mu(x) = (1-x^2)^{\mu/2}\frac{\mathrm{d}^\mu P_\lambda(x)}{\mathrm{d}x^\mu}, \tag{109}$$

where $x = \cos\theta$ and

$$P_\lambda(x) = \frac{1}{2^\lambda \lambda!}\frac{\mathrm{d}^\lambda (x^2-1)^\lambda}{\mathrm{d}x^\lambda}. \tag{110}$$

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

$$P_\mu^\mu(x) = (2\mu-1)!!\,(1-x^2)^{\mu/2}, \tag{111}$$

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

$$P_{\mu+1}^\mu(x) = x(2\mu+1)P_\mu^\mu(x). \tag{112}$$

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

$$(\lambda-\mu+1)\,P_{\lambda+1}^\mu(x) = (2\lambda+1)\,x\,P_\lambda^\mu(x) - (\lambda+\mu)\,P_{\lambda-1}^\mu(x), \tag{113}$$

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

Summarized algorithm

1. Compute the base case P_μ^μ from the closed-form formula.
2. If $\mu = \lambda$ the procedure ends, otherwise

3. Evaluate $P^{\mu}_{\mu+1}$, if $\lambda = \mu + 1$ the procedure ends, otherwise

4. Apply the recurrence relation $P^{\mu}_{\lambda+1}$ 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

$$P_{\lambda}^{-\mu}(x) = (-1)^{\mu} \frac{(\lambda - \mu)!}{(\lambda + \mu)!} P^{\mu}_{\lambda}(x), \tag{114}$$

7 Comparison with hfbcs-qrpa code

All the calculations are carried out using SLy5 parameters.

$$\left\langle r_p^2 \right\rangle = \frac{1}{Z} \int r^2 \rho_p(\mathbf{r}) d^3\mathbf{r} \tag{115}$$

$$\left\langle r_n^2 \right\rangle = \frac{1}{N} \int r^2 \rho_n(\mathbf{r}) d^3\mathbf{r} \tag{116}$$

$$\left\langle r_{ch}^2 \right\rangle = \left\langle r_p^2 \right\rangle + \left\langle r^2 \right\rangle_P + \left\langle r^2 \right\rangle_N + \frac{1}{Z} \left(\frac{\hbar}{mc} \right)^2 \sum_{\alpha} \mu_{\tau_\alpha} \left\langle \boldsymbol{\sigma} \cdot \boldsymbol{\ell} \right\rangle_\alpha \tag{117}$$

Table 5: ^{16}O Including spin-gradient terms, spin-orbit interaction, and Coulomb field

Physical quantities

		GCG	hfbcs_qrpa	$\Delta\%$
E_{TOT}	[MeV]	-128.424	-128.400	1.87×10^{-2}
$\left\langle r_n^2 \right\rangle^{1/2}$	[fm]	2.6581	2.6585	1.50×10^{-2}
$\left\langle r_p^2 \right\rangle^{1/2}$	[fm]	2.6832	2.6836	1.49×10^{-2}
$\left\langle r_{ch}^2 \right\rangle^{1/2}$	[fm]	2.7806	2.7803	1.08×10^{-2}

Neutron energy levels

		GCG	hfbcs_qrpa	$\Delta\%$
$1s_{1/2}$	[MeV]	-36.142	-36.137	1.38×10^{-2}
$1p_{3/2}$	[MeV]	-20.613	-20.611	9.70×10^{-3}
$1p_{1/2}$	[MeV]	-14.426	-14.428	1.38×10^{-2}

Proton energy levels

		GCG	hfbcs_qrpa	$\Delta\%$
$1s_{1/2}$	[MeV]	-32.349	-32.345	1.23×10^{-2}
$1p_{3/2}$	[MeV]	-17.139	-17.137	1.16×10^{-2}
$1p_{1/2}$	[MeV]	-11.081	-11.082	9.02×10^{-3}

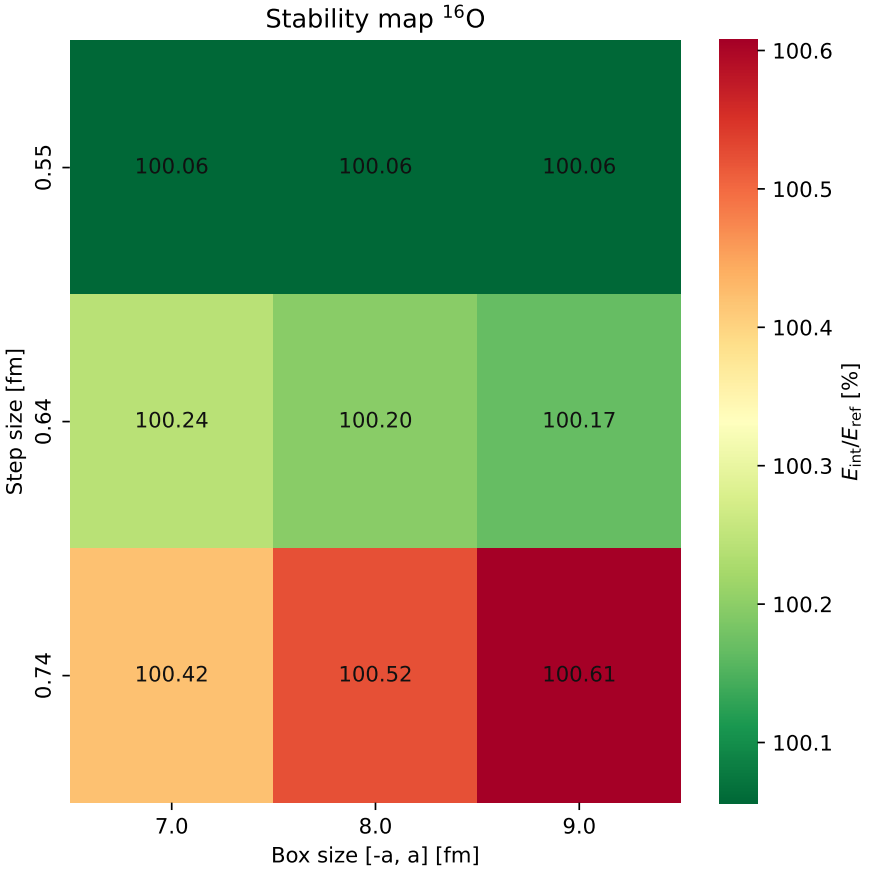

Figure 2: Stability heatmap for unconstrained GCG against hfbcs_qrpa reference value

8 Appendix

$$\mathcal{H} = \mathcal{K} + \mathcal{V} \tag{118}$$

$$= \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{\text{eff}} + \mathcal{H}_{\text{fin}} + \mathcal{H}_{\text{so}} + \mathcal{H}_{\text{sg}} + \mathcal{H}_{\text{coul}} \tag{119}$$

$$T = \int \mathcal{K} d^3r = \int \frac{\hbar^2}{2m} \tau(\mathbf{r}) d^3r \tag{120}$$

$$E_{\text{int}} = \int \mathcal{V} d^3r \tag{121}$$

$$E_1 = T + E_{\text{int}} \tag{122}$$

$$E_2 = \frac{1}{2}(T + \sum_\alpha \varepsilon_\alpha) + E_{\text{int}} - \frac{1}{2} \sum_q \int U_q \rho_q d^3r \tag{123}$$

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(\mathbf{r}) \psi = E\psi \tag{124}$$

$$\frac{\partial \psi}{\partial x} \to \frac{\psi_{i-2} - 8\psi_{i-1} + 8\psi_{i+1} - \psi_{i+2}}{12 h_x} \tag{125}$$

$$\frac{\partial^2 \psi}{\partial x^2} \to \frac{-\psi_{i-2} + 16\psi_{i-1} - 30\psi_i + 16\psi_{i+1} - \psi_{i+2}}{12 h_x^2} \tag{126}$$

$$M_{ijks,i'j'k's'} \psi_{i'j'k's'} = E \psi_{ijks} \tag{127}$$

$$M_{ab} \psi_b = E \psi_a \tag{128}$$