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1 | Energy functional

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.

The many-body hamiltonian of the system, given by

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

acts on the nucleus, a system of A nucleons described by the Slater determinant

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

That is, summing 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. Variational principle

It is possible to show [4] 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 equivalent to the

1.2.   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

$$E_{\text{HF}} = E_{\text{Skyrme}} + E_{\text{Coul}} + E_{\text{Kin}} \tag{1.4}$$

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

1.3.   Skyrme force and functional

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 interaction.
It was first proposed by Tony Skyrme in 1958 [5] as a zero range force between nucleons, and has been used successfully as the building block of theoretical nuclear structure.
Nowadays, the standard form is slightly enriched to be more general [1]. It comprises a two-body interaction, which reads

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

And a three body interaction, that is

$$v^{(3)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{6} t_3 \left(1 + x_3 P_\sigma\right) \left[\rho(\mathbf{R})\right]^\sigma \delta(\mathbf{r})$$

Where

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

Primed operators refer to the adjoint operator acting on the dual space.

This formulation respects all symmetries required of a non relativistic nuclear interaction

- Galilean boost

- Particle exchange

- Translation

- Rotation

- Parity

- Time reversal

The zero-range characteristic takes the form of a Dirac delta $\delta(\mathbf{r})$, which allows to write the exchange Fock term detailed in (REF) as a local one.

Taking the expectation value of the many body hamiltonian, in the Hilbert space of Slater determinants, yields

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int (\mathcal{E}_{\text{Skyrme}} + \mathcal{E}_{\text{Kin}}) d\mathbf{r} = \int \mathcal{E} d\mathbf{r} \tag{1.5}$$

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 [6]

$$\mathcal{E}_{\text{Kin}} = \frac{\hbar^2}{2m} \tau \tag{1.6}$$

$$\mathcal{E}_{\text{Skyrme}} = \sum_{t=0,1} \left\{ C_t^\rho [\rho_0] \rho_t^2 + C_t^{\Delta\rho} \rho_t \nabla^2 \rho_t + C_t^{\nabla \cdot J} \rho_t \nabla \cdot \mathbf{J}_t + C_t^\tau \rho_t \tau_t \right\} \tag{1.7}$$

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

$$C_0^\rho = +\frac{3}{8}t_0 + \frac{3}{48}t_3\rho_0^\sigma \tag{1.8}$$

$$C_1^\rho = -\frac{1}{8}t_0(1 + 2x_0) - \frac{1}{48}t_3(1 + x_3)\rho_0^\sigma \tag{1.9}$$

$$C_0^\tau = +\frac{3}{16}t_1 + \frac{1}{16}t_2(5 + 4x_2) \tag{1.10}$$

$$C_1^\tau = -\frac{1}{16}t_1(1 + 2x_1) + \frac{1}{16}t_2(1 + 2x_2) \tag{1.11}$$

$$C_0^{\Delta\rho} = -\frac{9}{64}t_1 + \frac{1}{64}t_2(5 + 4x_2) \tag{1.12}$$

$$C_1^{\Delta\rho} = +\frac{3}{64}t_1(1 + 2x_1) + \frac{1}{64}t_2(1 + 2x_2) \tag{1.13}$$

$$C_0^{\nabla \cdot J} = -\frac{3}{4}W_0 \tag{1.14}$$

$$C_1^{\nabla \cdot J} = -\frac{1}{4}W_0 \tag{1.15}$$

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

$$\left[-\nabla\left(\frac{\hbar^2}{2m_q^*(\mathbf{r})}\nabla\right) + U_q(\mathbf{r}) + \delta_{\text{q,proton}}U_C(\mathbf{r}) - i\mathbf{B}_q(\mathbf{r}) \cdot (\nabla \times \boldsymbol{\sigma})\right]\varphi_\alpha = \varepsilon_\alpha\varphi_\alpha \tag{1.16}$$

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

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = \frac{\delta\mathcal{E}}{\delta\tau_q} \tag{1.17}$$

$$U_q(\mathbf{r}) = \frac{\delta\mathcal{E}}{\delta\rho_q} \tag{1.18}$$

$$\mathbf{B}_q(\mathbf{r}) = \frac{\delta\mathcal{E}}{\delta\mathbf{J}_q} \tag{1.19}$$

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 1.4.

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

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = + \frac{\hbar^2}{2m} \tag{1.20}$$

$$+ \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho(\mathbf{r}) \tag{1.21}$$

$$- \frac{1}{8}[t_1(1+2x_1) + t_2(1+2x_2)]\rho_q(\mathbf{r}) \tag{1.22}$$

$$\tag{1.23}$$

$$U_q(\mathbf{r}) = + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho \tag{1.24}$$

$$+ \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\rho_q \tag{1.25}$$

$$+ \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau \tag{1.26}$$

$$+ \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\tau_q \tag{1.27}$$

$$+ \frac{1}{16}[t_2(2+x_2) - 3t_1(2+x_1)]\nabla^2\rho \tag{1.28}$$

$$+ \frac{1}{16}[3t_1(2x_1+1) + t_2(2x_2+1)]\nabla^2\rho_q \tag{1.29}$$

$$\tag{1.30}$$

$$\mathbf{W}_q(\mathbf{r}) = + \frac{1}{2}W_0[\nabla\rho + \nabla\rho_q] \tag{1.31}$$

$$- \frac{1}{8}(t_1x_1 + t_2x_2)\mathbf{J} + \frac{1}{8}(t_1 - t_2)\mathbf{J}_q \tag{1.32}$$

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

1.4.   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 [2], which gives a local exchange interaction.
In this approximation, the Coulomb energy reads

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

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

Which gives

$$U_C(\mathbf{r}) = \frac{\delta \mathcal{E}_{\text{Coul}}}{\delta \rho_p} = \frac{e^2}{2} \left[\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' - 2\left(\frac{3}{\pi}\right)^{\frac{1}{3}} \rho_p^{1/3}(\mathbf{r}) \right] \tag{1.33}$$

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)

$$\nabla^2 V_c = 4\pi e^2 \rho_p \tag{1.34}$$

Given the proton density, we can impose Dirichlet boundary conditions, which can be extracted from a quadrupole expansion of the charge density [3]

$$V_c(\mathbf{r}) = 4\pi e^2 \sum_{\lambda=0}^{2} \sum_{\mu=-\lambda}^{\lambda} \frac{\langle Q_{\lambda\mu} \rangle Y_{\lambda\mu}}{r^{1+\lambda}} \quad \text{on } \partial\Omega \tag{1.35}$$

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

$$\langle Q_{\lambda\mu} \rangle = \int r^\lambda Y_{\lambda\mu}^*(\mathbf{r}) \rho_p(\mathbf{r}) d^3\mathbf{r} \tag{1.36}$$

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

$$V_c(\mathbf{r}) = \frac{Ze^2}{r} + e^2 \sum_{\mu=-2}^{2} \frac{\langle Q_{2\mu} \rangle Y_{2\mu}}{r^3} \quad \text{on } \partial\Omega \tag{1.37}$$

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

1.5. 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 1.16 stands true, summarized as

$$(\hat{t} + U)\varphi_k = \varepsilon_k \varphi_k \tag{1.38}$$

We can multiply 1.38 on the left by φ_k^* and integrate to get

$$\int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\mathbf{r} + \int \varphi_k^* U \varphi_k d\mathbf{r} = \int \varphi_l^* \varepsilon_k \varphi_k d\mathbf{r} \tag{1.39}$$

The integral on the right hand side of 1.39 evaluates to ε_k due to the orthonormality constraint. If we sum over all states k we get

$$\sum_k \left\{ \int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\mathbf{r} + \int \varphi_k^* U \varphi_k d\mathbf{r} \right\} = \sum_k \varepsilon_k \tag{1.40}$$

$$\sum_k t_k + \int \rho U = \sum_k \varepsilon_k \tag{1.41}$$

Since U is calculated as 1.18, 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*

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

$$\tag{1.42}$$

If we explicit ρU in equation 1.41 using 1.42, 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

$$\int \mathcal{E}_{\text{Skyrme}} d\mathbf{r} = \sum_k (\varepsilon_k - t_k) + \int \mathcal{E}_{\text{rea}} d\mathbf{r} \tag{1.43}$$

and given the total energy of the system from 1.5

$$E = \sum_k t_k + \frac{1}{2} \int \mathcal{E}_{\text{Skyrme}} d\boldsymbol{r} \tag{1.44}$$

substituting 1.43 in 1.44 yields

$$E_{\text{HF}} = \frac{1}{2} \sum_k (\varepsilon_k + t_k) + \int \mathcal{E}_{\text{rea}} d\boldsymbol{r} = \frac{1}{2} \left(T + \sum_k \varepsilon_k \right) + E_{\text{rea}} \tag{1.45}$$

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 1.45 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

$$i = 0, \ldots, N_x - 1, \; h_x = \frac{2a_x}{N_x - 1}$$
$$j = 0, \ldots, N_y - 1, \; h_y = \frac{2a_y}{N_y - 1}$$
$$k = 0, \ldots, N_z - 1, \; h_z = \frac{2a_z}{N_z - 1}$$

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 [7], 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 1.16.

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

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

$\hat{h}_{\text{SO}}$ acts linearly on the spinor ψ_{ijk}. Finally, the mean field terms U_q, U_c are just multiplicative.

Given that the 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

$$
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & A & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
\psi \\
0 \\
0
\end{bmatrix}
= E
\begin{bmatrix}
0 \\
0 \\
\psi \\
0 \\
0
\end{bmatrix}
\tag{2.5}
$$

Meaning that ignoring the outside points while constructing the A matrix is equivalent to setting the desired boundary conditions on a box slightly larger than the one considered.

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 1.4, 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.

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

$$
\tag{2.6}
$$

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 2.6.

$$\frac{-30V_0 + 16V_1 - V_2}{12h^2} = 4\pi e^2 \rho_0 + \frac{V_{-2} - 16V_{-1}}{12h^2} = \tilde{\rho}_0 \qquad (2.7)$$

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

$$\frac{+16V_0 - 30V_1 + 16V_2 - V_3}{12h^2} = 4\pi e^2 \rho_1 + \frac{V_{-1}}{12h^2} = \tilde{\rho}_1 \qquad (2.8)$$

The proper system to solve will then be

$$AV = \tilde{\rho} \qquad (2.9)$$

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.   Conjugate gradient methods

This section is devoted to exploring the idea behind the Conjugate Gradient (CG) algorithm and its use in the General Conjugate Gradient (GCG).

2.2.1.   Conjugate Gradient

The CG method is used for solving linear systems of the form

$$Ax = b \tag{2.10}$$

Where A is an $n \times n$ matrix, and x and b are n-dimensional vectors. The quadratic form $f(x)$ associated to this system

$$f(x) = \frac{1}{2}x^T Ax - b^T x \tag{2.11}$$

If A is symmetric, positive-definite, the

2.3.   Functional minimization

2.4.   Constraints

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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 $(2\mu - 1)!! = 1 \cdot 3 \cdot 5 \dots (2\mu - 1)$ 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.