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Abstract

Here goes the Abstract in English of your thesis followed by a list of keywords. The Abstract is a concise summary of the content of the thesis (single page of text) and a guide to the most important contributions included in your thesis. The Abstract is the very last thing you write. It should be a self-contained text and should be clear to someone who hasn't (yet) read the whole manuscript. The Abstract should contain the answers to the main scientific questions that have been addressed in your thesis. It needs to summarize the adopted motivations and the adopted methodological approach as well as the findings of your work and their relevance and impact. The Abstract is the part appearing in the record of your thesis inside POLITesi, the Digital Archive of PhD and Master Theses (Laurea Magistrale) of Politecnico di Milano. The Abstract will be followed by a list of four to six keywords. Keywords are a tool to help indexers and search engines to find relevant documents. To be relevant and effective, keywords must be chosen carefully. They should represent the content of your work and be specific to your field or sub-field. Keywords may be a single word or two to four words.

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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 | Energy 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

$$E_{\text{HF}} = E_{\text{Skyrme}} + E_{\text{Coul}} + E_{\text{Kin}} \quad (1.1)$$

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

1.1. Skyrme force and functional

Now that the theoretical and numerical 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 [4] 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

$$v^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = t_0 (1 + x_0 P_\sigma) \delta(\mathbf{r}) \quad (1.2)$$

$$+ \frac{1}{2} t_1 (1 + x_1 P_\sigma) [\mathbf{P}'^2 \delta(\mathbf{r}) + \delta(\mathbf{r}) \mathbf{P}^2] \quad (1.3)$$

$$+ t_2 (1 + x_2 P_\sigma) \mathbf{P}' \cdot \delta(\mathbf{r}) \mathbf{P} \quad (1.4)$$

$$+ \frac{1}{6} t_3 (1 + x_3 P_\sigma) [\rho(\mathbf{R})]^\sigma \delta(\mathbf{r}) \quad (1.5)$$

$$+ i W_0 \boldsymbol{\sigma} \cdot [\mathbf{P}' \times \delta(\mathbf{r}) \mathbf{P}] \quad (1.6)$$

And a three body interaction, that is

$$v^{(3)}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{6} t_3 (1 + x_3 P_\sigma) [\rho(\mathbf{R})]^\sigma \delta(\mathbf{r}) \quad (1.7)$$

Where

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

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

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

- Galilean boost
- Particle exchange
- Translation
- Rotation
- Parity
- Time reversal

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

$$\langle H \rangle = \langle \Psi | H | \Psi \rangle = \int (\mathcal{E}_{\text{Skyrme}} + \mathcal{E}_{\text{Kin}}) d\mathbf{r} = \int \mathcal{E} d\mathbf{r} \quad (1.8)$$

In the case of even-even nuclei, time-odd components of the functional reduce to zero, leaving [5]

$$\mathcal{E}_{\text{Kin}} = \frac{\hbar^2}{2m} \tau \quad (1.9)$$

$$\mathcal{E}_{\text{Skyrme}} = \sum_{t=0,1} \left\{ C_t^\rho [\rho_0] \rho_t^2 + C_t^{\Delta\rho} \rho_t \nabla^2 \rho_t + C_t^{\nabla \cdot J} \rho_t \nabla \cdot \mathbf{J}_t + C_t^\tau \rho_t \tau_t \right\} \quad (1.10)$$

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

$$C_0^\rho = +\frac{3}{8}t_0 + \frac{3}{48}t_3\rho_0^\sigma \quad (1.11)$$

$$C_1^\rho = -\frac{1}{8}t_0(1+2x_0) - \frac{1}{48}t_3(1+x_3)\rho_0^\sigma \quad (1.12)$$

$$C_0^\tau = +\frac{3}{16}t_1 + \frac{1}{16}t_2(5+4x_2) \quad (1.13)$$

$$C_1^\tau = -\frac{1}{16}t_1(1+2x_1) + \frac{1}{16}t_2(1+2x_2) \quad (1.14)$$

$$C_0^{\Delta\rho} = -\frac{9}{64}t_1 + \frac{1}{64}t_2(5+4x_2) \quad (1.15)$$

$$C_1^{\Delta\rho} = +\frac{3}{64}t_1(1+2x_1) + \frac{1}{64}t_2(1+2x_2) \quad (1.16)$$

$$C_0^{\nabla \cdot J} = -\frac{3}{4}W_0 \quad (1.17)$$

$$C_1^{\nabla \cdot J} = -\frac{1}{4}W_0 \quad (1.18)$$

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

$$\left[-\nabla \left(\frac{\hbar^2}{2m_q^*(\mathbf{r})} \nabla \right) + U_q(\mathbf{r}) + \delta_{q,\text{proton}} U_C(\mathbf{r}) - i\mathbf{B}_q(\mathbf{r}) \cdot (\nabla \times \boldsymbol{\sigma}) \right] \varphi_\alpha = \varepsilon_\alpha \varphi_\alpha \quad (1.19)$$

The index $q = n, p$ refers respectively to the neutron and proton quantites.

Where the different terms are given by

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = \frac{\delta \mathcal{E}}{\delta \tau_q} \quad (1.20)$$

$$U_q(\mathbf{r}) = \frac{\delta \mathcal{E}}{\delta \rho_q} \quad (1.21)$$

$$\mathbf{B}_q(\mathbf{r}) = \frac{\delta \mathcal{E}}{\delta \mathbf{J}_q} \quad (1.22)$$

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 (REF).

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

$$\frac{\hbar^2}{2m_q^*(\mathbf{r})} = + \frac{\hbar^2}{2m} \quad (1.23)$$

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

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

$$(1.26)$$

$$U_q(\mathbf{r}) = + \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\rho \quad (1.27)$$

$$+ \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\rho_q \quad (1.28)$$

$$+ \frac{1}{8}[t_1(2+x_1) + t_2(2+x_2)]\tau \quad (1.29)$$

$$+ \frac{1}{8}[t_2(1+2x_2) - t_1(1+2x_1)]\tau_q \quad (1.30)$$

$$+ \frac{1}{16}[t_2(2+x_2) - 3t_1(2+x_1)]\nabla^2\rho \quad (1.31)$$

$$+ \frac{1}{16}[3t_1(2x_1+1) + t_2(2x_2+1)]\nabla^2\rho_q \quad (1.32)$$

$$(1.33)$$

$$\mathbf{W}_q(\mathbf{r}) = + \frac{1}{2}W_0[\nabla\rho + \nabla\rho_q] \quad (1.34)$$

$$- \frac{1}{8}(t_1x_1 + t_2x_2)\mathbf{J} + \frac{1}{8}(t_1 - t_2)\mathbf{J}_q \quad (1.35)$$

For ease of notation and implementation, unindexed densities refer to isovector quantities.

1.2. Coulomb interaction

In the Slater approximation [2], the Coulomb energy contribution to the total energy is

$$E_{\text{Coul}} = \int \mathcal{E}_{\text{Coul}}(\mathbf{r}) d\mathbf{r} \quad (1.36)$$

$$\mathcal{E}_{\text{Coul}}(\mathbf{r}) = \frac{e^2}{2} \left[\int \frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\mathbf{r}' - \frac{3}{2} \left(\frac{3}{\pi} \right)^{\frac{1}{3}} \rho_p^{4/3}(\mathbf{r}) \right] \quad (1.37)$$

Which gives

$$U_C(\mathbf{r}) = \frac{\delta \mathcal{E}_{\text{Coul}}}{\delta \rho_p} = \frac{e^2}{2} \left[\int \frac{\rho_p(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' - 2 \left(\frac{3}{\pi} \right)^{\frac{1}{3}} \rho_p^{1/3}(\mathbf{r}) \right] \quad (1.38)$$

The direct contribution is what one would get classically, computing the energy of a charge distribution.

The exchange part, arising from fermionic nature of nucleons, would be non-local, hence the need for a practical and robust approximation.

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)

$$\nabla^2 V_c = 4\pi e^2 \rho_p \quad (1.39)$$

The boundary conditions are of Dirichlet type, which can be extracted from a quadrupole expansion of the charge density [3]

$$V_c(\mathbf{r}) = 4\pi e^2 \sum_{\lambda=0}^2 \sum_{\mu=-\lambda}^{\lambda} \frac{\langle Q_{\lambda\mu} \rangle Y_{\lambda\mu}}{r^{1+\lambda}} \text{ on } \partial\Omega \quad (1.40)$$

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

$$\langle Q_{\lambda\mu} \rangle = \int r^\lambda Y_{\lambda\mu}^*(\mathbf{r}) \rho_p(\mathbf{r}) d^3\mathbf{r} \quad (1.41)$$

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

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

$$V_c(\mathbf{r}) = \frac{Ze^2}{r} + e^2 \sum_{\mu=-2}^2 \frac{\langle Q_{2\mu} \rangle Y_{2\mu}}{r^3} \text{ on } \partial\Omega \quad (1.42)$$

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

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 in the 5 points finite difference scheme, explained in

(REF), will look like

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

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

$$c_{0,-2}V_{-2} + c_{0,-1}V_{0,-1} + c_{0,0}V_0 + c_{0,1}V_1 + c_{0,2}V_2 = 4\pi e^2 \rho_0 \quad (1.43)$$

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 $i = 1$

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

After imposing the boundary conditions, we can easily solve the linear system of equations.

1.3. Energy calculation

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

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

$$E_{\text{int}} = E[\rho, \tau, J_{\mu\nu}] = \int \mathcal{E} d\mathbf{r} \quad (1.44)$$

An alternative approach is to realize that, in a stationary point $\delta E = 0$, the single particle eigenvalue equation stands true

$$(\hat{t} + U)\varphi_k = \varepsilon_k \varphi_k \quad (1.45)$$

We can multiply 1.45 on the left by φ_k^* and integrate to get

$$\int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\mathbf{r} + \int \varphi_k^* U \varphi_k d\mathbf{r} = \int \varphi_k^* \varepsilon_k \varphi_k d\mathbf{r} \quad (1.46)$$

The integral on the right hand side of 1.46 evaluates to ε_k due to the orthonormality constraint. If we sum over all states k we get

$$\sum_k \left\{ \int -\varphi_k^* \frac{\hbar^2}{2m} \nabla^2 \varphi_k d\mathbf{r} + \int \varphi_k^* U \varphi_k d\mathbf{r} \right\} = \sum_k \varepsilon_k \quad (1.47)$$

$$\sum_k t_k + \int \rho U = \sum_k \varepsilon_k \quad (1.48)$$

Since U is calculated as 1.21, assuming that the functional has a power dependence from ρ of the form $\mathcal{E} = A\rho^{\sigma+1}$ as in our case, we get the *rearrangement energy*

$$\rho U = \rho \frac{\delta \mathcal{E}}{\delta \rho} = \rho(\sigma + 1)A\rho^\sigma = (\sigma + 1)A\rho^{\sigma+1} = \mathcal{E} + \sigma \mathcal{E} = \mathcal{E} + \mathcal{E}_{\text{rea}} \quad (1.49)$$

Given the energy of the total system from 1.8, we have

$$\sum_k t_k + \frac{1}{2} \int \mathcal{E} d\mathbf{r} = E \quad (1.50)$$

If we explicit \mathcal{E} in equation 1.48 using 1.49, we finally get to

$$\int \mathcal{E} d\mathbf{r} = \sum_k (\varepsilon_k - t_k) - \sigma \int \mathcal{E} d\mathbf{r} \quad (1.51)$$

Substituting it in equation 1.49 yields

$$E_{\text{HF}} = \frac{1}{2} \sum_k (\varepsilon_k + t_k) - \sigma \int \mathcal{E} d\mathbf{r} = \frac{1}{2} \left(T + \sum_k \varepsilon_k \right) + E_{\text{rea}} \quad (1.52)$$

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

Sidenote: actual calculation

As shown in 1.11, the actual functional has a plethora of ρ terms, which can be summarized as

$$\mathcal{E} = \sum_j A_j \rho^{\sigma_j+1} \implies E_{\text{rea}} = - \sum_j \sigma_j A_j \rho^{\sigma_j+1} \quad (1.53)$$

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

Since equation 1.52 is valid only in the minimum of the functional, it's useful in Hartree-Fock calculations to check its equivalence with the integrated energy, so one can be sure to actually be in a minimum.

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A | Appendix

A.1. Spherical harmonics

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

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

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)

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

where $x = \cos \theta$ and

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

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

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

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

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

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

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

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

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

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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.

