



POLITECNICO
MILANO 1863

SCUOLA DI INGEGNERIA INDUSTRIALE
E DELL'INFORMAZIONE

Title

TESI DI LAUREA MAGISTRALE IN
XXXXXXX ENGINEERING - INGEGNERIA XXXXXXX

Author: **Name Surname**

Student ID: 000000

Advisor: Prof. Name Surname

Co-advisors: Name Surname, Name Surname

Academic Year: 20XX-XX

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.

Keywords: here, the keywords, of your thesis

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

Contents

Abstract	i
Abstract in lingua italiana	iii
Contents	v
1 Energy functional	1
1.1 Skyrme force and functional	1
Bibliography	5
A Appendix A	7
B Appendix B	9
List of Figures	11
List of Tables	13
List of Symbols	15
Acknowledgements	17

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 [2] as a zero range force between nucleons, and has been used successfully as the building block of 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 complex conjugate 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 and translation).

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

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

In the case of even-even nuclei, time-odd components of the functional reduce to zero, leaving [3]

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

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

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

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

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

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

The coulomb field U_C , which is present only in the single particle equation for protons, doesn't come from the skyrme interaction, but from the Coulomb part of the complete functional. It will be properly derived in section (REF).

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

particular case, we have

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

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

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

$$(1.26)$$

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

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

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

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

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

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

$$(1.33)$$

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

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

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

Bibliography

- [1] E. Chabanat, P. Bonche, P. Haensel, J. Meyer, and R. Schaeffer. A skyrme parametrization from subnuclear to neutron star densities. *Nuclear Physics A*, 627(4):710–746, 1997. ISSN 0375-9474. doi: [https://doi.org/10.1016/S0375-9474\(97\)00596-4](https://doi.org/10.1016/S0375-9474(97)00596-4). URL <https://www.sciencedirect.com/science/article/pii/S0375947497005964>.
- [2] T. Skyrme. The effective nuclear potential. *Nuclear Physics*, 9(4):615–634, 1958. ISSN 0029-5582. doi: [https://doi.org/10.1016/0029-5582\(58\)90345-6](https://doi.org/10.1016/0029-5582(58)90345-6). URL <https://www.sciencedirect.com/science/article/pii/0029558258903456>.
- [3] P. Stevenson and M. Barton. Low-energy heavy-ion reactions and the skyrme effective interaction. *Progress in Particle and Nuclear Physics*, 104:142–164, 2019.

A | Appendix A

If you need to include an appendix to support the research in your thesis, you can place it at the end of the manuscript. An appendix contains supplementary material (figures, tables, data, codes, mathematical proofs, surveys, . . .) which supplement the main results contained in the previous chapters.

B | Appendix B

It may be necessary to include another appendix to better organize the presentation of supplementary material.

List of Figures

List of Tables

List of Symbols

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

Acknowledgements

Here you might want to acknowledge someone.

