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Sensitivity of Nuclear Matter Properties to the Range of the Effective Interaction

Relatore:
Dott. Xavier Roca-Maza

Candidato:
Giacomo Accorto
Matricola 810361

Correlatore:
Prof. Gianluca Colò

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Contents

List of Tables

List of Figures

Introduction

At present, a nuclear model that describes phenomenology *tout court* is not yet available. A very successful theoretical approach is the self-consistent mean-field (SCMF) one. The approach is based on an independent particle picture, where nucleons are considered to be self-bound by the average of the two-body interactions over the states occupied by the other particles. The resulting field is created in a self-consistent way. Such a field is considered to be static, so that dynamical corrections are neglected. Specifically, this approach can be realized by means of an adopted effective interaction, solved at the level of the Hartree-Fock approximation. In atomic physics, energy density functionals of high accuracy can be derived from the electron gas theory. In contrast, in nuclear physics, the form of the effective interaction might be at most motivated from some *ab initio* theory, which is not as reliable as it is for electronic systems. In fact, in this field we do not know in detail the force acting between nucleons. Expressly, the functionals start directly from an effective theory, which considers fit parameters to be fixed on nuclear structure data.

During the past years the Milan nuclear physics research group, as well as many others, has mainly investigated the nuclear effective interaction by using a zero-range force, such as the one introduced by T. Skyrme in 1959 [12]. In this work we decided to adopt a finite-range potential, as first presented by D. M. Brink and E. Boeker in 1967 [4]. In their paper two ranges are introduced as parameters of the interaction. They physically indicate the distance at which the force acts. In the literature [4, 11], guided by some physical estimates, the ranges of the nucleon-nucleon effective interaction have been fixed at the start of the fitting protocol, and hence could not have been considered as fit parameters to be properly investigated. Another reason for this choice to be made is that as the ranges are allowed to be fit parameters, the work winds up in a numerical analysis, while many authors have often sticked to the idea that a physical guidance, coming e.g. from the meson-exchange picture, should dictate the values of the ranges. In these papers, the ranges have been chosen as $\mu_1 \approx 0.5 - 0.7$ fm and $\mu_2 \approx 1.0 - 1.2$ fm. Although these values bear some resemblance with the ranges associated with the one- and two-pion exchange, we work here along the idea that the interaction is purely effective.

Thus, the main aim of this work is to give an explanation of the role of the range in the nuclear effective interaction, and to clarify the sensitivity of nuclear matter properties to it. In particular, we did that by studying the Equation of State of symmetric nuclear matter, an infinite system with equal proton and neutron densities, totally spin unpolarized. The system choice and the effective interaction explored in this thesis make the Equation of State analytic. Furthermore, in this case we know that the wave functions expression has a simple plane-wave form. Nuclear matter properties, that characterize the Equation of State around the saturation density, have been used both as benchmark tools and as information to find the parameters.

In chapter one, we give a general overview about the main empirical information on the nucleon-nucleon interaction, a brief review regarding the SCMF models, a thorough definition of the symmetric uniform nuclear matter limit, and lastly we present the fundamentals of the Hartree-Fock approximation method.

In chapter two, with a couple of examples, we present how the Hartree-Fock calculations can be technically carried out for uniform nuclear matter. First, we use a zero-range density-dependent interaction as a preparatory example: this shows how to handle the kinetic term and a two-body term in a simple case. In addition, this kind of interaction is very popular in the field [12, 5], being one of the first to have been proposed. Second, for the finite-range potential, we also compute the Equation of State and we give most of the expressions and definitions used in chapter three.

How to determine the parameters of the adopted effective interaction is the main topic of chapter three. We first present some nuclear matter properties that characterize the symmetric matter Equation of State around the saturation density, and that we have employed to find the parameters. By using as an example a zero-range density-dependent effective interaction, we show how one may evaluate the parameters of the potential. Thereby we first study an interaction whose expression is made of just a single Gaussian function, and then we add a second Gaussian term to it. The main purpose of this chapter is to understand what is the behavior of nuclear properties, such as the incompressibility and the effective mass, as a function of the range. In fact, we have many models relating some observables to these properties. One important example is given by the giant monopole resonance (GMR) [8], which is linked to the incompressibility and to its derivative with respect to density, M. Another example is the giant quadrupole resonance (GQR), which depends on the effective mass of the system. Thus, physical values for these properties does impact on the accuracy of models describing, e.g., GMR or GQR. We also studied if having an extra Gaussian make the model more flexible or not. Many results are analytic, some others numerical, others obtained using a fit protocol. The analysis of the errors affecting the obtained results is not a purpose of this work.

Chapter 1

Nuclear Systems

1.1 Main Empirical Information on the Nucleon-Nucleon Interaction

We would like to recall the main features a nuclear interaction should reproduce. The following explanation does not mean to be thorough. For more details see, e.g., [7, 10].

1.1.1 Nucleon-Nucleon force

1. *Attractive* : Being the deuteron[1], with total angular momentum $J = 1$ and even parity, a bound system, the nuclear force shows a basically attractive character. It is also clear, from the existence of stable self-bound atomic nuclei, that the interaction between two nucleons is attractive, too.

2. *Spin-dependent and Hard Core* : The triplet system has a bound state (i.e. the deuteron), while singlet state fails to be bound. Moreover, if the two particles are identical and close enough, spins cannot be aligned because of the Pauli principle. Thus, the deuteron is bound because neutrons and protons are different particles and then they can stay close with aligned spins.

   Also related to Pauli repulsion, measurements show that nucleon-nucleon potential has a hard repulsive core with a range $r \approx 0.4$ fm.

3. *Short range* : Rough estimates of the range of the nucleon-nucleon force give $r \approx$ few fm. For example, one can consider the pion's Compton wavelength, which is, in fact, $\lambda_C^{\pi} = 1.4$ fm. Otherwise, the inter-particle distance between nucleons in nuclei is found to be around 1.1 fm. We will give a further example of these estimates in section 3.3.

4. *Noncentral* : Since the deuteron has a quadrupole moment, the orbital angular momentum cannot be a constant of the motion, although total angular momentum J is.

5. *Charge independence* : Charge independence implies the same forces in those states that can be occupied by all three kinds of pairs nn, pp, and np.

[1] A deuteron is a bound system composed by a neutron and a proton.

6. *Exchange character* : The differential cross section for neutron-proton scattering up to 600 MeV is full of backward scattering events, and shows a symmetry around $\pi/2$. Thereby, only even angular momentum states contribute to the scattering amplitude. With the aim to explain this behavior, the idea of an exchange force has been introduced as follows:

$$V_M = V(x)P_M, \tag{1.1}$$

where P_M is the Majorana space-exchange operator, so that

$$P_M\phi(\vec{x}_i,\vec{x}_j) = \phi(\vec{x}_j,\vec{x}_i). \tag{1.2}$$

Since

$$P_M Y_{lm}(\hat{x}) = Y_{lm}(-\hat{x}) = (-1)^l Y_{lm}(\hat{x}), \tag{1.3}$$

odd-l terms in scattering amplitude can be eliminated by means of a Serber force, defined by

$$V_{Serber} = V(x)\frac{1}{2}(1+P_M). \tag{1.4}$$

7. *Spin-orbit force* : In nucleon-nucleon scattering, large polarization of scattered nucleons has been observed perpendicular to the plane of scattering. A spin-orbit force is introduced to understand this polarization. Its contribution is effective only at high energy, since it vanishes in s states. In addition, the spin-orbit term has a huge relevance, since it explains shell effects, such as level splitting and magic numbers.

1.1.2 Size and Charge Distribution

Elastic electron scattering indicates an average charge distribution of the type given by a Woods-Saxon expression $\rho = \rho_0(1+e^{(r-R)/a})^{-1}$. The charge distribution expression is illustrated in figure 1.1.

1. The central nuclear density is approximately constant at $\rho_0 = 0.16$ particles/fm^3 from nucleus to nucleus. In fact, because of the short-range nature of the force, nucleons interacts only with their neighbors, so that, when one adds a new particle to the system, most of the others are not directly affected by its presence. Thus, interior density does not substantially change by increasing the number of the nucleons A.

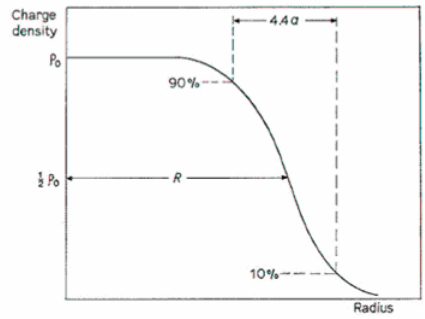

Figure 1.1: The nuclear charge-density distribution saturates inside the nucleus, as one stays far from the surface.

2. Empirically, it has been seen that the radius of a nucleus is given by $r_0 A^{\frac{1}{3}}$, where $r_0 \approx 1$ fm. By assuming nuclei to be spherical, one finds that the particle density in nuclear matter is a constant ${\rho_0}^2$, independent of the size of the nucleus.

$$\rho_0 = \frac{A}{V} = \frac{3}{4\pi r_0^3}. \tag{1.5}$$

3. Inter-particle distance in nuclei, characterized by $l = \rho^{-\frac{1}{3}} \approx 2$ fm, is found to be greater than the root-mean-square radius of the proton. This observation implies that interacting nucleons, within some energy range where distances shorter than their radius are not involved, may be used as degrees of freedom to understand the properties of the nuclei. Thereby, nucleons almost do not feel the repulsive hard core of the nuclear interaction, but rather a smooth potential, which is in good approximation the average interaction with the others.

[2] Except that at the nucleus surface, where the binding energy quickly drops.

1.2 Self-Consistent Mean-Field Models

The self-consistent mean-field (SCMF) approach is very useful to understand the structure of the nuclear systems. This approach takes place midway between *ab initio* models, that begin with a given nucleon-nucleon potential, and macroscopic models (such as the famous liquid drop model), that predict the nucleon binding energy, the nucleon radius, and so on, by looking at some global properties of nuclear systems. The first kind of models are very effective in reproducing nucleon-nucleon scattering data, but tend to fail in predicting quantitatively the saturation point, if three-body interactions are not taken into account. Moreover, even at the state of art, there are lot of issues when one tries to describe many-body systems using them. Many *Ansatz* for the potential have been employed to fit experimental data. The outcome shows different results for different choices of the nucleon-nucleon interaction fitting the same data. Moreover, the results are different for different many-body techniques used to solve each system. On the other hand macroscopic models are able to reproduce quite well some average trends (such as the binding energy trend) but are entirely based on the phenomenology. Most of these models do not take into account the important shell structure effects.

Hence it comes the idea to find a kind of compromise. SCMF approach begins at a microscopic nucleon-nucleon interaction level, although it considers effective interactions working well for many-body systems. The method consists in finding a self-consistent[3] mean nuclear field with as few as possible phenomenological hints. Thus, we have a theory at the level of the Hartree-Fock approximation. To build up a mean field just from a nucleon-nucleon interaction has revealed to be very cumbersome, and it seems to fail on a quantitative point of view. Thereby, it is much easier to motivate from these nucleon-nucleon interactions at most the expression for the potential, while some parameters are determined to fit the nuclear structure data. For more advanced details on SCMF state of art, see [2].

1.2.1 The Gogny Interaction

Zero-range interactions have been first introduced by T. Skyrme [12]. A finite-range interaction has been introduced by Brink and Boeker as a sum of two Gaussian potential [4]. Dechargé and Gogny [6] have put together these ideas, obtaining one of the most general forms for an effective interaction we have so far: the so-called Gogny force

$$\begin{aligned} V_{Gogny}(|\vec{r}_1-\vec{r}_2|) = \sum_{i=1,2} e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau) + \\ + t_3(1+x_0 P_\sigma)\delta(|\vec{r}_1-\vec{r}_2|)\rho^\alpha\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right) + \\ + iW_{ls}(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}^\dagger\times\delta(|\vec{r}_1-\vec{r}_2|)\vec{k}, \end{aligned} \tag{1.6}$$

where

$$P_\sigma = \frac{1+\vec{\sigma}_1\cdot\vec{\sigma}_2}{2} \tag{1.7}$$

[3] A self-consistent method is an iterative process that begin with a reasonable starting guess for the quantity to be determined (e.g. the eigenfunction of the system) to converge to the self-consistent result. A possibility, as it happens in Hartree-Fock approximation, is to find some functional of the eigenfunctions to be minimized.

is the spin-exchange operator,

$$P_\tau = \frac{1+\vec{\tau}_1\cdot\vec{\tau}_2}{2} \tag{1.8}$$

is the isospin-exchange operator, and the relative momentum is

$$\vec{k} = -\frac{i}{2}(\nabla_1 - \nabla_2). \tag{1.9}$$

The quantities B_i, H_i, M_i, W_i, μ_i, t_3, x_0, α and W_{ls} are parameters of the interaction. The Gogny force is composed by a finite range term, modeled by two Gaussian, including some (iso)spin exchange terms, a zero-range density-dependent term, and lastly a spin-orbit component, which is a function of the relative momentum.

In particular, we have focused on some simpler forms of Gogny force, the zero-range density-dependent potential

$$V_{zrdd}(|\vec{r}_1-\vec{r}_2|) = t_0\delta(|\vec{r}_1-\vec{r}_2|)(1+x_0P_\sigma) + \frac{t_3}{6}\delta(|\vec{r}_1-\vec{r}_2|)\rho^\alpha(1+x_3P_\sigma), \tag{1.10}$$

and the sum of two Gaussian potential, the latter as presented by Brink and Boeker in 1967,

$$V_{B\&B}(|\vec{r}_1-\vec{r}_2|) = \sum_{i=1,2} S_i(1-m_i+m_iP_M)e^{-\frac{|r_1-r_2|^2}{\mu_i^2}}. \tag{1.11}$$

One can rename parameters to lead back these potentials to the Gogny force. As an example, by calling $W_i = S_i(1-m_i)$ and $M_i = S_im_i$ we obtain a part of (1.6), actually the direct radial term plus an exchange term, showing the Serber force nature of this interaction. [4]

[4] Here we took advantage of the fact that $P_{12} = P_MP_\sigma P_\tau = -1$, and then $P_M = -P_\sigma P_\tau$, if we use the interaction to compute just anti-symmetric matrix elements, or rather if we always have the arrangement $V(1-P_{12})$. Since this will be the case all along this thesis, it is then true that when inside the potential we find a term like $f(x)P_{12}$ we have

$$(f(x)P_{12})(1-P_{12}) = -f(x)(1-P_{12}). \tag{1.12}$$

1.3 The Hartree-Fock Approximation

In the following we give a detailed explanation of Hartree-Fock approximation, that is the framework in which we shall use the chosen effective interaction to get the Equation of State per particle $e(\rho)$. Calculations that use second quantization formalism can be found in, e.g., [7, 10].

The starting point is the Hamiltonian H_0, which describes the free motion of N particles moving, eventually, in a local external potential:

$$H_0 = \sum_i^N h(i) = \sum_i^N \Big(-\frac{\hbar^2 \nabla_i^2}{2m} + U_{ext}(i) \Big), \tag{1.13}$$

where $\hbar c = 197.3269788$ MeV$\cdot$fm[5] is the Planck constant over 2π times the light velocity c, $mc^2 = 939.0 MeV$ is the rest mass of a nucleon, taken as an average between proton and neutron's ones[6]. $\nabla_i^2 = \sum_{i=1}^3 \partial_i \partial_i$ is the Laplacian operator that gives the kinetic term, while $U_{ext}(i)$ is some external potential acting on the i-th particle[7]. We have to add then a two-body interaction term H_1:

$$H_1 = \frac{1}{2} \sum_{i \neq j}^N v(i,j). \tag{1.14}$$

In the ground state, every particle occupies a given single-particle state, in such a way that its motion is not far to be independent of the other N-1 particles. We know that this provides an excellent approximation for a lot of systems; hence we assume that every particle, with wave function u_i, feels the potential

$$U_H(\vec{x}) = \sum_i^N \int d_3 y \, v(\vec{x} - \vec{y}) |u_i(\vec{y})|^2 = \int d_3 y \, v(\vec{x} - \vec{y}) n(\vec{y}), \tag{1.15}$$

given by its average interaction with all the others. Energy is therefore composed by two terms. The first one is the expectation value of H_0, the energy of the particle that moves within an external potential. The second one is the potential energy term related to the inter-particle interaction (the Hartree potential), essentially obtained as an average of the two-body interaction over the states occupied by the other particles. Thereby, we are not considering the contribution to the energy deriving from instantaneous interaction of the background N-1 particles, which are considered as static and independent ones. We get to the eigenvalues equation

$$\Big(-\frac{\hbar \nabla_{\vec{x}}^2}{2m} + U_{ext}(\vec{x}) + U_H(\vec{x}) \Big) u_i(\vec{x}) = E_i u_i(\vec{x}). \tag{1.16}$$

The real ground state energy is $E_{GS} = \langle \Psi_{GS} | H | \Psi_{GS} \rangle$. It is clear that in almost every realistic situation the ground state wave functions are not known, and should be evaluated in a self-consistent way. It is clear too, that by only taking the local Hartree potential, we are including self-interaction of particles and we are not considering Fermi statistics. This issues can be solved by considering a non-local exchange term (Fock term). Thus, we guarantee the anti-symmetric behavior under particles exchange, and we make self-interaction contribution vanish, too.

[5] `http://physics.nist.gov/cgi-bin/cuu/Value?hbcmevf|search_for=plank`

[6] `https://en.wikipedia.org/wiki/Nucleon`

[7] In atomic physics $U_{ext}(i)$ would be the nucleus central potential that keeps the electron system bound.

1.3.1 Hartree-Fock equations

By using variational methods we can get the Hartree-Fock equations. We start with N orthonormal single-particle wave functions u_i, and find the set that minimizes the expectation value of the Hamiltonian. In particular one considers the Slater determinants, defined by

$$|\Psi_{HF}\rangle = \frac{1}{\sqrt{N!}}\sum_{\sigma}(-1)^{\sigma}P_{\sigma}|u_1 \dots u_n\rangle\,, \tag{1.17}$$

$$\langle u_i|u_j\rangle = \delta_{ij}, \tag{1.18}$$

where σ indicates a possible permutation with its parity, performed by P_σ exchange operator on the state $|u_1 \dots u_n\rangle$. Thereby, we discover an upper bound to the ground state energy using an independent particles approximation. The energy difference is called correlation energy, and it is negative by definition:

$$E_c = E_{GS} - E_{HF} \leq 0. \tag{1.19}$$

Remember the Hamiltonian H_0 affects only the i-th particle. Two-body interaction H_1 affects instead only i-th and j-th particles. Thanks to the orthonormality of the Slater states, it is straightforward that for one-body operators the bra permutation must be the same as the ket permutation . As regards the two-body operators, the bra permutation can differ from the ket permutation at most for an exchange of the i-th particle with the j-th particle. Thus, we find:

$$\langle\Psi_{HF}|H_0|\Psi_{HF}\rangle = \frac{1}{N!}\sum_{\sigma,\sigma'}(-1)^{\sigma+\sigma'}\sum_{i}^{N}\langle u_1 \dots u_n|P_\sigma h(i)P_{\sigma'}|u_1 \dots u_n\rangle \tag{1.20}$$

$$= \frac{1}{N!}\sum_{\sigma,\sigma'}(-1)^{\sigma+\sigma'}\delta_{\sigma\sigma'}\sum_{i}^{N}\langle u_i|h(i)|u_i\rangle \tag{1.21}$$

$$= \sum_{i}^{N}\langle u_i|h(i)|u_i\rangle\,, \tag{1.22}$$

$$\langle\Psi_{HF}|H_1|\Psi_{HF}\rangle = \frac{1}{N!}\sum_{\sigma,\sigma'}(-1)^{\sigma+\sigma'}\frac{1}{2}\sum_{i\neq j}^{N}\langle u_1 \dots u_n|P_\sigma v(i,j)P_{\sigma'}|u_1 \dots u_n\rangle \tag{1.23}$$

$$= \frac{1}{N!}\sum_{\sigma,\sigma'}(-1)^{\sigma+\sigma'}\delta_{\sigma\sigma'}\frac{1}{2}\sum_{i\neq j}^{N}\langle u_i u_j|v(i,j)|u_i u_j - u_j u_i\rangle \tag{1.24}$$

$$= \frac{1}{2}\sum_{i,j}^{N}\langle u_i u_j|v(i,j)|u_i u_j - u_j u_i\rangle\,, \tag{1.25}$$

$$\langle\Psi_{HF}|H|\Psi_{HF}\rangle = \sum_{i}^{N}\langle u_i|h(i)|u_i\rangle + \frac{1}{2}\sum_{i,j}^{N}\langle u_i u_j|v(i,j)|u_i u_j - u_j u_i\rangle\,. \tag{1.26}$$

We consider the functional $E_{HF}[u_1 \dots u_n]$ to be minimized. By imposing the othonormality of the single-particle states by means of the Lagrange coefficients ϵ_{ij}, we get

$$E_{HF}[u_1 \dots u_n] = \langle\Psi_{HF}|H|\Psi_{HF}\rangle - \epsilon_{ij}(\langle u_i|u_j\rangle - \delta_{ij}). \tag{1.27}$$

Let us search for the minimum by considering a small variation δu_i of the i-th single-

particle state u_i:

$$0 = E_{HF}[\dots u_i + \delta u_i \dots] - E_{HF}[u_1 \dots u_n] \tag{1.28}$$

$$= \langle \delta u_i | h(i) | u_i \rangle + \frac{1}{2} \sum_j \Big[\langle \delta u_i u_j | v(i,j) | u_i u_j - u_j u_i \rangle + \\ + \langle u_j \delta u_i | v(i,j) | u_j u_i - u_i u_j \rangle \Big] - \sum_j \epsilon_{ij} \langle \delta u_i | u_i \rangle + c.c. \tag{1.29}$$

to find N Hartree-Fock equations

$$h(i) | u_i \rangle + \sum_j \langle \cdot \, u_j | v(i,j) | u_i u_j - u_j u_i \rangle = \sum_j \epsilon_{ij} | u_j \rangle . \tag{1.30}$$

Since every linear combination of solutions again solves these equations, we have a degree of freedom to diagonalize the matrix ϵ_{ij}. Furthermore, multiplying on the left by $\langle u_i |$, we obtain the usual form of the equations

$$\langle u_i | h(i) | u_i \rangle + \sum_j \langle u_i u_j | v(i,j) | u_i u_j - u_j u_i \rangle = \epsilon_i . \tag{1.31}$$

In the coordinate space we have N integro-differential equations:

$$(h + U_H) u_i(\vec{x}) - \int d_3 y u_i(\vec{y}) v(\vec{x}, \vec{y}) \sum_j u_j(\vec{x}) u_j^*(\vec{y}) = \epsilon_i u_i(\vec{x}), \tag{1.32}$$

1.3.2 Some Useful Results on the Hartree-Fock Equations

We can use equation (1.31) to get a simpler form of energy expectation value (1.26):

$$\langle \Psi_{HF} | H | \Psi_{HF} \rangle = \sum_i^N \epsilon_i - \frac{1}{2} \langle u_i u_j | v(i,j) | u_i u_j - u_j u_i \rangle = \frac{1}{2} \sum_i^N \Big(\langle u_i | h | u_i \rangle + \epsilon_i \Big). \tag{1.33}$$

These last expression put in evidence a really non-obvious fact: the expectation value of the Hamiltonian *is not* the sum of the single-particle Hartree-Fock energies.

We would also like to recall Koopmans' theorem

$$\mu \equiv E_{HF}(N+1) - E_{HF}(N) = \epsilon_{N+1}, \tag{1.34}$$

relating the Fermi's energy $\epsilon_F = \mu(T=0)$ to the eigenvalues ϵ_i.

1.4 Symmetric Nuclear Matter

We can imagine the nucleons to be contained in a box of volume Ω, which in the end will tend to infinity. In such a limit we consider only the volume contribution to the energy, without any surface term. We also neglect electric charge effects. Symmetric nuclear matter (SNM) is characterized by the fact that for every neutron there is a corresponding proton, so that:

$$N = Z = \frac{A}{2}. \tag{1.35}$$

Moreover, we ask the system to be homogeneous, i.e. with a constant density. Thereby

$$\rho_n = \rho_p = \frac{\rho}{2}. \tag{1.36}$$

We also know, by imposing the boundary box conditions, that the wave functions for a system like that have a simple plane-wave form. We will make use of the fact that this system does not vary under translations in space, so that in particular the momentum is a constant of the motion. Thereby, we can diagonalize the Hamiltonian together with the momentum operator, and choose momentum eigenstates to Hamiltonian's, too. In coordinate space one finds the eigenfunctions

$$\phi_{\vec{k}}(\vec{x}) = \langle \vec{x} | \vec{k} \rangle \tag{1.37}$$

$$= \frac{e^{i\vec{k}\cdot\vec{x}}}{\sqrt{\Omega}}. \tag{1.38}$$

It is interesting to point out, however, that in most of the Hartree-Fock calculations, wave-functions for finite nuclei have to be found in a self-consistent numerical way. Since in this case we know their exact expressions, it is possible to carry out the HF method in a totally analytic way.

Furthermore, the symmetry matter has no spin-polarization. This means that there is not a favorite spin alignment, or rather spins have a random distribution. If we choose the quantum numbers $|nlm_z\rangle$ to describe the system, then for every spin-up particle there will be a spin-down particle. From now on we assume to handle infinite, uniform, symmetric nuclear matter. This symmetry properties entail a remarkable simplification of the Hartree-Fock calculations, since all the (iso)spin-dependent terms will, on average, vanish. Specifically, this means that every time one finds a term containing $\langle \vec{\sigma}_1 \cdot \vec{\sigma}_2 \rangle$ or $\langle \vec{\tau}_1 \cdot \vec{\tau}_2 \rangle$, these vanish in the average over all the eigenstates[8].

We always consider zero temperature matter, a completely degenerate Fermi gas model. In fact, this is a very good approximation for nuclear matter, valid for a very wide range of energies. The saturation density for the nuclear matter is found to be at $\rho_0 = 0.16$ fm^{-3}, implying the Fermi momentum

$$k_F = \left(\frac{3\pi^2}{2}\rho_0\right)^{\frac{1}{3}} = 1.33 \text{ fm}^{-1}. \tag{1.39}$$

From this result, one easily obtains the Fermi energy

$$\epsilon_F = \frac{\hbar^2 k_F^2}{2m} \approx 37 \text{ MeV}, \tag{1.40}$$

[8] This is quite straightforward to be understood naively, thanks to rotational symmetries of the system. For a rigorous proof, see [13].

while the average kinetic energy is found to be, as we will see in chapter two, at $(3/5)\epsilon_F \approx 22$ MeV. Thus, only a small fraction of the nucleons in a nucleus with nucleon number A can be excited, unless the energy involved is comparable to ϵ_F, which dovetails a temperature of $\approx 10^8$K. To get an idea on the order of magnitude of this temperature, we recall that, e.g., Sun internal temperature is $T_I \approx 10^6$K.

Chapter 2

Hartree-Fock Calculations for Uniform Matter

2.1 The Kinetic Term

First of all, we show how to handle kinetic term within the Hartree Fock calculations.

Imagine the nucleons being confined in a spherical volume Ω, reminding that, as we said above, infinite uniform symmetric matter wave functions have the expression

$$\phi_{\vec{k}}(\vec{r}) = \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{\Omega}}. \tag{2.1}$$

We shall make use of the continuous limit

$$\sum_i \to \frac{g\Omega}{(2\pi)^3}\int d_3k, \tag{2.2}$$

where g is the degeneracy of the system. The limit becomes exact as we have infinite nuclear matter.

Furthermore, recall that the integration in momentum space runs over the Fermi sphere $\Omega_k = \{|\vec{k}| < k_F\}$.

Thus,

$$\langle T\rangle = \sum_\alpha^F \langle\alpha|\left(-\frac{\hbar^2\nabla^2_{\vec{r}}}{2m}\right)|\alpha\rangle \tag{2.3}$$

$$= \frac{g\Omega}{(2\pi)^3}\int_{\Omega_k} d_3k \int_\Omega d_3r \frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{\Omega}}\left(-\frac{\hbar^2\nabla^2_{\vec{r}}}{2m}\right)\frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{\Omega}} \tag{2.4}$$

$$= \frac{g\Omega k_F^3}{10\pi^2}\frac{\hbar^2k_F^2}{2m} \tag{2.5}$$

$$= \frac{g\Omega k_F^3}{10\pi^2}\epsilon_F, \tag{2.6}$$

where we used the Fermi energy definition

$$\epsilon_F = \frac{\hbar^2k_F^2}{2m}. \tag{2.7}$$

By imposing $g = 4$[1] and by taking advantage of the relation between the density and the Fermi momentum

$$k_F = \left(\frac{3\pi^2}{2}\rho\right)^{\frac{1}{3}}, \tag{2.8}$$

thanks to the fact that $A = \Omega\rho$, one can compute kinetic energy per particle

$$< t >= \frac{3}{5}\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}\epsilon_F = \frac{3}{5}\frac{\hbar^2}{2m}\left(\frac{3\pi^2}{2}\rho\right)^{\frac{2}{3}}. \tag{2.9}$$

[1] Since there is both spin and isospin degeneracy.

2.2 A Zero-Range Density-Dependent Potential

We consider here a zero-range interaction with a density-dependent term. This delta-modeled potential can be viewed as a part of the Skyrme potential. The main aim of this section is to show how a potential term has to be handled at the level of the Hartree-Fock approximation. The potential expression is:

$$V_{zrdd}(|\vec{r}_1-\vec{r}_2|) = t_0\delta(|\vec{r}_1-\vec{r}_2|)(1+x_0P_\sigma) + \frac{t_3}{6}\delta(|\vec{r}_1-\vec{r}_2|)\rho^\alpha(1+x_3P_\sigma). \tag{2.10}$$

We point out again that this potential explicitly depends on the density of the system, which is a constant for symmetric nuclear matter. It is commonly accepted that some nuclear properties, such as incompressibility and effective mass, are strongly related to the density dependence of the effective force.

Let us begin by computing the anti-symmetric form of the potential. There is a standard procedure to do that, and we will make use of the technique in next section, too.

$$V_{zrdd,AS} = V_{zrdd}(1-P_{12}) \tag{2.11}$$

In general, $P_{12} = P_M P_\sigma P_\tau$, where P_M is the Majorana space exchange operator, while P_σ and P_τ are instead spin and isospin exchange operators respectively. Since we are considering the contact interaction potential (2.10), it follows that here $P_M = 1$. In fact, the presence of the Dirac δ function implies that the wave functions will be evaluated for $|\vec{r}_1-\vec{r}_2| = 0$ only. This definitely simplifies calculations, because the exchange term becomes trivial.

We can then express the action of operators P_σ and P_τ by making use of the Pauli matrices in the (iso)spin space

$$P_\sigma = \frac{1+\vec{\sigma}_1\cdot\vec{\sigma}_2}{2}, \tag{2.12}$$

$$P_\tau = \frac{1+\vec{\tau}_1\cdot\vec{\tau}_2}{2}. \tag{2.13}$$

In what follows, we will consider only the first term of (2.10), since the calculations involving the second term would be analogous. By taking advantage of the previous expressions we find

$$V_{zrdd,AS} = t_0\delta(r)\left(\frac{3}{4}+\frac{x_0}{2}\vec{\sigma}_1\cdot\vec{\sigma}_2-\frac{1}{4}\vec{\sigma}_1\cdot\vec{\sigma}_2-\frac{x_0}{2}\vec{\tau}_1\cdot\vec{\tau}_2-\frac{1}{4}\vec{\tau}_1\cdot\vec{\tau}_2-\frac{1}{4}\vec{\sigma}_1\cdot\vec{\sigma}_2\vec{\tau}_1\cdot\vec{\tau}_2\right). \tag{2.14}$$

As we have already explained above, for the forthcoming calculations of $\langle V_{zrdd,AS}\rangle$ we will use the fact that the terms containing $\langle\vec{\sigma}_1\cdot\vec{\sigma}_2\rangle$ or $\langle\vec{\tau}_1\cdot\vec{\tau}_2\rangle$ vanish in the average process.

Thus, changing the frame of reference to the center of mass and the relative coordinates one, defined by

$$\vec{R} = \frac{\vec{r}_1+\vec{r}_2}{2}, \tag{2.15}$$

$$\vec{r} = \vec{r}_1-\vec{r}_2, \tag{2.16}$$

$$|det(\mathbf{J})| = 1, \tag{2.17}$$

where **J** is the Jacobian matrix, in spherical coordinates, we get

$$\langle V_{zrdd,AS}\rangle = \frac{1}{2}\sum_{\alpha\neq\beta}^{F}\langle\alpha\beta|\frac{3t_0}{4}\delta(r)|\alpha\beta\rangle \tag{2.18}$$

$$= \frac{1}{2}\left(\frac{g\Omega}{(2\pi)^3}\right)^2\int_{\Omega_k}\int_{\Omega_k} d_3k_1\, d_3k_2$$
$$\int_{\Omega}\int_{\Omega} d_3r_1\, d_3r_2\frac{e^{-i\vec{k}_1\cdot\vec{r}_1}}{\sqrt{\Omega}}\frac{e^{-i\vec{k}_2\cdot\vec{r}_2}}{\sqrt{\Omega}}\frac{3t_0}{4}\delta(|\vec{r}_1-\vec{r}_2|)\frac{e^{i\vec{k}_1\cdot\vec{r}_1}}{\sqrt{\Omega}}\frac{e^{i\vec{k}_2\cdot\vec{r}_2}}{\sqrt{\Omega}} \tag{2.19}$$

$$= \frac{3t_0g^2\Omega}{32\pi^4}\left(\frac{k_F^3}{3}\right)^2 \tag{2.20}$$

$$= \frac{3t_0\Omega}{8}\rho^2. \tag{2.21}$$

Thanks to tranlational invariance of the system, the change of the frame of reference does not affect the integration region. Moreover, Ω can be considered as large as we want, since in the end it will become infinite.

The latter calculation is going to be similar to the finite-range direct term one in the next section. In fact, in that calculation, too, we will not find any explicit momentum-dependence in the space integral. The only difference will be the substitution of the δ function with a Gaussian function.

Lastly, one can divide by the number of particle $A = \Omega\rho$, and add the kinetic term (2.9), to obtain the Equation of State

$$e[\rho] = \frac{3}{5}\frac{\hbar^2k_F^2}{2m} + \frac{3t_0}{8}\rho + \frac{t_3}{16}\rho^{\alpha+1}, \tag{2.22}$$

which does not depend on the number of particles and volume, as we expected for nuclear matter.

2.3 A Sum of Two Gaussian Potential

We shall consider here the finite-range effective interaction modeled by a sum of two Gaussian functions. As we said, the interaction is taken from Brink and Boeker [4], and it is possible to read it as a part of the more general Gogny force given in the equation (1.6).

$$V_{B\&B}(|\vec{r}_1-\vec{r}_2|)=\sum_{i=1,2} S_i(1-m_i+m_iP_M)e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}}. \tag{2.23}$$

In this case, to compute the exchange term is not as trivial as for a contact interaction. In fact, here $P_M=1$ is not valid anymore, since the force has a finite range character. We first build up the anti-symmetric form of potential (2.23), in the same way as in the previous section, except that here we must be careful in keeping the direct term separated from the exchange one. In fact, from now on we will treat them separately. We take advantage of the expressions (2.12) and (2.13).

$$V_{B\&B,AS}(|\vec{r}_1-\vec{r}_2|)=\sum_{i=1,2} S_i(1-m_i+m_iP_M)(1-P_MP_\sigma P_\tau)e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} \tag{2.24}$$

$$=\sum_{i=1,2} S_i\left(1-\frac{5}{4}m_i-\frac{m_i}{4}(\vec{\sigma}_1\cdot\vec{\sigma}_2+\vec{\tau}_1\cdot\vec{\tau}_2+\vec{\sigma}_1\cdot\vec{\sigma}_2\vec{\tau}_1\cdot\vec{\tau}_2)\right)e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} \tag{2.25}$$

$$+\sum_{i=1,2} S_i\left(\frac{5}{4}m_i-\frac{1}{4}-\frac{1-m_i}{4}(\vec{\sigma}_1\cdot\vec{\sigma}_2+\vec{\tau}_1\cdot\vec{\tau}_2+\vec{\sigma}_1\cdot\vec{\sigma}_2\vec{\tau}_1\cdot\vec{\tau}_2)\right)P_Me^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} \tag{2.26}$$

As we can see, (2.25) is the direct contribution to the potential, while (2.26) is the exchange one.

2.3.1 The Direct Hartree Term

We aim now to compute the direct term contribution to the mean field.

$$\langle V_d\rangle=\frac{1}{2}\sum_{i=1,2}\sum_{\alpha,\beta=1}^{F}\langle\alpha\beta|S_i(1-\frac{5}{4}m_i)e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}}|\alpha\beta\rangle \tag{2.27}$$

$$=\frac{1}{2}\sum_{i=1,2}S_i(1-\frac{5}{4}m_i)\left(\frac{4\Omega}{(2\pi)^3}\right)^2\int_{\Omega_k}\int_{\Omega_k}d_3k_1\,d_3k_2$$

$$\int_\Omega\int_\Omega d_3r_1\;d_3r_2\;\frac{e^{-i\vec{k}_1\cdot\vec{r}_1}}{\sqrt{\Omega}}\frac{e^{-i\vec{k}_2\cdot\vec{r}_2}}{\sqrt{\Omega}}e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}}\frac{e^{i\vec{k}_1\cdot\vec{r}_1}}{\sqrt{\Omega}}\frac{e^{i\vec{k}_2\cdot\vec{r}_2}}{\sqrt{\Omega}}. \tag{2.28}$$

Let us change frame of reference for space coordinates, using center of mass and relative coordinates.

$$\vec{R}=\frac{\vec{r}_1+\vec{r}_2}{2}, \tag{2.29}$$

$$\vec{r}=\vec{r}_1-\vec{r}_2, \tag{2.30}$$

$$|det(\mathbf{J})|=1. \tag{2.31}$$

Again, the change of the frame of reference does not affect the region of the integration. Another way to see where this possibility of shifting the integration region comes from, is to think that that $\mu^3 \ll \Omega$, so that all in all we can use the limit for infinite matter right here. Thanks to the symmetries of the system and of the integrand, it is very convenient to pass through spherical coordinates. Thus, we have

$$\begin{aligned}\langle V_d\rangle &= \sum_{i=1,2}\frac{S_i}{32\pi^6}(4-5m_i)\int_0^{k_F}\int_0^{k_F} dk_1\,dk_2(4\pi)^2k_1^2k_2^2\int_\Omega d_3R\int_0^\infty dr(4\pi)r^2e^{-\frac{r^2}{\mu_i^2}}\\ &= \sum_{i=1,2}\frac{S_i}{32\pi^6}(4-5m_i)(4\pi)^3\left(\frac{k_F^3}{3}\right)^6\Omega\sqrt{\pi}\frac{\mu^3}{4}\\ &= \sum_{i=1,2}\frac{S_i\Omega\mu_i^3\pi^{\frac{3}{2}}}{8}(4-5m_i)\rho^2, \end{aligned} \tag{2.32}$$

and the direct contribution to the energy per nucleon is

$$\langle v_d\rangle = \sum_{i=1,2}\frac{S_i\mu_i^3\pi^{\frac{3}{2}}}{8}(4-5m_i)\rho. \tag{2.33}$$

The direct term strongly depends on the range, expressly as a cubic power. Beside that, it grows as ρ. As we will see this is the term dominating in the high density limit.

2.3.2 The Exchange Fock Term

As we said above Fock term is the one that derives from line (2.26).

$$\langle V_e\rangle = \frac{1}{2}\sum_{i=1,2}\sum_{\alpha,\beta=1}^{F}\langle\alpha\beta|S_i(\frac{5}{4}m_i-\frac{1}{4})e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}}|\beta\alpha\rangle \tag{2.34}$$

$$= \frac{1}{2}\sum_{i=1,2}S_i(\frac{5}{4}m_i-\frac{1}{4})\left(\frac{4\Omega}{(2\pi)^3}\right)^2\int_{\Omega_k}\int_{\Omega_k}d_3k_1\,d_3k_2 \tag{2.35}$$

$$\int_\Omega\int_\Omega d_3r_1\;d_3r_2\;\frac{e^{-i\vec{k}_1\cdot\vec{r}_1}}{\sqrt{\Omega}}\frac{e^{-i\vec{k}_2\cdot\vec{r}_2}}{\sqrt{\Omega}}e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}}\frac{e^{i\vec{k}_2\cdot\vec{r}_1}}{\sqrt{\Omega}}\frac{e^{i\vec{k}_1\cdot\vec{r}_2}}{\sqrt{\Omega}} \tag{2.36}$$

$$= \frac{1}{2}\sum_{i=1,2}S_i(\frac{5}{4}m_i-\frac{1}{4})\frac{1}{4\pi^6}\int_{\Omega_k}\int_{\Omega_k}d_3k_1\,d_3k_2$$

$$\int_\Omega\int_\Omega d_3r_1\;d_3r_2\;e^{-i(\vec{k}_1-\vec{k}_2)\cdot(\vec{r}_1-\vec{r}_2)}e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} \tag{2.37}$$

There is a non-vanishing dependence of the integrand on the momentum. By changing the space frame of reference in the last integral to the center of mass and relative coordinates one, it is straightforward to notice that

- The center of mass integral is nothing but the volume Ω;
- The space integral can be written as follows:

$$\int_\Omega d_3re^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{r}}e^{-\frac{|\vec{r}|^2}{\mu_i^2}} = e^{-|\vec{k}|^2\frac{\mu_i^2}{4}}\int_\Omega d_3re^{-\left(\frac{\vec{r}}{\mu_i}+i(\vec{k}_1-\vec{k}_2)\frac{\mu_i}{2}\right)^2}. \tag{2.38}$$

Let us shift the integration variable:

$$\frac{\vec{r}}{\mu_i} + i(\vec{k_1} - \vec{k_2})\frac{\mu_i}{2} \to \vec{r'}, \tag{2.39}$$

$$d_3 r = \mu_i^3 \, d_3 r. \tag{2.40}$$

The transformed integration region can be shifted back again to Ω, thanks to translational invariance. Thus, we can use spherical coordinates and choose Ω as big as we want to take advantage of the known result

$$\int_0^\infty dx \, x^2 e^{-x^2} = \frac{\sqrt{\pi}}{4}. \tag{2.41}$$

Thereby,

$$\langle V_e \rangle = \sum_{i=1,2} S_i (\frac{5}{4} m_i - \frac{1}{4}) \frac{\Omega \mu_i^3}{8\pi^{\frac{9}{2}}} \int_{\Omega_k} \int_{\Omega_k} d_3 k_1 \, d_3 k_2 e^{-(\vec{k_1} - \vec{k_2})^2 \frac{\mu_i^2}{4}}. \tag{2.42}$$

To solve the momentum space integral is much more cumbersome. In fact, it becomes necessary to change variables in $\vec{k}$-space, too. Unfortunately, in this case the frame of reference choice *does* affect the integration region. In fact the change of the frame of reference

$$\vec{K} = \frac{\vec{k_1} + \vec{k_2}}{2}, \tag{2.43}$$

$$\vec{k} = \vec{k_1} - \vec{k_2}, \tag{2.44}$$

$$|det(\mathbf{J})| = 1, \tag{2.45}$$

implies the integration region Ω_k to be transformed in the region L, defined by

$$L = f(\Omega_k) = \{|\vec{k}_1(\vec{K}, \vec{k})|, |\vec{k}_2(\vec{K}, \vec{k})| < k_F\} = \{|\vec{K} + \frac{1}{2}\vec{k}| < k_F, |\vec{K} - \frac{1}{2}\vec{k}| < k_F\}. \tag{2.46}$$

It is easy to see that that the new region is nothing but a two spheres intersection, each sphere having radius k_F. Their centers stay at distance $|\vec{k}|$. Thanks to the rotational and the translational symmetries, to define this region is totally analogous to solve the system of the equations

$$x^2 + y^2 + z^2 = k_F^2, \tag{2.47}$$

$$(x - d)^2 + y^2 + z^2 = k_F^2, \tag{2.48}$$

which has solution $x_0 = \frac{d}{2}$, being at the present case $d = |\vec{k}|$. Thereby, we obtain circumferences lying on planes parallel to yz-plane. One can find the surface to be $A = \pi(K_F^2 - x^2)\Theta(K_F - \frac{d}{2})$. This is sketched in figure 2.1. With these ingredients we are able to find the volume of the region $|L|$.

$$|L| = 2\int_{\frac{d}{2}}^{k_F} dx \pi (k_F^2 - x^2) \tag{2.49}$$

$$= \frac{4\pi}{3} k_F^3 (1 - \frac{3}{4k_F} d + \frac{1}{16 k_F} d^3) \Theta(k_F - \frac{d}{2}). \tag{2.50}$$

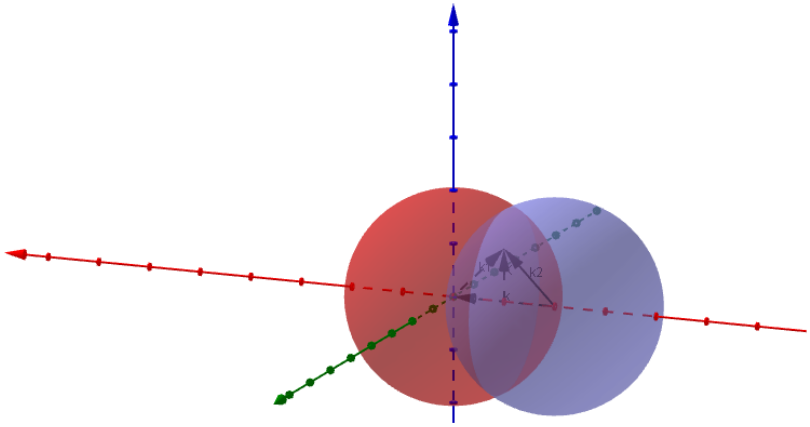

Figure 2.1: The intersection of two spheres with same radius k_F is a circumference. Vectors $\vec{k}_1$, $\vec{k}_2$, $\vec{k}$ and $\vec{K}$ are showed, too. The integration region L is the lentil-shaped one.

We can finally compute the integral (2.42). For convenience, let us define the quantities

$$x = \frac{|\vec{k}|}{2k_F}, \tag{2.51}$$

$$q_i = \mu_i k_F. \tag{2.52}$$

$$\tag{2.53}$$

Thereby, by taking advantage of the following three integral results[2]:

$$\int_0^1 dx x^2 e^{-(qx)^2} = \frac{\sqrt{\pi}\,\mathrm{erf}(q) - 2qe^{-q^2}}{4q^3}, \tag{2.54}$$

$$-\frac{3}{2}\int_0^1 dx x^3 e^{-(qx)^2} = \frac{3}{4q^4}(q^2 e^{-q^2} + e^{-q^2} - 1), \tag{2.55}$$

$$\frac{1}{2}\int_0^1 dx x^5 e^{-(qx)^2} = \frac{1}{4q^6}(q^4 e^{-q^2} + 2q^2 e^{-q^2} + 2e^{-q^2} - 2), \tag{2.56}$$

with error function defined as usual by

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x dt e^{-t^2}, \tag{2.57}$$

[2] Those expressions can be obtained by parameter differentiation or by integration by parts

one has

$$\begin{aligned}\langle V_e\rangle &= \sum_{i=1,2} S_i(\frac{5}{4}m_i-\frac{1}{4})\frac{\Omega\mu_i^3}{8\pi^{\frac{9}{2}}}\int_L\int_L d_3K\,d_3k e^{-\frac{\mu_i^2}{4}\vec{k}^2}\Theta(k_F-|\vec{K}+\frac{1}{2}\vec{k}|)\Theta(k_F-|\vec{K}-\frac{1}{2}\vec{k}|)\\ &= \sum_{i=1,2} S_i(5m_i-1)\frac{2q_i^3\rho\Omega}{\sqrt{\pi}}\int_0^1 dx x^2 e^{-(q_i x)^2}(1-\frac{3}{2}x+\frac{1}{2}x^3).\end{aligned} \tag{2.58}$$

This result implies

$$< v_e >= \frac{1}{2}\sum_{i=1,2} S_i(5m_i-1)\frac{1}{\sqrt{\pi}}g(\mu_i k_F). \tag{2.59}$$

where the dimensionless function g has been defined by

$$g(q) = \frac{2}{q^3}-\frac{3}{q}-(\frac{2}{q^3}-\frac{1}{q})e^{-q^2}+\sqrt{\pi}\,\mathrm{erf}(q). \tag{2.60}$$

We would like to point out that the range dependence is totally contained in the function g, which saturates at the value $\sqrt{\pi}$ as the product q grows. Furthermore,for $q \ll 1$, $g \sim -q$. We recall that $q = \mu_i k_F \sim \mu_i \rho^{\frac{1}{3}}$. Thus, this is the leading term in the low density limit. It is important to note that the behavior g has for small densities is as we expected at a qualitative level. In the low-density limit the energy must tend to zero as the density do the same.

2.3.3 Equation of State and Related Quantities

We can eventually write down the energy per particle as a function of the density. That one as well as the following expressions are widely used through the entire chapter three.

$$e(\rho) = \frac{3}{5}\frac{\hbar^2}{2m}k_F^2+\frac{1}{2}\sum_{i=1,2}\frac{\pi^{\frac{3}{2}}}{4}S_i\mu_i^3(4-5m_i)\rho+\frac{1}{2}\sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5m_i-1)g(\mu_i k_F). \tag{2.61}$$

As expected for an extensive quantity such as energy, again energy per particle is finite and does not depend on volume.

We point out that the parameters m_i appear with opposite sign in the direct term respect to the exchange term. Thus, once negative(positive) strength parameters S_i sign has been fixed, both the direct and the exchange term contribute with an attractive(repulsive) Gaussian term, having strength proportional to S_i. As regards the second terms, they have opposite behavior (and strength $|S_i 5m_i|$).

Let us consider for a moment a single Gaussian potential, as we will do in chapter three. As we just noted, the exchange term is leading the low density behavior, while the direct term leads for high densities. Since symmetric nuclear matter is expected to have a negative minimum, the previous fact explicitly restricts the parameter value to satisfy:

$$S(4-5m) > 0, \tag{2.62}$$

$$S(5m-1)g(\mu_i k_F) < 0. \tag{2.63}$$

A study of the behavior of the function g would give us even stricter constraints on the parameter m.

It is interesting to compute here some physical quantities related to derivatives of (2.61) with respect to the density[3]. In particular, in this work we will make use of the expressions of the pressure, of the incompressibility, and of the skewness [4].

$$P(\rho) = \rho^2 \frac{\partial e}{\partial \rho} \tag{2.64}$$

$$= \frac{2}{5}\frac{\hbar^2}{2m}k_F^2\rho + \frac{1}{2}\sum_{i=1,2}\frac{\pi^{\frac{3}{2}}}{4}S_i\mu_i^3(4-5m_i)\rho^2 + \tag{2.65}$$

$$+ \sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5m_i-1)p(\mu_i k_F)\rho, \tag{2.66}$$

$$K(\rho) = 9\rho^2\frac{\partial^2 e}{\partial \rho^2} \tag{2.67}$$

$$= -\frac{6}{5}\frac{\hbar^2}{2m}k_F^2 - 3\sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5m_i-1)k(\mu_i k_F), \tag{2.68}$$

$$Q(\rho) = 27\rho^3\frac{\partial^3 e}{\partial \rho^3} \tag{2.69}$$

$$= \frac{24}{5}\frac{\hbar^2}{2m}k_F^2 + 3\sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5.m_i-1)q(\mu_i k_F) \tag{2.70}$$

where the dimensionless functions p, k, q are defined by

$$p(q) = -\frac{1}{q^3} + \frac{1}{2q} + (\frac{1}{q^3} + \frac{1}{2q})e^{-q^2}, \tag{2.71}$$

$$k(q) = -\frac{6}{q^3} + \frac{2}{q} + (\frac{1}{q^3} + \frac{4}{q} + q)e^{-q^2}, \tag{2.72}$$

$$q(q) = -\frac{54}{q^3} + \frac{14}{q} + (\frac{54}{q^3} + \frac{40}{q} + 13q + 2q^3)e^{-q^2}. \tag{2.73}$$

We point out that neither the incompressibility nor the skewness contain any contribution coming down from the direct term.

We also note that for $q \ll 0$ the functions p, k, and q behave as the variable q, so that the related physical quantities vanish as the density drops to zero. They behave as q^{-1} if $q \gg 1$.

[3] An overview of these properties will be given in the first section of chapter three.

[4] For example, the incompressibility and the skewness are related to the excitation energy of the giant monopole resonance.

Chapter 3

Nuclear Matter Properties and Fit Parameters

3.1 Some Symmetric Nuclear Matter Properties

Symmetric nuclear matter around the saturation point can be characterized by some properties, related to quantities that can be experimentally measured. Nevertheless, the way these properties are determined is not unique, so that some comments are in order. Such a system is an idealized one. A neutron star is by far the closest object to an infinite system of nuclear matter we know, although it is a very neutron-rich one and spans a much wider range than the one we discuss here. It is obviously difficult to obtain experimental observations on neutron stars, and even more those of direct interest to nuclear physics. Therefore, most of the information must be inferred from the knowledge we have on finite nuclei. We recall that the inside part of a stable $N\sim Z$ nucleus can be sketched as a piece of symmetric nuclear matter.

In this section we face the issue by presenting some properties we used to build or confirm the phenomenological potentials.

1. *Saturation density* : As we discussed in section 1.1, empirically it has been found that the radius of a nucleus grows with the number of particle, specifically as $A^{\frac{1}{3}}$. Thereby, the density
$$\rho = \frac{A}{V} \sim \frac{1}{r_0^3} \tag{3.1}$$
is a constant for the nuclear matter. By knowing the saturation density, one can easily obtain the optimal value for r_0 in all nuclei. The equilibrium density value has been measured quite precisely[1], so that [14]
$$\rho_0 = 0.16 \pm 0.02 \text{ particles/fm}^3. \tag{3.2}$$

2. *Saturation energy* : The binding energy of the nuclear matter, or rather its volume contribution, that grows as A^2, computed at the saturation density, is

[1] e.g. with neutron or electron elastic scattering

[2] We can ignore the surface term, proportional to $A^{\frac{2}{3}}$, as well as the Coulomb repulsion contribution, the symmetry energy contribution, since $N = Z$, and the pairing effects.

evaluated to be [14]

$$e(\rho_0) = -16 \pm 1 \text{ MeV}. \tag{3.3}$$

3. *Pressure* : Saturation energy is a global minimum for infinite nuclear matter. Thus, the derivative of the energy per nucleon with respect to the density must vanish when evaluated at the saturation density. Pressure is a quantity which is proportional to that first derivative, and must therefore vanish, too.

$$P(\rho_0) = \rho^2 \frac{\partial e}{\partial \rho}\Big|_{\rho=\rho_0} = 0 \text{ MeV/fm}^3. \tag{3.4}$$

We used the previous properties in every further calculation, to be reproduced by the fit parameters of the adopted effective potentials. As regards the next properties, we sometime took advantage of them as properties to be reproduced, sometimes as references.

4. *Incompressibility* : We can show that the incompressibility is another quantity related to the derivatives of the energy with respect to the density. In fact, one usually defines compressibility as the relative sensitivity of the nuclear volume to small pressure variations:

$$\chi = -\frac{1}{V}\left(\frac{\partial P}{\partial V}\right)^{-1}. \tag{3.5}$$

In a system at zero temperature, with a constant number of particles $A = \rho V$, pressure is related to the energy by

$$P = -\frac{\partial E}{\partial V} = \rho^2 \frac{\partial e}{\partial \rho}. \tag{3.6}$$

Thus, by using the relation between volume and density to derive the latter equation with respect to the volume, we find

$$\chi^{-1} = \rho \frac{\partial^2 P}{\partial \rho^2}. \tag{3.7}$$

By making use of the last two equations, one finds the compressibility dependence on the density:

$$\chi^{-1}(\rho) = 2\rho^2 \frac{\partial e}{\partial \rho} + \rho^3 \frac{\partial^2 e}{\partial \rho^2} \tag{3.8}$$

$$= 2P(\rho) + \rho^3 \frac{\partial^2 e}{\partial \rho^2}. \tag{3.9}$$

Taking advantage of the equilibrium condition $P(\rho_0) = 0$, the Taylor expansion for the energy around its minimum reads as follows:

$$e(\rho) = e(\rho_0) + \frac{1}{18} K_\infty \left(\frac{\rho - \rho_0}{\rho_0}\right)^2 + \ldots. \tag{3.10}$$

Thus, one can finally define the incompressibility as

$$K_\infty = 9\rho^2 \frac{\partial^2 e}{\partial \rho^2}\Big|_{\rho=\rho_0} \tag{3.11}$$

$$= \frac{9}{\rho_0}\chi^{-1} \tag{3.12}$$

$$= 240 \pm 40 \text{ MeV } (\approx 20\% \text{ uncertainty}) \tag{3.13}$$

We have a quantity related to the curvature of the Equation of State. We point out that K_∞ coincides with $K(\rho_0)$, given in equation (2.67). The value of the incompressibility shows clearly how exotic nuclear matter is, being 24 orders of magnitude more incompressible than a liquid. The best way to infer its value is to measure the excitation energy of the GMR, related to the incompressibility.

5. *Giant Monopole Resonance* : The excitation energy of this important nuclear resonance is related to the incompressibility of the finite nucleus. The latter property can be related with the incompressibility of symmetric nuclear matter, and corrected by its derivative with respect to the density, to take into account surface effects. It is however a fact that the third derivative of the Equation of State can be derived from experimental data with a better precision than the incompressibility [8]. The main reason of that lies in the fact that this quantity is defined at the (almost)model-independent cross density $\rho_c = 0.7\rho_0$. Considering the equations (3.8) and (3.9), one defines a density-dependent incompressibility as

$$K(\rho) = \frac{9\chi^{-1}(\rho)}{\rho} \tag{3.14}$$

$$= \frac{18}{\rho} P(\rho) + 9\rho^2 \frac{\partial^2 e}{\partial \rho^2}. \tag{3.15}$$

Its derivative with respect to the density, once evaluated at ρ_c, is called M. This quantity is related to the giant monopole resonance (GMR) excitation energy, and it is defined by [8]

$$M = 3\rho \frac{\partial K}{\partial \rho}\Big|_{\rho=\rho_c} \tag{3.16}$$

$$= 27\rho_c \left(2\frac{\partial e}{\partial \rho}\Big|_{\rho=\rho_c} + 4\rho \frac{\partial^2 e}{\partial \rho^2}\Big|_{\rho=\rho_c} + \rho_c^2 \frac{\partial^3 e}{\partial \rho^3}\Big|_{\rho=\rho_c} \right) \tag{3.17}$$

$$= 54\frac{P(\rho_c)}{\rho_c} + 12K(\rho_c) + Q(\rho_c) \tag{3.18}$$

$$= 1100 \pm 70 \text{ MeV } (\approx 6\% \text{ uncertainty}). \tag{3.19}$$

6. *Effective mass* : It is the mass that nucleons that move inside the mean field would have if they were freely moving particles, but with an effective mass m^*. In fact, one computes the Fourier transform of the Schrödinger equation of the system, and sets it equal to the Fourier transform of the Schrödinger equation of a freely moving, m^* massive, particle:

$$\frac{\hbar^2}{2m} k^2 + U(k) = \frac{\hbar^2}{2m^*} k^2. \tag{3.20}$$

The latter equation can be derived with respect to the momentum, to get to the definition of the effective mass:

$$\frac{m}{m_\tau^*} = 1 + \frac{m}{\hbar^2 k} \frac{\partial U_\tau(k)}{\partial k}. \tag{3.21}$$

The main issue is then to obtain the single-particle potential $U_\tau(k)$ of a neutron or a proton, labeled by τ, having momentum k. That potential is defined by

$$U_\tau(k) = \frac{1}{2} \sum_{\sigma',\tau'} \int_{\Omega_k} \frac{d_3 k'}{(2\pi)^3} \langle k\sigma\tau k'\sigma'\tau' | V(1 - P_{12}) | k\sigma\tau k'\sigma'\tau' \rangle . \tag{3.22}$$

We recall that we always stayed within the Hartree Fock approximation. Beside that, in symmetric nuclear matter (iso)spin average over the Fermi sphere vanishes. Thus, the latter expression can be analytically computed for the sum of two Gaussian potential, in a way that is not technically different from the calculations we made in chapter two to find the Equation of State of the system. We note that the momentum dependence of the mean field is totally due to the exchange term, since the direct term is a constant in the momentum space.

3.2 A Zero-Range Density-Dependent Potential

The Equation of State (2.22) depends on the three parameters t_0, t_3 and α. We can fix them by imposing some nuclear matter properties to be predicted by the model. If $\rho_0 = 0.16\ \text{fm}^{-3}$, we ask to the Equation of State:

$$e[\rho_0] = -16\,\text{MeV}, \tag{3.23}$$

$$P(\rho_0) = \rho^2 \frac{\partial e}{\partial \rho}\Big|_{\rho=\rho_0} = 0, \tag{3.24}$$

$$K_\infty = 9\rho_0^2 \frac{\partial^2 e}{\partial \rho^2}\Big|_{\rho=\rho_0} = 240\,\text{MeV}. \tag{3.25}$$

Equations (3.23) and (3.24) show the saturation point for nuclear matter, while (3.25) exhibits the curvature of the Equation of State around its minimum. It is possible to solve analytically the three equations-three variables system. The roots are

$$\alpha = \frac{9e(\rho_0) + k_\infty + A(2\rho_0^{\frac{2}{3}} - 3)\rho_0^{\frac{2}{3}}}{3A\rho_0^{\frac{2}{3}} - 9e(\rho_0)} = 0.203 \tag{3.26}$$

$$t_0 = -\frac{k_\infty + 2A\rho_0^{\frac{2}{3}}(3\alpha + \rho_0^{\frac{2}{3}})}{9B\alpha\rho_0} = -2552\,\text{MeV}\cdot\text{fm}^3 \tag{3.27}$$

$$t_3 = \frac{k_\infty + 2A\rho_0^{\frac{4}{3}}}{9C\alpha(\alpha+1)\rho_0^{\alpha+1}} = 16694\,\text{MeV}\cdot\text{fm}^{3(\alpha+1)} \tag{3.28}$$

where we defined:

$$A = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{\frac{2}{3}} \frac{\hbar^2}{2m}, \tag{3.29}$$

$$B = \frac{3}{8}, \tag{3.30}$$

$$C = \frac{1}{16}. \tag{3.31}$$

We point out that t_0 is the attractive term. t_3 term dominates at high densities, thanks to the positive α value, and it is repulsive. In figure 3.1 we illustrated the Equation of State for that parameter choice. We point out here some general considerations about its shape.

1. Zero density entails zero energy, as we expected.

2. At small densities, the system is always found to be bound, although the pressure is negative. This can be seen as a weak evidence that mean-field models do not describe very well low-density systems. In fact, it is known that at low densities the nucleons tend to form nuclei. Since the fact is not taken into account into our approach, we do not expect to find the exact functional behavior of the Equation of State as $\rho \ll 1$.

3. The system is unbound in the high density limit. Specifically, that happens as ρ approaches the value $\approx 3\rho_0$.

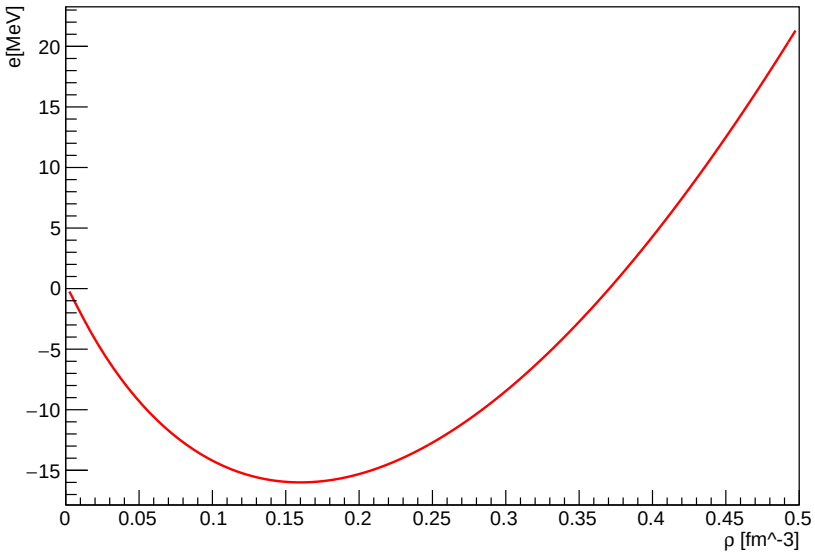

Figure 3.1: The Equation of State for the zero-range density-dependent potential (2.10), for the computed t_0, t_3 and α fit parameters.

3.3 A Single Gaussian Potential

We would like to begin the discussion on the role of the range in the nuclear interaction by considering a reduced form of the Brink and Boeker potential (1.11). In particular, we take only a single Gaussian potential, to see how well it can predict nuclear properties. Thus, in this section the adopted effective interaction is

$$V(|\vec{r}_1-\vec{r}_2|) = S(1-m+mP_M)e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu^2}}. \tag{3.32}$$

As we showed in chapter two, it entails the equation of state being

$$e(\rho) = \frac{3}{5}\frac{\hbar^2}{2m}k_F^2 + \frac{1}{2}\frac{\pi^{\frac{3}{2}}}{4}S\mu^3(4-5m)\rho + \frac{1}{2}\frac{1}{\sqrt{\pi}}S(5m-1)g(\mu k_F), \tag{3.33}$$

where

$$g(q) = \frac{2}{q^3} - \frac{3}{q} - (\frac{2}{q^3} - \frac{1}{q})e^{-q^2} + \sqrt{\pi}\,\mathrm{erf}(q), \tag{3.34}$$

and erf(x) is the well known error function, already defined in equation (2.57).

3.3.1 Two Strength Parameters and Fixed Range

First of all, we computed the Gaussian strength parameters S and m for a fixed range μ, by imposing the equation of state to reproduce the saturation properties at $\rho_0 = 0.16$ fm^{-3}:

$$e(\rho_0) = -16 \text{ MeV} \tag{3.35}$$

$$= \frac{3}{5}\frac{\hbar^2}{2m}k_{F0}^2 + \frac{1}{2}\frac{\pi^{\frac{3}{2}}}{4}S\mu^3(4-5m)\rho_0 + \frac{1}{2}\frac{1}{\sqrt{\pi}}S(5m-1)g(\mu k_{F0}), \tag{3.36}$$

$$P(\rho_0) = 0 \text{ MeV}\cdot\text{fm}^{-3} \tag{3.37}$$

$$= \frac{2}{5}\frac{\hbar^2}{2m}k_{F0}^2\rho_0 + \frac{1}{2}\frac{\pi^{\frac{3}{2}}}{4}S\mu^3(4-5m)\rho_0^2 + \frac{1}{\sqrt{\pi}}S(5m-1)p(\mu k_{F0})\rho. \tag{3.38}$$

That is a linear system in S and m, which we solved analytically, finding the roots

$$m = \frac{1}{5}\Bigg\{1 + 3\frac{\pi^{\frac{3}{2}}}{8}\mu^3\rho_0\Big(e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_{F0}^2\Big) \tag{3.39}$$

$$\Bigg[\Big(\frac{\pi^{\frac{3}{2}}}{8}\mu^3\rho_0 - \frac{g(\mu k_{F0})}{2\sqrt{\pi}}\Big) + \frac{\Big(g(\mu k_{F0}) - 2p(\mu k_{F0})\Big)\Big(e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_{F0}^2\Big)}{2\sqrt{\pi}}\Bigg]^{-1}\Bigg\}, \tag{3.40}$$

$$S = 2\sqrt{\pi}\frac{e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_{F0}^2}{\Big(5m-1\Big)\Big(g(\mu k_{F0}) - 2p(\mu k_{F0})\Big)}. \tag{3.41}$$

In table 3.1 we record some of these solutions, for the range μ varying between 0.5 fm and 1.5 fm. We have chosen the range to take physically acceptable values. We would like to briefly show an alternative way (with respect to those given in chapter one) to compute the order of magnitude of the range.

Table 3.1: Strength parameters and incompressibility for the single Gaussian potential with fixed range.

μ (fm)	m	S (MeV)	K_∞ (MeV)
0.5	2.68	-1835	281
0.7	1.64	-700	258
0.9	1.21	-350	231
1.1	1.02	-207	201
1.3	0.91	-138	170
1.5	0.85	-100	141

It is known that for incident nucleon energies up to ≈ 10 MeV in the center of mass frame of reference, the differential cross section for neutron-proton scattering is isotropic. Scattering occurs then in s-wave states. We can therefore roughly estimate range value of the nucleon-nucleon force from a classical limit on the maximum angular momentum $\hbar l_{max} = r\,p$ that can give a contribution to scattering amplitude:

$$1 < l_{max} = r\sqrt{\frac{m_N E}{\hbar^2}} \approx r(\text{fm})\sqrt{\frac{\text{E}}{40\ \text{MeV}}} \tag{3.42}$$

For energy up to ≈ 10 MeV we get $r \approx$ few fm.

Coming back to the outcomes of our work, we note that the Gaussian strength S is always negative, while the exchange parameter is positive. Moreover, we point out that as the range increases, the strength parameter S diminishes together with the exchange one m. Thus, it seems that a larger range helps forces being smoother. Physically, one could think that the system is held together more easily if the force has a more far-reaching arm. At a mathematical level that means that if the Gaussian function is allowed to be larger (greater μ), it does not need to be too high (larger strength parameters S and m) to reproduce the saturation equilibrium point. There is a more rigorous way to explain the result. The volume integral of the interaction

$$\int d_3 r\, V(\vec{r}) \tag{3.43}$$

has to be preserved for different parameters choices. In fact, this quantity appears expressly in the direct term of the Equation of State through μ^3. Thus, a greater range entails a lower strength of the Gaussian and vice versa.

On the other side, one cannot even choose a range too large. In fact, calculations also show that once range goes beyond the reasonable limit of 2 fm, one find the absurd of the saturation density being just an inflection point of the Equation of State, rather than its global minimum. In this case, the system tends to be more and more bound as the density grows. We showed in figure 3.2 how the equation of state becomes if range is chosen as $\mu = 3$ fm. Besides, in the fourth column of table 3.1 we computed the incompressibility K_∞, which has an expected value of 240 ± 40 MeV. It is interesting to point out that our model can reproduce the incompressibility value for a very wide set of ranges: we are less than one standard deviation far from the K_∞ best known value while $0.5 < \mu < 1.1$. We note too that as μ increases, K_∞ falls off. We plotted this tendency in figure 3.3.

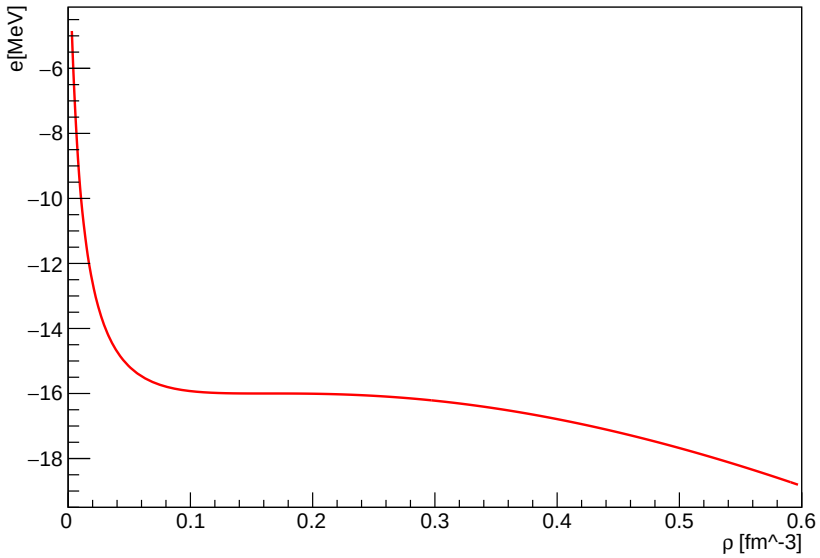

Figure 3.2: The equation of state for $\mu = 3$ fm shows that if one chooses a range too much long the saturation properties cannot be reproduced.

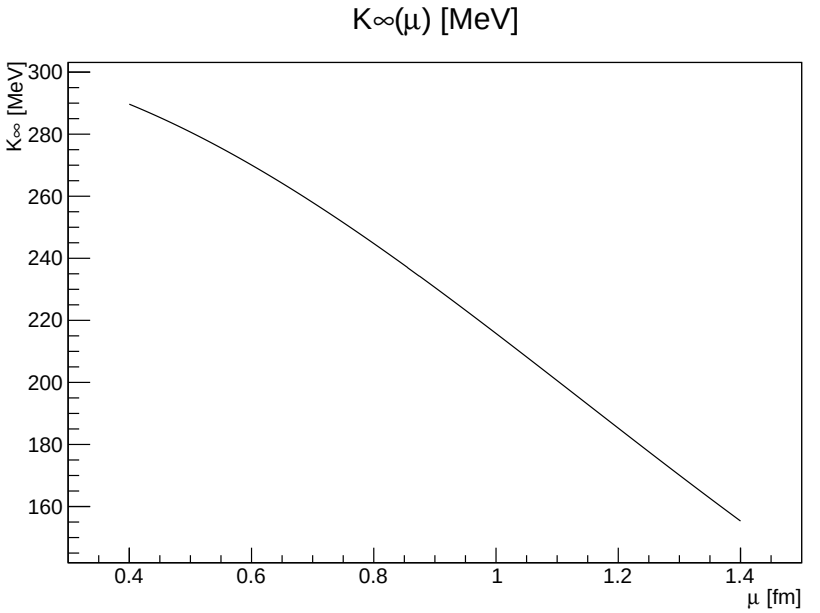

Figure 3.3: The incompressibility as a function of the range decreases with a quasi-linear tendency.

By looking at $K(\rho)$ expression given in equation (2.67), we can see that all its range dependence stays inside the dimensionless function $k(q)$, where $q = \mu k_F$. For convenience, we recall here their expressions:

$$K(\rho) = -\frac{6}{5}\frac{\hbar^2}{2m}k_F^2 - 3\frac{1}{\sqrt{\pi}}S(5m-1)k(\mu k_F), \tag{3.44}$$

$$k(q) = -\frac{6}{q^3} + \frac{2}{q} + (\frac{1}{q^3} + \frac{4}{q} + q)e^{-q^2}. \tag{3.45}$$

As we just said, no contribution to $K(\rho)$ comes from the direct term. Thereby, we can explain the (almost)linear decrease of the incompressibility to a mathematical level, since one can check that q^{-1} and q^{-3} terms almost exactly cancel when $k_F \approx 1$ fm^{-1}. Anyway, it is not trivial at all to give a physical explanation to its decrease as the range grows. One could naively think that by diminishing the range of the nucleon-nucleon force, the system becomes smaller, entailing greater momenta of the particles, together with a greater resistance to physical compression. An involved discussion on this latter result can be found in [3], too.

3.3.2 Two Strength Parameters and Range

It is interesting to see that as one imposes the incompressibility to be exactly 240 MeV, by using the range as a free parameter, one gets to a specific value for the range itself. We did that by adding to the conditions about the saturation point the extra constraint

$$K(\rho) = 240 \text{ MeV} \tag{3.46}$$

$$= -\frac{6}{5}\frac{\hbar^2}{2m}k_F^2 - 3\frac{1}{\sqrt{\pi}}S(5m-1)k(\mu k_F), \tag{3.47}$$

where now range is meant to be allowed to vary to reproduce the properties we have chosen. That is no more a linear system, and we solved it by using numerical methods. Actually, we carried out a C++ version of the Broyden's method for root finding of non-linear systems of equations. The method is a multi-dimensional version of secant's method. For more details about its routine and about how it works see [9] and appendix A. That brings us to the following results:

$$S = -430 \text{ MeV}, \tag{3.48}$$

$$m = 1.32, \tag{3.49}$$

$$\mu = 0.834 \text{ fm}. \tag{3.50}$$

To get an idea on how good the present model is, we computed the quantity M, related to the giant monopole resonance, expected having the value $M_{\text{exp}} = 1100 \pm 70$MeV [8]. We recall its definition:

$$M = 3\rho\frac{\partial K(\rho)}{\partial \rho}\Big|_{\rho=\rho_c} \tag{3.51}$$

$$= \frac{54}{\rho_c}P(\rho_c) + 12K(\rho_c) + Q(\rho_c). \tag{3.52}$$

Using parameters (3.48), (3.49) and (3.50), one finds $M = 1180.5455$ MeV, very near to the experimental value. This surely signals the goodness of the model.

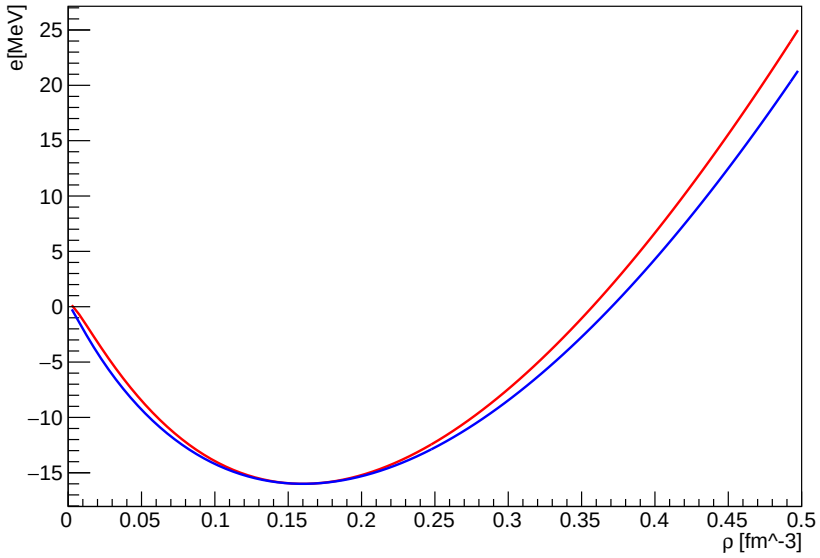

Figure 3.4: The comparison between the Equation of State coming out from the zero-range density-dependent potential (red) and the Equation of State of the single Gaussian potential (3.32)(blue). In the high-density limit the first grows as $\rho^{\alpha+1}$, while the second as ρ.

Moreover, we compared the Equation of State that the model predicts to the Equation of State coming from the zero-range interaction computed in equation (2.22) and displayed in figure 3.1. The visual comparison is made in figure 3.4. The two curves show a similar behavior, at least until the high density limit, where they deviate.

3.4 A Sum of Two Gaussian Potential

In this section we add a second Gaussian term, trying to understand if the model can improve the description of symmetric nuclear matter. We consider then the entire Brink and Boeker interaction, as presented above in equation (1.11):

$$V_{B\&B}(|\vec{r}_1-\vec{r}_2|)=\sum_{i=1,2} S_i(1-m_i+m_iP_M)e^{-\frac{|r_1-r_2|^2}{\mu_i^2}}. \tag{3.53}$$

We can now investigate the two ranges, together with the four strength fit parameters, whose signs establish the repulsive or attractive role of the Gaussian terms. In particular, we are interested in understanding if the first Gaussian term has, or has not, the same behavior as the second one, regarding the strength parameters S_i and m_i.

3.4.1 Four Strength Parameters and Two Fixed Ranges

Analytic solution

We begin by fixing some values for the ranges, to find S_1, m_1, S_2 and m_2. As in the paper of Brink and Boeker [4], for further calculations we will fix them to be $\mu_2=2\mu_1$. We will try to justify this choice at the end of the section.

The properties we aim to reproduce are the saturation energy, the equilibrium zero-pressure condition, the incompressibility, and the M value, so that

$$e(\rho_0)=\frac{3}{5}\frac{\hbar^2}{2m}k_{F0}^2+\frac{1}{2}\sum_{i=1,2}\frac{\pi^{\frac{3}{2}}}{4}S_i\mu_i^3(4-5m_i)\rho_0+\frac{1}{2}\sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5m_i-1)g(\mu_i k_{F0}), \tag{3.54}$$

$$P(\rho_0)=\frac{2}{5}\frac{\hbar^2}{2m}k_{F0}^2\rho_0+\frac{1}{2}\sum_{i=1,2}\frac{\pi^{\frac{3}{2}}}{4}S_i\mu_i^3(4-5m_i)\rho_0^2+ \tag{3.55}$$

$$+\sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5m_i-1)p(\mu_i k_{F0})\rho_0, \tag{3.56}$$

$$K_\infty=-\frac{6}{5}\frac{\hbar^2}{2m}k_{F0}^2-3\sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5m_i-1)k(\mu_i k_{F0}), \tag{3.57}$$

$$M=\frac{54}{\rho_c}P(\rho_c)+12K_0(\rho_c)+Q_0(\rho_c). \tag{3.58}$$

Thus, we get a linear four equations-four variables system, that can be analytically solved.

En passant, one could ask himself why not to use here the numerical Broyden's method. In fact, when one attempts to solve multi-dimensional systems in a numerical way, this entails multi-dimensional function minimum finding [9]. Thereby, when the dimensions of the problem raise, it raises at the same time the possibility of finding local mimima of the vectorial function defining the system. As it happens for every locally convergent method, a huge relevance must be given to the starting guesses the user gives for the roots. Since, starting from the next calculation, Broyden's method gave us such issues, we decided not to use it here.

However, the analytic solution attempt exhibits a couple of interesting outcomes:

- First, if we choose the two ranges to be equal, we find that the system is under-determined in two equations. What we do mean is that one can think to assign some values to a couple of parameters, let's say S_2 and m_2, to obtain the expression of , e.g., the incompressibility. Its expression is

$$K_\infty = 6\frac{k(\mu_1 k_F)}{g(\mu_1 k_F) - 2p(\mu_1 k_F)}(e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_F^2) - \frac{6}{5}\frac{\hbar^2}{2m}k_F^2. \tag{3.59}$$

  However, this is not such an surprising result. In fact, we are just saying that, if we have an unique range, we can get back to the one Gaussian-two parameters problem by simply renaming the parameters definitions.

- If we instead allow the fixed ranges to be different, we get to a more enlightening result. In fact, we find out *again* the system to be under-determined, but now for one equation only. Therefore, by assigning a value to, e.g., m_2, one find that M must have the expression

$$\begin{aligned}
M =& 27\Bigg[\frac{4}{9}\frac{\hbar^2}{2m}k_F^2 + (4p(\mu_1 k_{Fc}) - \frac{8}{3}k(\mu_1 k_{Fc}) + \\
&+ \frac{2}{9}q(\mu_1 k_{Fc}))\frac{e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_F^2 - \frac{(K_\infty + \frac{6}{5}\frac{\hbar^2}{2m}k_{F0}^2)(g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0})) + 6k(\mu_1 k_{F0})(e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_F^2)}{2p(\mu_1 k_{F0})(g(\mu_2 k_{F0}) - 2p(\mu_2 k_{F0})) - 2p(\mu_2 k_{F0})(g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0}))}}{g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0})} + \\
&+ (4p(\mu_2 k_{Fc}) - \frac{8}{3}k(\mu_2 k_{Fc}) + \\
&+ \frac{2}{9}q(\mu_2 k_{Fc}))\frac{(K_\infty + \frac{6}{5}\frac{\hbar^2}{2m}k_{F0}^2)(g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0})) + 6k(\mu_1 k_{F0})(e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_F^2)}{2p(\mu_1 k_{F0})(g(\mu_2 k_{F0}) - 2p(\mu_2 k_{F0})) - 2p(\mu_2 k_{F0})(g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0}))} + \\
&- \frac{\rho_c}{\rho_0}\Bigg(\frac{g(\mu_1 k_{F0})}{g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0})} + ak_F^2 + \\
&+ g(\mu_2 k_{F0})\frac{(K_\infty + \frac{6}{5}\frac{\hbar^2}{2m}k_{F0}^2)(g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0})) + 6k(\mu_1 k_{F0})(e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_F^2)}{2p(\mu_1 k_{F0})(g(\mu_2 k_{F0}) - 2p(\mu_2 k_{F0})) - 2p(\mu_2 k_{F0})(g(\mu_1 k_{F0}) - 2p(\mu_1 k_{F0}))} - e(\rho_0)\Bigg)\Bigg]
\end{aligned} \tag{3.60}$$

  This result shows that the Equation of State coming out from this potential does not allow us to have a third derivative (read M) independent of the second derivative (read K_∞). We point out in particular the fact that M depends only on the nuclear matter properties. Specifically, the saturation density ρ_0 and the cross density ρ_c appear only through their ratio $\rho_0/\rho_c \approx 0.7$.

Thus, it seems that the model predictive power is strongly related to the freedom of choice of the two ranges.

Fit

We search then some brand new conditions to fit the parameters, since the constraint on M cannot be used. In fact, in this subsection, and in the next one, too, we used six different density-energy points, as listed in the table 3.2. This benchmark energies are taken from [1], where a more fundamental calculation of symmetric nuclear matter, starting from the bare nucleon-nucleon potential, has been done. We

Table 3.2: The density-energy points we used in the fit protocols.

ρ_i (fm^{-3})	e(ρ) (MeV)
0.0400	-6.6894
0.0800	-12.263
0.1200	-15.166
0.1600	-16.000
0.2000	-15.336
0.2400	-13.606

Table 3.3: Strength parameters fit results for three couples of ranges.

μ_1 (fm)	μ_2 (fm)	S_1 (MeV)	m_1	S_2 (MeV)	m_2
0.4	0.8	-1675	-1.767	-278	2.73
0.6	1.2	-22.5	52.4	-143	0.54
0.8	1.6	-13.1	40.2	-59.6	0.26

just remind here that the nuclear Equation of State is not directly observable. Thus, we have the six conditions

$$e(\rho_j) = \frac{3}{5}\frac{\hbar^2}{2m}k_{Fj}^2 + \frac{1}{2}\sum_{i=1,2}\frac{\pi^{\frac{3}{2}}}{4}S_i\mu_i^3(4-5m_i)\rho_j + \frac{1}{2}\sum_{i=1,2}\frac{1}{\sqrt{\pi}}S_i(5m_i-1)g(\mu_i k_{Fj}) \quad (3.61)$$

We found here more suitable to perform a χ^2 fit to the benchmark calculations, rather than to use the above mentioned root finding method. In particular we used MINUIT tool to minimize the χ^2 function of the system with respect to the fit parameters. The χ^2 function is defined as usual as the sum of the squares deviations, between measured values and predictions of the theoretical model, those latter depending on parameters:

$$\chi^2 = \frac{1}{N}\sum_k^N \left(\frac{f_k^{(\mathrm{exp})} - f_k^{(\mathrm{th})}}{\sigma_k}\right)^2 \quad (3.62)$$

where σ_k are the errors on the fitted energies. Every fit in this work is characterized by $\chi^2 \approx 10^{-2}$. First, we fixed some ranges in the fit process. Some of the results are in table 3.3. In table 3.4 we show then the corresponding values of the saturation energy, pressure, and incompressibility. The values are quite reasonable. We find again the fact that as the ranges of the two Gaussian increase, the strength parameters fall off, taking lower values.

Table 3.4: Saturation energy, equilibrium pressure, and incompressibility for the fit results given in table 3.3. Note that in the fit protocol we did not include the saturation point as we did before. Hence the result for the equilibrium pressure $P(\rho_0)$ needs not to be zero at exactly ρ_0 , but just close to it.

$e(\rho_0)$ (MeV)	$P(\rho_0)$ (MeV/fm^3)	K_∞ (MeV)
-16.0664	-3.70441	226.883
-16.0661	-4.13202	229.56
-16.0734	-3.97359	230.505

3.4.2 Four Strength Parameters and Two Ranges

Let the ranges be fit parameters, restricted to be positive and to satisfy the reasonable requests 0.2 fm $< \mu_1 <$ 1 fm and 1 fm $< \mu_2 <$ 2 fm. One finds:

$$S_1 = -25.36 \text{ MeV}, \tag{3.63}$$
$$m_1 = 25.38, \tag{3.64}$$
$$S_2 = -81.22 \text{ MeV}, \tag{3.65}$$
$$m_2 = 0.316, \tag{3.66}$$
$$\mu_1 = 0.749 \text{ fm}, \tag{3.67}$$
$$\mu_2 = 1.44 \text{ fm}. \tag{3.68}$$

The Equation of State for these parameters is illustrated in figure 3.5. The first information that stands out is the fact that ranges almost perfectly satisfy $\mu_2 = 2\mu_1$. This is in line with the guess made by Brink and Boeker in their paper. Regarding the strength parameters, the two Gaussian terms behave in the same way: S_1 and S_2 are negative, while m_1 and m_2 are positive. The fit tool also gives us the parameter

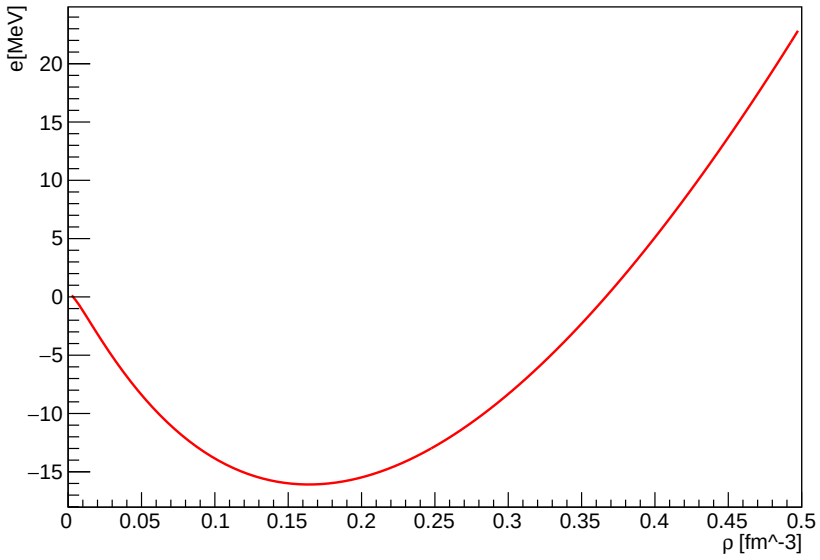

Figure 3.5: The Equation of State for the six parameter fit.

correlation coefficients, showed in table 3.5. In particular, that table shows that the ranges are more related to their respective strength parameters rather than to the others. We can also see a small correlation between the strength parameters S_i and their respective exchange parameters m_i. Correlation between parameters with different index, referring to the two different Gaussian, can be completely neglected.

Table 3.5: The parameter correlation coefficients in the six parameters fit.

Parameter	S_1	m_1	S_2	m_2	μ_1	μ_2
S_1	1.000	0.398	-0.043	0.243	-0.382	0.043
m_1	0.398	1.000	-0.016	-0.229	0.345	0.016
S_2	-0.043	-0.016	1.000	-0.201	0.024	0.758
m_2	0.243	-0.229	-0.201	1.000	0.235	0.201
μ_1	-0.382	0.345	0.024	0.235	1.000	-0.023
μ_2	0.043	0.016	0.758	0.201	-0.023	1.000

As a benchmark, one computes the values of the energy, pressure, and incompressibility at the empirical saturation density of $\rho_0 = 0.16$ fm^{-3} for those parameters. We get:

$$e(\rho_0) = -16.081 \text{ MeV}, \tag{3.69}$$

$$P(\rho_0) = -4.06 \text{ MeV/fm}^3, \tag{3.70}$$

$$K_\infty = 231 \text{ MeV}. \tag{3.71}$$

The saturation energy and the incompressibility have values compatible with those expected. We point out again that the zero pressure condition at ρ_0 is not taken into account in the fit protocol. Hence we only expect $P(\rho) = 0$ in a neighborhood of the saturation density ρ_0. In fact, the solution of the equation

$$P(\rho) = 0, \tag{3.72}$$

with respect to the density, and using the fit parameters of this subsection, results

$$\rho_0 = 0.164 \text{ fm}^{-3}. \tag{3.73}$$

The expression of the pressure is given by equation (2.64). Thus, our guess is confirmed, and the saturation density is near to the expected value 0.16 fm^{-3}. In the fit protocol we set at 1 MeV the error on the benchmark energies of table 3.2. It would be interesting to estimate the corresponding uncertainty on the density to see if the two values are really compatible.

Let us come back to the single Gaussian potential. We just learned that using the sum of two Gaussian interaction it is possible to reproduce the Equation of State of [1]. The question is if by using just the single Gaussian potential it is possible to do the same. The fit protocol is arranged fixing the parameter $S_2 = 0$, i.e. neglecting the second Gaussian contribution to the Equation of State. The results for that fit are the following:

$$S_1 = -372 \text{ MeV}, \tag{3.74}$$

$$m_1 = 1.24, \tag{3.75}$$

$$\mu_1 = 0.876 \text{ fm}. \tag{3.76}$$

We point out that these values for the parameters are very similar to those obtained in section 3.3.2 imposing as nuclear properties the saturation point and the incompressibility value. However, one finds the parameters correlation to be extremely high, around ≈ 1. Thus, having only one Gaussian term permit yet to reproduce the Equation of State given by [1], but parameters become much less flexible and more correlated.

3.5 Effective Mass

We derive the effective mass m^*, as defined in equation (3.21). For the potential

$$V_{B\&B}(|\vec{r}_1-\vec{r}_2|)=\sum_{i=1,2}S_i(1-m_i+m_iP_M)e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} \tag{3.77}$$

one can compute its Fourier transform [11]

$$U(k)=\sum_{i=1,2}\left(\frac{\pi^{\frac{3}{2}}\mu_i^3}{4}S_i(4-5m_i)\rho+\frac{1}{\sqrt{\pi}}S_i(5m_i-1)u(\mu_i k,\mu_i k_F)\right), \tag{3.78}$$

where $k=|\vec{k}_1-\vec{k}_2|$, and the dimensionless function u is

$$u(q,q_F)=\frac{1}{q}\left[e^{-\frac{(q+q_F)^2}{4}}-e^{-\frac{(q-q_F)^2}{4}}\right]+\frac{\sqrt{\pi}}{2}\left[\mathrm{erf}\left(\frac{(q+q_F)}{2}\right)-\mathrm{erf}\left(\frac{(q-q_F)}{2}\right)\right]. \tag{3.79}$$

To obtain the effective mass[3] we have to derive equation (3.78). Before giving its expression we point out again that the direct term does not contribute to it, as it happens for the incompressibility. Thus,

$$\frac{m^*}{m}(k)=\left(1+\frac{m}{\hbar^2}\sum_{i=1,2}\mu_i^2\frac{1}{\sqrt{\pi}}S_i(5m_i-1)h(\mu_i k,\mu_i k_F)\right)^{-1}, \tag{3.80}$$

being h essentially the derivative of u:

$$h(q,q_F)=\frac{1}{q^3}\left[(2-qq_f)e^{-\frac{(q-q_F)^2}{4}}-(2+qq_f)e^{-\frac{(q+q_F)^2}{4}}\right]. \tag{3.81}$$

Usually the effective mass is computed at the Fermi surface, where the function h becomes

$$h(q_F,q_F)=\frac{1}{q_F^3}\left[2(1-e^{-q_F^2})-q_F^2(1+e^{-q_F^2})\right]. \tag{3.82}$$

We analyze the behavior of the effective mass of a system of nucleons interacting through the finite-range potentials we considered previously. For the one Gaussian interaction, given in equation 3.32, we impose strength parameters to reproduce the saturation point, and then we compute the effective mass as a function of the range. The result is illustrated in figure 3.6. The plot shows that the effective mass takes values around 0.25, which is not in agreement with the expected value of $\approx 0.6-0.8$ [10]. On the other side we get the information about its sensitivity to the range. In particular, the effective mass seems not to strongly depend on the range, and there is a slightly increase as the range increases. At $\mu\approx 2$ fm the effective mass saturates. For the parameter shown in equations (3.48), (3.49), (3.50), reproducing the incompressibility $K_\infty=240$ KeV, one finds

$$\frac{m*}{m}=0.254. \tag{3.83}$$

[3] Or rather the ratio between the effective mass and the nucleon mass.

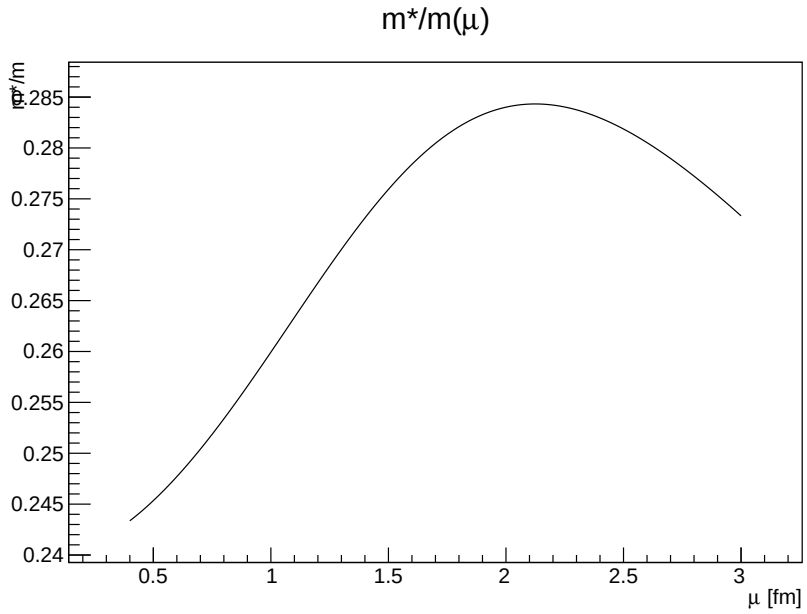

Figure 3.6: The effective mass grows together with the range from 0.24 to 0.29. Its value saturates for $\mu \approx 2$ fm, then it falls off.

One could ask if by adding a second Gaussian term, and using then the entire Brink and Boeker interaction (1.11), it is possible to obtain a better effective mass value. Our answer would be that it is not possible. In fact, in the analytic system given in section 3.4, we swap M equation (3.58) with equation (3.80), to find out that again the system is under-determined in one equation. Thus, we find a parameters-independent[4] equation, relating the effective mass to the other nuclear matter properties:

$$\frac{m^*}{m} = 1 + 2\frac{m}{\hbar^2}\left[\mu_1^2 h(\mu_1 k_F, \mu_1 k_F)\frac{D}{E_1} + \mu_2^2 h(\mu_2 k_F, \mu_2 k_F)\frac{I}{6L}\right] \tag{3.84}$$

where we defined

$$D = e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_F^2 - E_2\frac{I}{6L}, \tag{3.85}$$

$$E_i = g(\mu_i k_F) - 2p(\mu_i k_F), \tag{3.86}$$

$$I = \left(K_\infty + \frac{6}{5}\frac{\hbar^2}{2m}k_F^2\right)E_1 + 6k(\mu_1 k_F)\left(e(\rho_0) - \frac{1}{5}\frac{\hbar^2}{2m}k_F^2\right), \tag{3.87}$$

$$L = k(\mu_1 k_F)E_2 - k(\mu_2 k_F)E_1. \tag{3.88}$$

We focus on the relation between the effective mass and the incompressibility, as Cochet et al. did for the Skyrme interaction in [5]. As an example, using equation (3.84), the reference values for the nuclear matter properties, and by choosing $\mu_1 = 0.7$ and $\mu_2 = 1.4$, we report some of these results in table 3.6. It is clear that in the present case there is no relation between the two quantities, being the effective mass approximately constant over a wide range of values of the incompressibility. Moreover, we point out that the addition of a second Gaussian function does

[4] Let us recall that here ranges are *not* fit parameters yet.

Table 3.6: The effective mass as a function of the incompressibility.

K_∞ (MeV)	m^*/m
200	0.257
220	0.255
240	0.253
260	0.250
280	0.248

not improve the value of the effective mass, too small. In fact, making use of the six parameters of section 3.4.2, fitted to the benchmark calculations of [1], the result for the effective mass, computed using equation (3.80) does not improve as could be expected. In that case,

$$\frac{m*}{m} = 0.260. \tag{3.89}$$

The effective mass is a property that lies on a different level respect to the other properties we used, directly related to the Equation of State of the entire many-body system. Conversely, the effective mass is a single particle property, and we did not directly impose any single particle property to the system. Thereby, it seems that other interaction terms are necessary to reproduce an effective mass value compatible with the expected one. Let us consider the Gogny force, given above in equation (1.6).

$$\begin{aligned} V_{Gogny}(|\vec{r}_1-\vec{r}_2|) = \sum_{i=1,2} e^{-\frac{|\vec{r}_1-\vec{r}_2|^2}{\mu_i^2}} (W_i + B_i P_\sigma - H_i P_\tau - M_i P_\sigma P_\tau) + \\ + t_3(1+x_0 P_\sigma)\delta(|\vec{r}_1-\vec{r}_2|)\rho^\alpha\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right) + \\ + iW_{ls}(\vec{\sigma}_1+\vec{\sigma}_2)\cdot\vec{k}^\dagger\times\delta(|\vec{r}_1-\vec{r}_2|)\vec{k}, \end{aligned} \tag{3.90}$$

The effective mass is not affected neither by the direct term, which is proportional to $W_i = S_i(1-m_i)$, nor by the density-dependent contact term, nor by the spin-orbit term. As one can see in equations (A6), (A7), (A8), and (A9) in [11], the effective mass only depends on the parameter B_0^i, defined by Sellahewa and Rios in equation (8) of their paper as

$$B_0^i = -\frac{1}{\sqrt{\pi}}[W_i + 2B_i - 2H_i - 4M_i]. \tag{3.91}$$

In the case of the sum of two Gaussian interaction we adopted, $W_i = S_i(1-m_i)$, $B_i = 0$, $H_i = 0$, $M_i = S_i m_i$. The lack, in our interaction, of the parameters B_i and H_i related to (iso)spin exchange terms, may explain the low value we found for the effective mass. It is a fact that once those parameters are considered, the effective mass take values between ≈ 0.6 and ≈ 0.8, as it is shown in figure 4 of [11].

Conclusions

The nuclear many-body problem still challenges theorists, despite a remarkable progress in the recent years. To investigate nuclear spectroscopy, many groups have employed zero-range forces, that allow great simplifications. In this work, we wished to study some general, albeit simple, features of finite range forces. In particular we studied the Equation of State of symmetric nuclear matter by employing a finite-range effective interaction, solved at the Hartree-Fock level. The interaction has been taken from [4], and it is composed by four strength parameters and two ranges. We have focused on the investigation of the role of the range(s) as fit parameter(s), since in the literature such a discussion has not been dealt in detail yet.

In chapter one we gave a brief overview on many-body nuclear systems, such as the symmetric matter, focusing on the mean-field approach.

In chapter two we carried out the calculation of the Equation of State for the adopted potential. Moreover, we computed the expressions of some nuclear properties related to the Equation of State. Functional behaviour of those quantities has been studied. The chapter has been thought to give an adequate mathematical background to the analyses made all along chapter three.

One of the purposes of chapter three has been to study the differences between a potential build only by a single Gaussian term and the Brink and Boeker potential, made of two Gaussian functions. Thus, we started by considering the single Gaussian potential given in equation (3.32).

- By imposing the saturation point conditions, a study has been made about the sensitivity of the incompressibility to the range. The incompressibility decreases with a linear tendency as the range grows.

- The simple single Gaussian interaction has been able to reproduce the expected value of the incompressibility, within one standard deviation, for a very wide set of ranges. The interaction also produces an acceptable value for the quantity M, related to the excitation energy of the giant monopole resonance.

- Six points of the Equation of State given by [1] have been fitted by the interaction, but the parameters were not flexible and extremely correlated.

- We studied the effective mass of the system, to find out that an acceptable value could not be obtained by means of the employed interaction. Nevertheless, we noticed that the effective mass slightly grows with the range, but saturates when the range overtakes the reasonable value of ≈ 2 fm.

Also because of those limitations, we considered the sum of two Gaussians interaction given in equation (3.53).

- We imposed the conditions of the saturation point, incompressibility, and M, keeping the two ranges fixed. By making use, as fit parameters, of Gaussian strengths only, the resulting system has been found under-determined, meaning that, for this simple interaction, M cannot be considered independent of the the other nuclear matter properties.

- The same happens if one swap the condition on M with a condition on the effective mass. Specifically, we showed that the effective mass is approximately a constant over a wide set of incompressibilities. Thus, the model predictive power is strongly related to the freedom of choice of the two ranges.

  We let then the two ranges to be fit parameters.

- The EoS given by [1] has been reproduced, giving a $\chi^2 \approx 10^{-2}$ value, and lower parameters correlation coefficients than before. Specifically, we pointed out that the ranges are more correlated to their strength parameters rather than to the other parameters, and that the two Gaussians parameters are very uncorrelated. That fact signals that the second Gaussian term is not redundant.

- The previous literature fixed, instead of fitting, the ranges. We showed that the guess to fix them at $\mu_2 = 2\mu_1$, by following some simple physical considerations also discussed in section 1.1 and 3.3, is a very reasonable one. In fact, the fit result shows that the ranges almost perfectly satisfy $\mu_2 = 2\mu_1$.

- The system again could not reproduce the effective mass of the system. A solution to that limitation of the interaction might be to add (iso)spin exchange terms as in the Gogny force.

The presented model is very efficient in reproducing the expected equation of state properties, such as the saturation point and the incompressibility: the range plays an important role in producing acceptable values of these quantities. Conversely, the range seems not to be directly correlated to single particle properties, such as the effective mass, whose values could not be reproduced, unless a more complex structure of the finite-range potential is considered.

Appendix A

Broyden's Method

If we have a system of equation to be zeroed

$$\vec{F}(\vec{x}) = 0, \tag{A.1}$$

by neglecting terms of second order or higher, one can expand it in Taylor series

$$\vec{F}(\vec{x} + \delta\vec{x}) = \vec{F}(\vec{x}) + \mathbf{J} \cdot \delta\vec{x}, \tag{A.2}$$

where **J** is the Jacobian matrix of the vectorial function $\vec{F}(\vec{x})$. One sets l.h.s. equal to zero, to obtain a set of linear equations for the corrections $\delta\vec{x}$ that move each function closer to zero simultaneously:

$$\vec{F}(\vec{x}) = -\mathbf{J} \cdot \delta\vec{x}. \tag{A.3}$$

The correction are then added to the solution vector, $x_{new} = x_{old} + \delta\vec{x}$ and the process is iterated until convergence. This method is known as the Newton-Raphson's method.

Newton-Raphson's method for root finding has several disadvantages. First, the Jacobian matrix is needed, while in many problems its determination is expensive. To overtake this issue there are methods that provide approximations to the Jacobian for zero finding. These methods are called secant method. Let us call the approximate Jacobian **B**. Then one has the quasi-Newton step $\delta\vec{x}_i$ solves

$$\mathbf{B}_i \cdot \delta\vec{x}_i = \vec{F}_i. \tag{A.4}$$

The secant condition is that $\mathbf{B}_{i+1}$ satisfies

$$\mathbf{B}_{i+1} \cdot \delta\vec{x}_i = \delta\vec{F}_i. \tag{A.5}$$

By the way, this latter equation does not determine $\mathbf{B}_{i+1}$ uniquely. Broyden's idea is to get $\mathbf{B}_{i+1}$ by making the least change to $\mathbf{B}_i$ consistent with the secant condition. Thus, he found

$$\mathbf{B}_{i+1} = \mathbf{B}_i + \frac{(\delta\vec{F}_i - \mathbf{B}_i \cdot \delta\vec{x}_i) \otimes \delta\vec{x}_i}{\delta\vec{x}_i \cdot \delta\vec{x}_i}. \tag{A.6}$$

Broyden's method converges super-linearly[1] once it gets close enough to the root. For more details on the routine we used, see [9].

[1] A sequence x_n converges super-linearly to its limit α if exists a sequence $c_n \to 0$ and there is N_0 satisfying $|x_n + 1 - \alpha| \leq c_{N_0}|x_n - \alpha|$

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