CHAPTER 1

INTRODUCTION

As a consequence of the antisymmetric properties of a fermion system, the expectation value of any two-body operator yields two terms: the direct term and the exchange term. This is the case for example of the Coulomb interaction. The resulting terms are called the direct Coulomb and the exchange Coulomb energies respectively. The computation of the direct term is relatively easy and straightforward while the exchange term is complicated by the presence of a non-local density term. One can compute the exchange term through an exact calculation which can be quite tedious and time consuming. In order to simplify the calculation, an approximation (dubbed as the Slater approximation) was used to calculate the exchange term. The Slater approximation has been employed in mean field approaches such as Hartree-Fock (see e.g. Vautherin and Brink (1972)) and Hartree-Fock-Bogoliubov (see e.g. Decharge and Gogny (1980)) calculations as well as in the density functional approach (see e.g. Bulgac and Shaginyan (1996)). It has been shown to be a reasonable approximation in some limited cases (Titin-Schnaider and Quentin, 1974 and Skalski, 2000). A more general study of the validity of this approximation is the purpose of this study.

In the Slater approximation, the Slater determinant which describes the nucleons inside the nucleus is written in terms of plane waves. As is well known, upon using plane waves the probability of finding a nucleon (in this case a proton) is equal for any position in space. The first study of the validity of different approximations used to calculate the exchange Coulomb energy was performed by Titin-Schnaider and Quentin

(1974) using the SIII Skyrme parametrization for the effective nucleon-nucleon strong interaction. They had calculated the error associated with these approximations for the ground state solutions for light nuclei (^{16}O to ^{56}Ni) mainly of deformed shapes. The results for the Slater approximation showed that the validity of the Slater approximation will be maximal when the relevance of a constant density ansatz will be expected. This consideration leads to the conclusion that this validity should be better in heavy than in light nuclei since in the former most of the nuclear matter is located in the saturated part of the density profile. Actually it showed a decreasing pattern as a function of mass number, A which was almost stabilized to about 5% for the last four heavier nuclei (Titin-Schnaider and Quentin, 1974). The same type of reasoning should imply that upon increasing the nuclear surface (as in extremely deformed nuclei) this validity should be arguably, less guaranteed. A more recent study having the same goal has been performed by Skalski (2000) who has calculated the differences in the exchange Coulomb energy for a wide range of only spherical nuclei starting from light to superheavy ones. The SkP and SkM* parameterizations were employed in the calculation in which the difference in the exchange Coulomb energy was found to be nearly identical for the two different sets of Skyrme parameters (Skalski, 2000) even though the single particle energies was found to be not the same. Incidentally, the exchange Coulomb energies for ^{16}O and ^{40}Ca did compare very well with those obtained in Titin-Schnaider and Quentin (1974) with the SIII Skyrme interaction. These findings prompted the author to suggest that the results are independent on the choice of realistic Skyrme force parameters being used in the Hartree-Fock calculation.

The next step to take is thus to verify the validity of the Slater approximation beyond the closed shells yet first preserving the spherical shape to disentangle the nucleon number effect from any deformation effects, even though, as well known, these

nuclei should be generally deformed in their ground states. It is the main goal of this study. Since the Coulomb interaction acts only between protons, it is safe to assume that the addition of neutrons into the nucleus (as in an isotopic series) would not affect much the order of magnitude of the correction of the exchange Coulomb energy. We then mostly look for the effect brought upon by the addition of extra protons into the nuclear system which can be made by studying different isotonic series. From another point of view, we have studied for a fixed proton number how the considered error would vary with moderately large deformations which is another way to change the single particle level density with proton valence configuration ranging between closed and open shell situation.

Beyond that study, it is also interesting to look into the validity of Slater approximation as nuclei undergo a large scale deformation process as e.g. in fission or fusion. Before a nucleus breaks apart through fission for instance, the shape of the nucleus will be distorted away from a compact almost spherical shape where the surface is minimal at constant volume. Then one may wonder how good the Slater approximation is, immediately after the scission point in which the nucleus breaks into two smaller fragments. In view of this, the effect of nuclear deformation onto the exchange Coulomb energy would therefore be very much interesting. Similar studies could be interesting when extending them to a system of two colliding nuclei before reaching the top of the fission barrier.

In Chapter 2 of this dissertation, we shall look into some theoretical aspects of the present work. Notably, the discussion will focus a) on the Hartree-Fock method which is the backbone of the microscopic method used in the present work, b) a discussion of the Slater approximation. The phenomenological Skyrme interaction used

to describe the nucleon-nucleon interaction and the Bardeen-Cooper-Schrieffer (BCS) approach to treat pairing correlations will be also discussed. Chapter 3 shall deal with the method of solving the Hartree-Fock equations through the computation of the various scalar functions entering the Hartee-Fock equations and of relevant matrix elements. Then, the results of the calculations will be presented in Chapter 4. In the present work, the focus is on heavy nuclei as suggested by the essay title. Nevertheless, the present study also applies very well to medium heavy nuclei which results have been included herein. Finally, we shall provide conclusions of the present work in Chapter 5.

CHAPTER 2

THEORETICAL BACKGROUND

2.1.1 NUCLEON-NUCLEON INTERACTION IN FREE SPACE

Two nucleons interact with one another through a nucleon-nucleon interaction which can be described by an attractive plus short range repulsive potential. There are three levels of invariance of the nucleon-nucleon interaction in the strong interaction sector with respect to changing the nucleon charge which are in decreasing order of stringency:

- Charge independence (i.e. neutron-neutron, neutron-proton and proton-proton interactions are the same. Since neutron-proton interaction belongs to the T=0 and T=1 subspaces where T is the total isospin quantum number, then it means in particular that the nucleon-nucleon interaction is the same in the two subspaces.)

- Isospin invariance (i.e. for rotations in the isospin space, the interaction may depend on T but not on T_z (third component of the total isospin)

- Charge symmetry (i.e. when changing neutron-neutron into proton-proton interaction or in other words the $T_z = \pm 1$ components of the nucleon-nucleon interaction are similar.)

We will adopt here the isospin invariance for the Hartree-Fock part of the approach (as in usual Skyrme forces) and only the charge symmetry for the treatment of pairing correlations. Apart from its repulsive core part, the nucleon-nucleon interaction is a

somewhat short range (~ 1 fm) attractive interaction. Such an interaction is only valid for free nucleons, where the two nucleons form an isolated system devoid of any other forces at work. However, the correct description of nucleon-nucleon interaction in a nuclear medium is complicated by the presence of other neighbouring nucleons.

To account for the presence of other nucleons, an effective potential, V_{eff} (r_1,r_2) is used. It describes the interaction between two nucleons at positions r_1 and r_2 while summing up the averaged contributions from other surrounding nucleons. There are two schools of thoughts to describe the effective interaction. On one hand, one has described it from an approximate account of free two-body nucleon-nucleon interactions in a more or less sophisticated many-body approach. While such approach is fundamentally sound, the actual process is nevertheless lengthy and time consuming if at all possible. On the other hand, one has undertaken a phenomenological approach whereby the effective interaction is described by some a priori mathematical expression with some adjustable parameters that are fitted to experimental data. The advantages and weaknesses of the phenomenological approach lie in its mathematical simplicity. Nevertheless, it has allowed to reproduce some experimental data quite satisfactory. Much work has been done in the development of phenomenological interactions giving rise to many types of phenomenological effective interactions (see e.g. Ring and Schuck (1980)) which were employed in the study of nuclear properties.

2.1.2   PHENOMENOLOGICAL SKYRME INTERACTIONS

One of the examples of phenomenological interactions is the so called Skyrme interaction. The application of Skyrme interaction in nuclear structure calculation was first attempted around the 1970's in studying the ground state of spherical and deformed

nuclei, as well as fission barriers of heavy nuclei. Skyrme initially proposed the average potential as a sum of two-body and three-body interaction (Skyrme, 1956):

$$V_{eff} = \sum_j^A \sum_{i<j}^A V(i,j) + \sum_k^A \sum_{j<k}^A \sum_{i<j}^A V(i,j,k) \tag{1}$$

The choice of the indices is made to avoid double counting the same interaction. The mathematical form of the local two-body interaction is such that its $\vec{r}$ representation is:

$$V(\vec{r}_1, \vec{r}_2) = t_0(1 + x_0 P^\sigma)\delta(\vec{r}_1 - \vec{r}_2) + \frac{1}{2}t_1[\delta(\vec{r}_1 - \vec{r}_2)k^2 + k'^2\delta(\vec{r}_1 - \vec{r}_2)]$$

$$+ t_2\overleftarrow{k}'\delta(\vec{r}_1 - \vec{r}_2)\vec{k} + iW_0(\sigma^{(1)} + \sigma^{(2)}) \cdot \overleftarrow{k}' \times \delta(\vec{r}_1 - \vec{r}_2)\vec{k} \tag{2}$$

while the three-body term is given by:

$$V(\vec{r}_1, \vec{r}_2, \vec{r}_3) = t_3\delta(\vec{r}_1 - \vec{r}_2)\delta(\vec{r}_2 - \vec{r}_3) \tag{3}$$

The momentum operator $\vec{k}$ acts on the right and is defined as:

$$\vec{k} = \frac{1}{2i}(\vec{\nabla}_1 - \vec{\nabla}_2) \tag{4}$$

while the adjoint operator of $\vec{k}$, $(\vec{k})^\dagger$ denoted here as $\overleftarrow{k}'$ acts on the left:

$$\overleftarrow{k}' = -\frac{1}{2i}(\overleftarrow{\nabla}_1 - \overleftarrow{\nabla}_2) \tag{5}$$

Here, the terms t_0, t_1, t_2, t_3, x_0 and W_o are parameters which are obtained by fitting nuclear experimental data and P^σ refers to the spin-exchange operator.

Further, one has rather considered the Skyrme force as purely a two-body interaction with the three-body interaction giving rise to a density dependence force which is written for even-even nuclei as (Vautherin and Brink, 1972):

$$V(\vec{r}_1, \vec{r}_2) = \frac{1}{6} t_3 (1 + P^\sigma) \delta(r_1 - r_2) \rho \left(\frac{r_1 + r_2}{2} \right) \tag{6}$$

The two approaches are consistent provided ρ is even with respect to time-reversal.

2.1.3   CHOICE OF A SKYRME PARAMETERISATION

As mentioned earlier, the parameters in the Skyrme force are fitted to some experimental results. Many sets of parameters have been obtained and some appear to be better suited for some given nuclear properties. In the present study, the SkM* parameterization is chosen as it is shown to give a good description of nucleus in fission process (somewhat better as compared to other sets of parameters (Bonneau, Quentin and Samsoen, 2004)). Historically, the SkM* set by Bartel *et al*. (1982) is an improvement over the earlier SkM set (Krivine, Treiner and Bihigas, 1980) and was able to describe correctly the fission barrier of ^{240}Pu. The values for the parameters within the SkM* set are given as below:

$t_0 = -2645.0 \quad t_1 = \quad 410.0 \quad t_2 = - \quad 135.0 \quad t_3 = \quad 15595.0$

$x_0 = \quad 0.09 \quad\quad x_1 = \quad 0.0 \quad\quad x_2 = 0.0 \quad\quad x_3 = 0.0 \quad\quad W = 130.0$

2.2   COULOMB INTERACTION AMONG PROTONS

2.2.1   Importance of Coulomb interaction

In addition to the nucleon-nucleon interaction, protons also interact among themselves through the long range Coulomb interaction. The Coulomb interaction plays a very important role in the study of nuclear properties. One of the first effects of the Coulomb energy can be seen in the existence of a "valley" of stable nuclei deviating from the N=Z line. The nuclear strong interaction up to a very good approximation is charge independent in that the interactions between proton-proton, neutron-neutron and proton-neutron are the same. Through the Pauli principle among nuclei composed of a given (even) number of nucleons (isobars) the one with the same amount of protons and neutrons will be preferred (through maximizing the exchange free interaction terms). However, moving towards heavier stable nuclei they are composed of more neutrons than protons. This is because even though one looses in them some energy due the loss in the symmetry energy, one gains more by reducing the repulsive Coulomb energy. This means that some protons are "converted" into neutrons leaving the nucleus with a lesser number of protons and thus a lesser repulsion due to Coulomb interaction. Therefore, a stable heavy nucleus has more neutrons than protons.

Coulomb interaction also plays some role in limiting the size of the nucleus. From the semi-empirical mass formula, one writes the total binding energy, BE, as (see e.g. Preston and Bhaduri (1975)):

$$BE(N,Z) = a_V A - a_S A^{2/3} - k_C Z^2 A^{-1/3} - \cdots \tag{7}$$

The terms on the right hand side of the equation correspond to the volume, surface and Coulomb energy terms respectively. If a nucleus has a large size assuming that the number of protons is about half or somewhat less than the total number of nucleons:

$$Z \lesssim \frac{1}{2}A \qquad (8)$$

then, the Coulomb term in the semi-empirical mass formula would vary roughly as $A^{5/3}$, thus varying more rapidly with A than the leading linear volume term.　　Assuming that a nucleus has a constant volume, there will be only two dominant energy terms that vary with deformation. They are the surface energy term and the Coulomb energy term. The surface energy term corrects for the volume term since nucleons near the surface interact with less nucleons compared to those near the inner part of the nucleus. Being a term reflecting the lack of binding, it is clearly positive. The expression for the surface energy, E_S term is:

$$E_S = ST \qquad (9)$$

with S and T being the nuclear surface and surface tension respectively. For a spherical nucleus $E_S = 4\pi R^2 T$ with $R = r_0 A^{1/3}$ so that:

$$E_S = 4\pi r_0^2 S A^{2/3} = a_S A^{2/3} \qquad (10)$$

The coefficient a_S is given (neglecting for the sake of simplicity of the present exposition the corresponding symmetry energy) by (see e.g. Preston and Bhaduri (1975)):

$$a_S \sim 18.56\ MeV \qquad (11)$$

The surface energy term varies proportionally to the surface area as shown in equation (9). Therefore, as a nucleus become more and more deformed from a spherical shape the surface area, and thus its surface energy, increases resulting in a higher energy and thus in a lower total binding energy (defined as positive quantity).

On the contrary, the Coulomb energy results in an opposite effect to the total binding energy with regards to deformation. For a spherically charged nucleus, the expression for the Coulomb energy, E_C for a spherical nucleus:

$$E_C = \frac{3}{5}\frac{(Ze)^2}{R} = \frac{3}{5}\frac{(Ze)^2}{r_0 A^{1/3}} = a_C \frac{Z^2}{A^{1/3}} \tag{12}$$

which is inversely proportional to the radius, R. The coefficient a_C has the value of ~ 0.717 MeV (see e.g. Preston and Bhaduri (1975)). The radius of a nucleus is minimal for a spherical shape nucleus and increases for a deformed shape. Therefore, as the shape of the nucleus grows in deformation the correction to the total binding energy due to the Coulomb energy (which is roughly inversely proportional to the global size) decreases which leads to more binding.

The possibility of a nucleus to undergo the fission process can then be viewed as resulting from the competition between the surface energy which decreases the binding energy and the Coulomb energy which increases the binding energy as the nucleus becomes more deformed. The radius of a deformed nucleus can be expanded in term of the spherical harmonics such that (see e.g. Irvine (1972) and Nilsson and Ragnarsson (1995)):

$$R(\theta, \phi) = R(\alpha_l)\left[1 + \sum_{l,m} \alpha_l Y_l^m(\theta, \phi)\right] \tag{13}$$

where $R(\alpha_l)$ is a deformation dependent radius (placed here to conserve the volume) while θ and ϕ are the azimuthal and polar angles of the cylindrical coordinates respectively. For a small deformation, the quadrupole ($l = 2$) term is found to be more important and since we are looking at axially symmetrical deformations, the expansion is taken only in the m=0 case. We then have:

$$R(\theta, \alpha_2) = R(\alpha_2)[1 + \alpha_2 P_2(cos\theta)] \tag{14}$$

Using this deformation dependent radius, the surface and Coulomb energies for a small distortion of the nuclear shape are given by the relation (see e.g. Nilsson and Ragnarsson (1995)):

$$E_S = E_{S_0}\left(1 + \frac{2}{5}\alpha_2^2 - \frac{4}{105}\alpha_2^3 + \cdots\right) \tag{15}$$

$$E_C = E_{C_0}\left(1 - \frac{1}{5}\alpha_2^2 - \frac{4}{105}\alpha_2^3\right) \tag{16}$$

with E_{S_0} and E_{C_0} being the surface and Coulomb energy of an undistorted (spherical) nucleus. With these relations, one can easily see that the surface energy increases while Coulomb energy decreases, with deformation. This is clearly demonstrated in Figure 2.1 which gives the plot of the Coulomb, surface and the net deformation energies (in MeV) as a function of quadrupole deformation, α_2. The near total cancellation of the surface and Coulomb energy makes it important to correctly calculate both contributions so as to obtain accurate deformation energy.
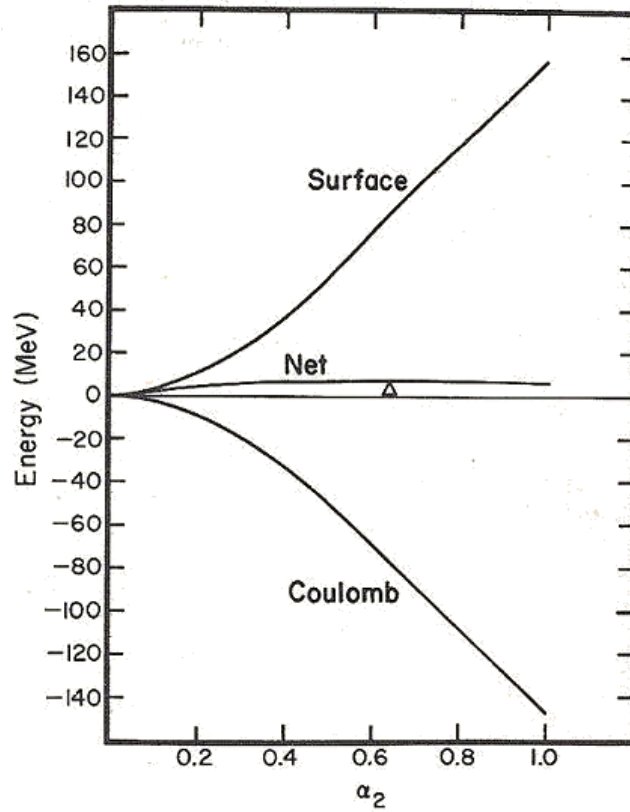
Figure 2.1: The surface and Coulomb energy as a function of quadrupole deformation for ^{252}Cf. The near cancellation of both terms give rise to a relatively small deformation energy (taken from R. Vandenbosch and J. R. Huizenga (1973))

For a nucleus to be stable against small deformation, the change in the Coulomb energy has to be smaller than the change in the surface energy, so that:

$$\frac{\Delta E_C}{\Delta E_S} \leq 1 \qquad (17)$$

By introducing the fissility parameter, X given by:

$$X = \frac{E_C}{2E_S} \qquad (18)$$

one can write the total deformation energy as:

$$\Delta E = E_S + E_C - E_{S_0} - E_{C_0} = E_{S_0} \left(\frac{2}{5}(1 - X)\alpha_2^2 - \frac{4}{105}(1 + 2X)\alpha_2^3 + \cdots \right) \quad (19)$$

The equation above shows that for $X < 1$, the deformation energy is increasing around $\alpha_2 = 0$ which means that there is a fission barrier for elements beyond iron that the nucleus needs to overcome before fission process could occur. On the other hand, the deformation energy has a downsloping character when $X > 1$ even for small deformation (small value of α_2). Thus, the nucleus is not stable against small deformation if the fissility parameter is greater than unity.

From the definition of the fissility parameter, one sees that:

$$X = \frac{3e^2}{40\pi r_0^3 S} \left(\frac{Z^2}{A} \right) \quad (20)$$

The heaviest nucleus that exists naturally, which is ^{238}U, has a fissility parameter $X \sim 0.8$. This is a typical value for nuclei with a mass number, A=230-240. One can see from equation (20) that spontaneous fission is more likely to occur for nuclei with a large number of protons for a given total number of nucleons A.

The two physical consequences discussed above highlights the importance of the Coulomb interaction on nuclear structure. It is therefore imperative that the Coulomb interaction is treated properly in most nuclear properties calculations.

2.2.2 Derivation of the direct and exchange Coulomb contribution

For any two-body interaction (in the present case the Coulomb interaction) described by the operator v_{12}. The expectation value of a two-body interaction in a Slater determinant, $|\Psi\rangle$ is equal to:

$$\langle\Psi|v_{12}|\Psi\rangle = \frac{1}{2}\Sigma_{i,j}^{A}\langle ij|v_{12}|\widetilde{ij}\rangle \tag{21}$$

with $|\widetilde{ij}\rangle = |ij\rangle - |ji\rangle$ resulting from the anti symmetric properties of the state $|\Psi\rangle$. Writing the above equation in coordinate space and for a local two-body interaction, one would get:

$$\frac{1}{2}\Sigma_{i,j}^{A}\langle ij|v_{12}|\widetilde{ij}\rangle = \frac{1}{2}\Sigma_{i,j}^{A}\int\int d^{3}\vec{r}\, d^{3}\vec{r}'\,\langle ij|\vec{r},\vec{r}'\rangle\langle\vec{r},\vec{r}'|v_{12}|\vec{r},\vec{r}'\rangle\langle\vec{r},\vec{r}'|\widetilde{ij}\rangle \tag{22}$$

Expanding the equation further with $v_{12}|\vec{r},\vec{r}'\rangle = v(\vec{r},\vec{r}')|\vec{r},\vec{r}'\rangle$, one gets:

$$E_{coul} = \frac{1}{2}\Sigma_{i,j}^{A}\int d^{3}\vec{r}d^{3}\vec{r}'\,\left|\langle ij|\vec{r},\vec{r}'\rangle\right|^{2}v(\vec{r},\vec{r}')$$

$$-\frac{1}{2}\Sigma_{i,j}^{A}\int d^{3}\vec{r}d^{3}\vec{r}'\,\langle ij|\vec{r},\vec{r}'\rangle v(\vec{r},\vec{r}')\langle\vec{r},\vec{r}'|ji\rangle \tag{23}$$

We shall denote the single particle wavefunction of the state in the coordinate space as:

$$\phi_i(\vec{r}) = \langle\vec{r}|i\rangle \tag{24}$$

so that $\langle\vec{r},\vec{r}'|ij\rangle = \phi_i(\vec{r})\phi_j(\vec{r}')$. Finally, the expression for the total Coulomb energy is thus:

$$E_{coul} = \frac{1}{2}\sum_{i,j}^{A} \int d^3\vec{r}\, d^3\vec{r}'\, |\phi_i(\vec{r})|^2 v(\vec{r},\vec{r}')|\phi_j(\vec{r}')|^2$$

$$-\frac{1}{2}\sum_{i,j}^{A} \int d^3\vec{r}\, d^3\vec{r}'\, \phi_i^*(\vec{r})\phi_j^*(\vec{r}')v(\vec{r},\vec{r}')\phi_j(\vec{r})\phi_i(\vec{r}') \qquad (25)$$

The first term on the right hand side refers to the direct Coulomb contribution while the second term is the exchange part. The direct Coulomb term gives rise to the repulsive part of the Coulomb interaction while the exchange part causes an extra binding between the nucleons. The calculation of the direct term is much easier as one needs only for computing the nucleon density $\rho(\vec{r}) = \sum_i^A |\varphi_i(\vec{r})|^2$ (or $\rho(\vec{r}')$) as a function of a single spatial variable. The direct term has been exactly included in all previous self-consistent calculations. In contrast, the exchange part is more complicated in that one now needs to know the non-local nucleon density, $\rho(\vec{r},\vec{r}') = \sum_i^A \varphi_i$ as a function of two space variables. The computational time for the exchange Coulomb part is therefore much longer than for the direct term. To overcome these problems, the Slater approximation detailed below is commonly used in place of the exact Coulomb expression for the exchange term.

2.2.3 Energy contribution from direct and exchange Coulomb term

We will adopt here an equivalent but somewhat different (from the rest of our text) point of view to obtain the expressions of the direct and exchange Coulomb energies. By taking nucleon as having a diffuse density rather than a point particle, the total Coulomb energy may be written in the form (Quentin, 1975):

$$E_C = \frac{e^2}{2}\int \mathrm{P}(\vec{r},\vec{r}')\frac{1}{|\vec{r}-\vec{r}'|}d^3\vec{r}\, d^3\vec{r}' \qquad (26)$$

The symbol $P(\vec{r}, \vec{r}')$ denotes the probability of finding two protons at position $\vec{r}$ and $\vec{r}'$.

The general form of this probability written for any wavefunction, $|\Psi\rangle$ is:

$$P(\vec{r}, \vec{r}') = \sum_k^Z \sum_{j<k}^Z \langle \Psi | [\delta(\vec{r} - \vec{r}_j)\delta(\vec{r}' - \vec{r}_k) + \delta(\vec{r} - \vec{r}_k)\delta(\vec{r}' - \vec{r}_j)] | \Psi \rangle \qquad (27)$$

Taking for $|\Psi\rangle$ a Slater determinant consisting of plane waves, it may be shown (see e.g. Quentin (1975)) that the probability $P(\vec{r}, \vec{r}')$ is given:

$$P(\vec{r}, \vec{r}') = \left(\rho_0^p\right)^2 \left\{ 1 - \frac{1}{2}\left[C\left(k_F^p |\vec{r} - \vec{r}'|\right)\right]^2 \right\} \qquad (28)$$

with the function C(x) defined as:

$$C(x) = \frac{3j_1(x)}{x} = \frac{3}{x^2}\left(\frac{\sin x}{x} - \cos x\right) \qquad (29)$$

where $j_n(x)$ is the spherical Bessel function of the first kind which is related to the Bessel function of the first kind, $J_n(x)$ by the relation $j_n(x) = \sqrt{\frac{\pi}{2x}} J_{n+\frac{1}{2}}(x)$; $n = 0,1,2 \ldots$. In the above, ρ_0^p is the average proton density at the Fermi surface which is related as well known with the Fermi momentum for a system of doubly spin-degenerated fermions by:

$$\left(k_F^p\right)^3 = 3\pi^2 \rho_0^p \qquad (30)$$

From equation (28), it is apparent that there are two terms contributing to the total Coulomb energy in equation (26). The first term on the right hand side of equation (28) represent the direct Coulomb part while the second term is the exchange Coulomb part.

One then has the expression for the Coulomb energy coming from direct and exchange part respectively as follows:

$$V_{coul\_dir}(\vec{r}) = \frac{e^2}{2} \int \left(\rho_0^p(\vec{r}')\right)^2 \frac{1}{|\vec{r}-\vec{r}'|} d^3\vec{r}\, d^3\vec{r}' \tag{31}$$

$$V_{coul\_exch}(\vec{r},\vec{r}') = \frac{e^2}{4} \int \left(\rho_0^p(\vec{r}')\right)^2 \frac{[C(k_F^p|\vec{r}-\vec{r}'|)]^2}{|\vec{r}-\vec{r}'|} d^3\vec{r}\, d^3\vec{r}' \tag{32}$$

2.2.4   Calculation of the direct Coulomb potential

One can see that a singularity point appears in equation (31) when $\vec{r}$ approaches $\vec{r}'$. To avoid this problem, one can use the substitution of the term as shown below as was employed for instance in Quentin (1975) and Vautherin (1973):

$$\vec{\nabla}_{\vec{r}'}^2 |\vec{r}-\vec{r}'| = \frac{2}{|\vec{r}-\vec{r}'|} \tag{33}$$

After the substitution, one then integrate by parts to obtain:

$$V_{coul\_dir}(\vec{r}) = \frac{e^2}{4} \int |\vec{r}-\vec{r}'| \vec{\nabla}^2 \rho_0^p(\vec{r}') d^3\vec{r}' \tag{34}$$

One then need to change the coordinate system into cylindrical coordinate considering the earlier fact that the nucleus is assumed to be axially symmetric along the z-direction. The expression for the direct Coulomb energy after integration over the azimuthal angle is (see for e.g. Quentin (1975)):

$$V_{coul\_dir}(\vec{\rho},\vec{z}) = e^2 \int_0^\infty \rho'\, d\rho' \int_{-\infty}^\infty dz\, [(z-z')^2 + (\rho-\rho')^2]^{1/2}$$

$$\times E\left(\left\{\frac{4\rho\rho'}{[(z-z')^2+(\rho-\rho')^2]^{1/2}}\right\}\right) \times \vec{\nabla}^2 \rho_0^p(\vec{\rho}',\vec{z}) \tag{35}$$

with the following expression for E(x):

$$E(x) = \int_0^{\pi/2}(1 - x\sin^2\theta)^2 d\theta \tag{36}$$

2.2.5 The Slater approximation of the Coulomb exchange within the Local Density Approximation

From equation (32) for the exchange Coulomb potential, one may further show (see e.g. Quentin (1975)) that upon changing into relative coordinate and center-of-mass coordinate,

$$\vec{r}_{rel} = \vec{r} - \vec{r}' \tag{37}$$

$$\vec{R}_{c.m} = \frac{1}{2}(\vec{r} + \vec{r}') \tag{38}$$

one gets:

$$E_{coul\_exch} = -\frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\left(\rho_0^p\right)^{4/3}\Omega \tag{39}$$

The symbol Ω represents the total volume of the system under study. One can then write the expression for exchange Coulomb energy density as:

$$\frac{E_{(coul\_exch)}}{\Omega} = -\frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\left(\rho_0^p\right)^{4/3} \equiv \varepsilon_{coul\_exch} \tag{40}$$

In nuclear matter, as was considered so far, the distribution of protons and neutrons in space is constant. This situation is very similar to the density distribution of nucleons inside the nucleus where the density is almost constant in the center and only fall off

gradually at the nuclear surface. Therefore, this allows one to take the Local Density Approximation in which the density inside a nucleus is taken to be locally constant and then one would have the total Coulomb exchange energy given as:

$$E_{coul\_exch} = -\frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3}\int\left(\rho_0^p\right)^{4/3}d^3\vec{r} \qquad (41)$$

Equation (41) for the coulomb exchange energy is called the Slater approximation for the exchange part of the Coulomb interaction (Slater, 1951). It amounts to consider locally (in $\vec{r}$) that the proton distribution is a piece of nuclear matter at the locally experienced proton density. This approximation has been regularly used in most self-consistent calculation, see for example Quentin and Flocard (1978).

2.3   HARTREE-FOCK-SKYRME APPROXIMATION

2.3.1   Introduction to Hartree-Fock approximation

The Hartree-Fock (HF) method was initially proposed for the study of atomic physics but its wide applicability in many other fields of physics makes it one of the most popular approximations of the quantal many-body problem used so far. In nuclear physics, the HF method has been found to be relevant to study the ground state energy and wavefunction of a specific nucleus. Much work in such a framework has been done thus far such as reviewed in Quentin and Flocard (1978), Aberg, Flocard and Nazarewicz (1990) and Bender, Heenen and Reinhard (2003), ranging from light nuclei up to heavy ones.

This method stems from a microscopic point of view, whereby the argument was that any proper description of the properties of nucleus under study should start from a

basic free nucleon-nucleon interaction. However, due to the mathematical difficulty encountered to treat at all orders the effect of such a two-body interaction, a mathematical ansatz was proposed instead, to describe the nucleonic interactions inside a nucleus. Hence, the name phenomenological effective interaction was given to it. In this approach, three main assumptions were made (see e.g. Bonneau (2003)):

   i. The kinetic energy of nucleons inside the nucleus is assumed to be non-relativistic, its average being about 20 MeV,

  ii. The nucleons interact with one another through an interaction which is described by an effective two-body phenomenological interaction (possibly density dependent)

 iii. Mesonic degrees of freedom are not taken into account.

In this approach, the many-body wavefunction of the A nucleons is a priori approximated by a product of single particle wavefunctions. However, since nucleons are fermions, they have to obey the Pauli antisymmetrization principle and as such the appropriate wavefunction would be an (antisymmetrized) Slater determinant written as:

$$\Psi(r) = \frac{1}{\sqrt{A}}\det|\Phi_i(r_i)| = \frac{1}{\sqrt{A}}\begin{bmatrix} \Phi_1(r_1) & \cdots & \Phi_1(r_A) \\ \vdots & \ddots & \vdots \\ \Phi_A(r_1) & \cdots & \Phi_A(r_A) \end{bmatrix} \tag{42}$$

For a two body system, the Slater determinant would thus be:

$$\Psi(r_1, r_2) = \frac{1}{\sqrt{2}}[\Phi_1(r_1)\Phi_2(r_2) - \Phi_1(r_2)\Phi_2(r_1)] \tag{43}$$

From this, one can see that in a Slater determinant two nucleons cannot be at the exactly same state (so-called Pauli exclusion principle).

2.3.2 Concept of an average potential

In a nucleus consisting of *A* nucleons, the total Hamiltonian is given (for a two body interaction) by:

$$H = \sum_i^A t_i + \sum_j^A \sum_{i<j}^A V_{ij} \tag{44}$$

The first term on the right hand side represents the kinetic energy of the nucleons, where the summation is taken over all constituent nucleons in the nucleus. The second term is the two-body interaction between nucleons with a choice of indices i and j made in order to avoid double counting the interaction.

The two-body interactions between all the nucleons can be averaged out to obtain an average one-body potential, U, which is felt by all nucleons. Adding U inside equation (44) would give:

$$H = \sum_i^A t_i + \sum_i^A U_i + \left(\sum_j^A \sum_{i<j}^A V_{ij} - \sum_i^A U_i \right) \tag{45}$$

$$= \sum_i^A h_{SP_i} + \left(\sum_j^A \sum_{i<j}^A V_{ij} - \sum_i^A U_i \right) \tag{46}$$

whereby h_{SP_i} is the single particle energy, which is defined as the sum of the kinetic energy and the one-body potential of the ith nucleon:

$$h_{SP_i} = t_i + U_i \tag{47}$$

In the Hartree-Fock approximation, the average one-body potential, U is derived from the two-body interaction, V above. The term on the right hand side inside the bracket in equation (46) is called the residual interaction, representing the remaining part of the interaction beyond the average potential. Examples of residual interactions generally

taken into account are designed to treat correctly pairing or vibrational correlations. For the Hartree-Fock approximation to be relevant, the residual interaction has to be as small as possible.

$$H \approx \sum_i^A h_{SP_i} = H_{HF} \tag{48}$$

One then has a reduction of an initial many-body problem into a one-body problem which is much easier to solve. Solving the Schrodinger equation for the Hamiltonian H_{HF} will give a result approximating the exact wavefunction, in the form of a Slater determinant. The residual part $H - H_{HF}$ then may be treated as a perturbation of the approximate result.

2.3.3 Solving the Hartree-Fock equation using variational method

To obtain the total energy of the nucleus, one would need to solve the Schrodinger equation. This can be done by employing the variational method as a mean of solving the static Schrodinger equation. An energy functional associated with a wavefunction $|\Psi\rangle$ for the Hamiltonian operator H_{HF} can be written as:

$$E[\Psi] = \frac{\langle \Psi | H_{HF} | \Psi \rangle}{\langle \Psi | \Psi \rangle} \tag{49}$$

in which $|\Psi\rangle$ is the Slater determinant as mentioned above and the denominator term here is to ensure that the wavefunction remains normalised during the variation. One arbitrary varies $|\Psi\rangle$ about any $|\Psi_n\rangle$ where $|\Psi_n\rangle$ is the solution to the eigenvalue equation $(H - E_n)|\Psi_n\rangle = 0$ to obtain a stationary total energy such that:

$$\delta E = \delta \frac{\langle \Psi | H_{HF} | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0 \tag{50}$$

The $|\Psi\rangle$ and $\langle\Psi|$ may be treated as independent variable in the variation process (this is related to the complex character of the wavefunction acssociated to $|\Psi\rangle$), so that the variation is carried out for either one of them. By varying $|\Psi\rangle$, one can get:

$$\delta E = \frac{\langle\Psi|H|\delta\Psi\rangle - E[\Psi]\langle\Psi|\delta\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{51}$$

If $|\Psi\rangle = |\Psi_n\rangle$ or in other words, $|\Psi\rangle$ is the eigenfunction of the Hamiltonian operator then one obtains a stationary energy and therefore solving the variational equation is equivalent to solving the Schodinger equation. Let us denote the ket of the true ground state of a system as $|\psi_0\rangle$. One may prove that for any $|\Psi\rangle$:

$$E[\psi] \geq E[\psi_0] \tag{52}$$

Therefore, one strives to minimize the value of $E[\psi]$ in order to get a better approximation to the real ground state of a system.

2.3.4   Local and non-local potential

The HF one body potential, U is defined as (see e.g. Preston and Bhaduri (1975)):

$$\langle l|U|m\rangle = \sum_{p,q}^{A}\langle lp|V|\widetilde{mq}\rangle \tag{53}$$

with

$$|\widetilde{mq}\rangle = |mq\rangle - |qm\rangle \tag{54}$$

The indices l,m,p and q label the single particle states and $|\widetilde{mq}\rangle$ represents the antisymmetric state of a two fermion system.

Defining the single particle states $|m\rangle$ as eigenfunctions of the single particle Hamiltonian operator, $(t + U)$ with eigenvalue, e_m, one has:

$$(t + U)| m \rangle = e_m |m\rangle \tag{55}$$

Writing equation (55) in coordinate space where $\emptyset_m(\vec{r}) = \langle \vec{r}|m \rangle$ is the single particle wavefunction would yield:

$$-\frac{\hbar}{2M}\nabla^2 \emptyset_m(\vec{r}_1) + U_H \emptyset_m(\vec{r}_1) - \int U_F(\vec{r}_1, \vec{r}_2) \emptyset_m(\vec{r}_2)\, d^3r_2 = e_m \emptyset_m(\vec{r}_1) \tag{56}$$

The first term on the right hand side is the kinetic energy term while U_H denotes the local part of U and U_F denotes its non-local part, with

$$U_H(\vec{r}_1) = \sum_{i=1}^{A} \int \emptyset_l^*(r_2)\, V(|r_1 - r_2|)\emptyset_l(r_2)d^3r_2 \tag{57}$$

and

$$U_F(\vec{r}_1, \vec{r}_2) = \sum_{i=1}^{A} \emptyset_l^*(r_2)\, V(|r_1 - r_2|)\emptyset_l(r_1) \tag{58}$$

The local potential term (Hartree term) reflects the total potential felt classically by a nucleon in position $\vec{r}_1$ due to the presence of other nucleons in $\vec{r}_2$. The summation, though, is taken for all nucleons inside the nucleus which means that the particular nucleon of interest itself contributes to the potential. This is obviously not physically true, and is corrected for, among other effects, by the non-local term (Fock term) or exchange term. As it turns out, the considered effective interaction depends on the local

density, ρ at the center of mass of the system, $\frac{(\vec{r}_1+\vec{r}_2)}{2}$ of the two interacting nucleons. The density dependence is indeed very important to reproduce the experimental total and single particle energies (see e.g. Preston and Bhaduri (1975)). This results in an extra term in equation (56) which now becomes:

$$-\frac{\hbar}{2M}\nabla^2\emptyset_m(r_1) + U_H\emptyset_m(r_1)\ -\int U_F(r_1,r_2)\emptyset_m(r_2)\,d^3r_2 +\ U_R(r_1)\emptyset_m(r_1)$$
$$=\ e_m\emptyset_m(r_1)$$

(59)

U_R is called the rearrangement potential due to the density dependence of the interaction.

(Note: the above simple local expression for U_R is only valid for a zero range density dependent two-body interaction as in the case of the Skyrme and Gogny interaction.)

2.3.5   General description of solving Hartree-Fock equation

To solve the eigenvalue equation (55), the expectation value of the single particle Hamiltonian is taken between single particle states $|\,l\rangle$ and $|\,m\rangle$.

$$\langle l|\,H_{SP}|m\rangle =\ e_m\delta_{lm}$$

(60)

The single particle states can be expanded in terms of certain basis states such as harmonic oscillator potential eigenstates denoted here as $|\beta\rangle$ (x_β^m being the expansion coefficient of the state m):

$$|m\rangle = \sum_\beta x_\beta^m|\beta\rangle$$

(61)

By introducing the HF single particle operator;

$$\rho = \sum_m^A |m\rangle\langle m| \tag{62}$$

one has:

$$\rho_{\delta\gamma} \equiv \langle\delta|\rho|\gamma\rangle = \sum_m^A (x_\gamma^m)^* (x_\delta^m) \tag{63}$$

where the symbols γ and δ label harmonic oscillator basis states.

Equation (60) can then be written as:

$$\forall\alpha; \qquad \sum_\beta \langle\alpha|t|\beta\rangle x_\beta^m + \sum_{\beta,\gamma,\delta} \langle\alpha\gamma|V|\widetilde{\beta\delta}\rangle \rho_{\delta\gamma} x_\beta^m = e_m x_\alpha^m \tag{64}$$

The set of equations (64) constitutes a system of non linear equations to be solved iteratively. In order to do this, an ansatz for ρ is needed. This is usually done firstly by approximating the one-body potential, U, to be that of, for example, a harmonic oscillator or a Wood-Saxon potential. Equation (64) may be solved taking the state $|m\rangle$ as being an eigenstate of the single particle Hamiltonian using one of these simple potentials. The left hand side of equation (64) is then solved as a linear system of equations yielding a new set of single particle states. From the new set of single particle states, the density operator of equation (63) can be calculated and is then used to get a new one-body potential, U. The calculation is then repeated as long as the convergence is not achieved. (The convergence being defined as the situation where the variation (in norm) of some chosen quantities is smaller than a given value.)

2.3.6   Hartree-Fock equation with Skyrme interaction

Vautherin and Brink found out that by using the Skyrme interaction, the total energy of a nucleus, E can be written in terms of a Hamiltonian density, $\mathcal{H}(\vec{r})$ such that:

$$E = \langle T + V \rangle \tag{65}$$

$$= \int \mathcal{H}(\vec{r}) d^3 r \tag{66}$$

The energy density is expressed in the Skyrme interaction case in terms of three local densities: the nucleon density, the kinetic energy density and the spin-orbit densities defined as follows (Vautherin and Brink, 1972):

$$\rho_q(\vec{r}) = \sum_{m,\sigma} |\Phi_m(\vec{r}, \sigma, q)|^2 \tag{67}$$

$$\tau_q = \sum_{m,\sigma} |\vec{\nabla} \Phi_m(\vec{r}, \sigma, q)|^2 \tag{68}$$

$$\vec{J}_q = (-i) \sum_{m,\sigma,\sigma'} \Phi_m^*(\vec{r}, \sigma, q) \left[\vec{\nabla} \Phi_m(\vec{r}, \sigma', q) \times \langle \sigma | \vec{\sigma} | \sigma' \rangle \right] \tag{69}$$

In these equations, $\Phi_m(\vec{r}, \sigma', q)$ represents the single particle state in space coordinate with $\Phi_m(\vec{r}, \sigma', q) = \langle (\vec{r}, \sigma', q) | m \rangle$. The operator $\vec{\sigma}$ is the spin operator with the relation $\vec{S}_i = \frac{\hbar}{2} \vec{\sigma}_i$; $(i = x, y, z)$ with $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$ and $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$.

The expression for the Hamiltonian density, $\mathcal{H}(\vec{r})$ in equation (66) was derived by Vautherin and Brink for the case of nucleus with an even number of neutrons and protons, taking into account the time reversal invariance symmetry (see Vautherin and Brink (1972) for more details):

$$\mathcal{H}(\vec{r}) = \frac{\hbar^2}{2m}\tau(\vec{r}) + \frac{1}{2}t_0\left[\left(1+\frac{1}{2}x_0\right)\rho^2 - \left(x_0 + \frac{1}{2}\right)\left(\rho_n^2 + \rho_p^2\right)\right] + \frac{1}{4}(t_1 + t_2)\rho\tau$$

$$+ \frac{1}{8}(t_2 - t_1)\left(\rho_n\tau_n + \rho_p\tau_p\right) + \frac{1}{16}(t_2 - 3t_1)\rho\nabla^2\rho$$

$$+ \frac{1}{32}(3t_1 + t_2)\left(\rho_n\nabla^2\rho_n + \rho_p\nabla^2\rho_p\right) + \frac{1}{16}(t_1 - t_2)\left(\vec{J}_n^2 + \vec{J}_p^2\right)$$

$$+ \frac{1}{4}t_3\rho_n\rho_p\rho - \frac{1}{2}W_0\left(\rho\vec{\nabla}\cdot\vec{J} + \rho_n\vec{\nabla}\cdot\vec{J}_n + \rho_p\vec{\nabla}\cdot\vec{J}_p\right) \tag{70}$$

By applying the varational principle, they then obtained the following Hartree-Fock equations (Vautherin and Brink, 1972):

$$\left[-\vec{\nabla}\frac{\hbar^2}{2m_q^*(\vec{r})}\vec{\nabla} + U_q(\vec{r}) + \vec{W}_q(-i)\left(\vec{\nabla}\times\vec{\sigma}\right)\right]\Phi_m = e_m\Phi_m \tag{71}$$

The symbol $m_q^*(\vec{r})$ denotes an effective mass (coming from the Fock part of the HF potential) which depends only on the nucleon density. The dependence of each term on the left hand side is given below. The first term is similar to the kinetic energy with a position dependent (effective) mass:

$$\frac{\hbar^2}{2m_q^*(\vec{r})} = \frac{\hbar^2}{2m} + \frac{1}{4}(t_1 + t_2)\rho + \frac{1}{8}(t_2 - t_1)\rho_q \tag{72}$$

The second and third terms are the one-body potential and spin-orbit potential respectively:

$$U_q(\vec{r}) = t_0\left[\left(1 + \frac{1}{2}x_0\right)\rho - \left(x_0 + \frac{1}{2}\right)\rho_q\right] + \frac{1}{4}t_3\left(\rho^2 - \rho_q^2\right)$$

$$- \frac{1}{8}(3t_1 - t_2)\nabla^2\rho + \frac{1}{16}(3t_1 - t_2)\nabla^2\rho_q + \frac{1}{4}(t_1 + t_2)\tau$$

$$+ \frac{1}{8}(t_2 - t_1)\tau_q - \frac{1}{2}W_0\left(\vec{\nabla}\cdot\vec{J} + \vec{\nabla}\cdot\vec{J}_q\right) + \delta_{q,\frac{1}{2}}V_C(\vec{r}) \tag{73}$$

$$\vec{W_q}(\vec{r}) = \frac{1}{2} W_0 (\vec{\nabla}\rho + \vec{\nabla}\rho_q) + \frac{1}{8}(t_1 - t_2)\vec{J_q}(\vec{r}) \tag{74}$$

In solving the Hartree-Fock equation with the Skyrme force as defined in equation (71), the matrix elements of the single particle Hamiltonian given by equation (72) to (74) have to be calculated and diagonalised. This part of the calculation is carried out in coordinate space.

2.4   TREATMENT OF PAIRING INTERACTION

2.4.1   The BCS Approximation

As was mentioned earlier, one of the residual interactions to be necessarily treated is the one leading to pairing correlations between nucleons. Let us call it the pairing interaction. It leads to the formation of a pair of two nucleons being in two states conjugated by time reversal. This nucleon pair is promoted to a higher unoccupied single particle energy level but results in a lower binding energy of the whole nuclear system due to the added specific binding correlation energy when summed on all pairs. To account for this phenomenon, one usually makes use of the Bardeen, Cooper and Schrieffer (BCS) formalism which was initially proposed for the study of superconductivity (see e.g. Bardeen, Cooper and Schrieffer (1957)).

One first makes the approximation that the ground state of an even-even nucleus can be written in terms of a BCS wavefunction given by (see e.g. Preston and Bhaduri (1975)):

$$|BCS\rangle = \prod_{\mu>0}(U_\mu + V_\mu a_\mu^+ a_{\bar{\mu}}^+)|0\rangle \tag{75}$$

The ket $|0\rangle$, here, denotes the vacuum state (a state devoid of any nucleon). The operators a_{μ}^{+} and $a_{\bar{\mu}}^{\pm}$ are the particle creation operators in state μ and its time-reverse state $\bar{\mu}$ (U_{μ} and V_{μ} being real non-negative numbers not larger than 1). In the present case, the Hamiltonian, H is a Hermitian operator satisfying time reversal invariance property which implies that if a state μ is an eigenstate of H its time-reverse state $\bar{\mu}$ is also an eigenstate of H with the same (energy) eigenvalue. In the case (considered here) of axial symmetry and parity symmetry the third component of the total angular momentum, K is a good quantum number as well as the parity π. If the state μ corresponds to the quantum number K^{π} the state $\bar{\mu}$ corresponds to $-K^{\pi}$. This property has been used to limit the product in the definition of the $|BCS\rangle$ state to only positive K value states only (denoted by $\mu > 0$).

One can see that the BCS wavefunction describes the nuclear system in a state where all nucleons are paired. A difference with regards to the independent particle description is that the occupation of the single particle states is given in terms of the probabilities of the state μ for being empty (U_{μ}^{2}) or being filled (V_{μ}^{2}) instead of an integer particle number 0 (unoccupied) and 1 (occupied) respectively (note that due to the analytical form of the $|BCS\rangle$ state, the probability of any state μ and its time-reversed state are equal).

The simplest Hamiltonian describing this case written in the second quantization notation is:

$$H = \sum_{v} e_{v} a_{v}^{+} a_{v} - G \sum_{v,\mu} a_{v}^{+} a_{\bar{v}}^{+} a_{\bar{\mu}} a_{\mu} \qquad (76)$$

The symbol a_{v}^{+} and a_{v} denotes the creation operator and annihilation operator respectively in the state v. The term G is the strength of the pairing force. It is positive

(attractive residual interaction). To solve the static Schrodinger equation associated with this Hamiltonian, a Lagrange multiplier λ is introduced to minimize the Hamiltonian given in equation (76) under the constraint of $\sum_v a_v^+ a_v = N$ where N is the number of considered fermions. The modified "Hamiltonian" can then be written as (see e.g. Preston and Bhaduri (1975)):

$$H^{'} = \sum_v (e_v - \lambda) a_v^+ a_v - G \sum_{v,\mu} a_v^+ a_{\bar{v}}^+ a_{\bar{\mu}} a_\mu \qquad (77)$$

One takes the expectation value of this operator with respect to the BCS trial wavefunction, thus obtaining:

$$\langle BCS|H^{'}|BCS \rangle = \sum_{\mu,v>0} [2(e_v - \lambda)V_v^2 - GV_v^4] - G(\sum_{v>0} U_v V_v)^2 \qquad (78)$$

In solving the BCS variational equation one will vary the coefficient, V_v in the trial wavefunction in order to minimize the expectation value of the Hamiltonian (note that U_v is determined when V_v is known).

$$\frac{\partial}{\partial V_v} \langle BCS|H^{'}|BCS \rangle = 0 \qquad (79)$$

Solving the equation (79), one obtains the equation:

$$2(e_v^{'} - \lambda)U_v V_v = \Delta(U_v^2 - V_v^2) \qquad (80)$$

with:

$$e_v^{'} = e_v - GV_v^2 \quad \text{and} \quad \Delta = G \sum_{v>0} U_v V_v \qquad (81)$$

From the above, using the relation $U_\nu^2 + V_\nu^2 = 1$, one will then obtain the occupation probabilities as:

$$U_\nu^2 = \frac{1}{2}\left[1 + \frac{e_\nu' - \lambda}{\sqrt{(e_\nu' - \lambda)^2 + \Delta^2}}\right] \tag{82}$$

$$V_\nu^2 = \frac{1}{2}\left[1 - \frac{e_\nu' - \lambda}{\sqrt{(e_\nu' - \lambda)^2 + \Delta^2}}\right] \tag{83}$$

The Lagrange multiplier, λ is the chemical potential or a kind of Fermi level of the nuclear system (Preston and Bhaduri, 1975) which is determined by using the constraint relation:

$$2\sum_{v>0} V_v^2 = N \tag{84}$$

where N is the total number of nucleons under consideration. An important consequence of the introduction of the pairing interaction is to smear the occupation of the particle states near the Fermi level (corresponding to the uncorrelated case) since in the absence of pairing correlation, the single particle states below and above the Fermi level are fully occupied and fully empty, respectively.

2.4.2 Quasiparticles and the Bogolyubov-Valatin transformation

In order to obtain the expression for the operator H' defined in equation (77), quasiparticle operators may be introduced through the Bogolyubov-Valatin transformation (Preston and Bhaduri, 1975).

$$\alpha_\nu^+ = U_\nu a_\nu^+ - V_\nu a_{\bar{\nu}} \quad \text{(and obviously } \alpha_\nu = U_\nu a_\nu - V_\nu a_{\bar{\nu}}^+\text{)} \tag{85}$$

The quasiparticle operators for the time-reverse state of ν are:

$$\alpha_{\bar{\nu}}^+ = U_\nu a_{\bar{\nu}}^+ + V_\nu a_\nu \quad (\text{and obviously} \quad \alpha_{\bar{\nu}} = U_\nu a_{\bar{\nu}} + V_\nu a_\nu^+) \tag{86}$$

These quasiparticle operators obey the same anti commutation relations as the particle creation and annihilation operators:

$$\{\alpha_\nu, \alpha_\mu^+\} = \delta_{\nu\mu} \quad \text{and} \quad \{\alpha_\nu, \alpha_\mu\} = \{\alpha_\nu^+, \alpha_\mu^+\} = 0 \tag{87}$$

Using these operators, one can deduce that the BCS wavefunction is a quasiparticle vacuum, since:

$$\alpha_\nu|BCS\rangle = 0 \tag{88}$$

The state $\alpha_\nu^+|BCS\rangle$ is called a single quasiparticle state. Single particle states lying deeper than the Fermi surface whose occupation probabilities, V_ν^2 are close to 1, are essentially one-hole states. On the other hand, states far above the Fermi level are one-particle states.

In order to obtain the expectation value of the operator H', one will need to inverse equations (85) and (86) to obtain:

$$a_\nu = U_\nu \alpha_\nu + V_\nu \alpha_{\bar{\nu}}^+ \quad and \quad a_{\bar{\nu}} = U_\nu \alpha_{\bar{\nu}} - V_\nu \alpha_\nu^+ \tag{89}$$

Using these equations, one can then work out the expectation value of the operator H' as given in equation (77). The energy of a single quasiparticle state can be obtained by

evaluating the expectation value of $\langle BCS|[(\alpha_\nu H'\alpha_\nu^+) - H']|BCS\rangle$ and has the following

expression (see e.g. Preston and Bhaduri (1975)):

$$E_{qp} = \sqrt{(e_\nu' - \lambda)^2 + \Delta^2} \tag{90}$$

2.4.3   On the treatment of pairing correlations in a self-consistent calculation

By introducing the occupation probabilities from the BCS equation, the three local

densities introduced earlier namely the nucleon density, the kinetic energy density and

spin-orbit density would now be written as (see e.g. Vautherin (1973)):

$$\rho_q(\vec{r}) = 2 \sum_{m,\sigma} V_m^2 \, |\Phi_m(\vec{r},\sigma,q)|^2 \tag{91}$$

$$\tau_q = 2 \sum_{m,\sigma} V_m^2 \, |\vec{\nabla}\Phi_m(\vec{r},\sigma,q)|^2 \tag{92}$$

$$\vec{J}_q = (-2i) \sum_{m,\sigma,\sigma'} V_m^2 \, \Phi_m^*(\vec{r},\sigma,q)\left[\vec{\nabla}\Phi_m(\vec{r},\sigma',q) \times \langle \sigma|\vec{\sigma}|\sigma'\rangle\right] \tag{93}$$

where the sum sums on "positive" states as defined above. We shall then extend the

variational method discussed earlier to account for the variation of the occupation

probability of the single particle states. The pairing energy from the BCS formalism is

given as (see e.g. Vautherin (1973)):

$$E_p = -G\{\textstyle\sum_\nu U_\nu V_\nu\}^2 \tag{94}$$

One can write the energy functional, E as:

$$E[\phi_m, V_m^2] = \int \mathcal{H}(\vec{r})d^3r - G\{\textstyle\sum_\nu U_\nu V_\nu\}^2 \tag{95}$$

The term inside the integral is the Hamiltonian density related to the Skyrme interaction which is added to the pairing energy to constitute the total energy. To get the minimum total energy of the nuclear system, one will need the functional E to be stationary with respect to the variation of the single particle states ϕ_m and the occupation probability V_m^2. From this variational process, one will obtain two equations that will be solved iteratively (see Vautherin (1973)). The first one (Hartree-Fock equation) is similar to the one obtained without pairing interaction:

$$\left[-\vec{\nabla}\frac{\hbar^2}{2m_q^*(\vec{r})}\vec{\nabla} + U_q(\vec{r}) + \vec{W}_q(-i)(\vec{\nabla}\times\vec{\sigma})\right]\Phi_m = e_m\Phi_m \tag{96}$$

where the various terms of the Hartree-Fock equation have been defined earlier in terms of densities (91-93) including now V_m^2 probabilities. The second equation is related to the pairing interaction and is identical to the equation (80) above:

$$2\left(e_m - \lambda_{q_m}\right)\{V_m^2(1 - V_m^2)\}^{1/2} - \Delta(1 - 2V_m^2) = 0 \tag{97}$$

whose solution is the occupation probability (as we have seen):

$$V_m^2 = \frac{1}{2}\left[1 - \frac{e_m - \lambda_q}{\sqrt{\left(e_m - \lambda_q\right)^2 + \Delta^2}}\right] \tag{98}$$

With the inclusion of the BCS formalism, one has an additional loop inside the Hartree-Fock equation to calculate the occupation probability, V_m^2.

To recapitulate the calculation process, one first begins from a deformed harmonic oscillator approximation of the one-body potential solving for the energy and single particle wavefunction. One would then enter the BCS calculation loops from which the results would be the occupation probabilities that will be utilized in the next step for the calculation of the local densities. Subsequent calculation steps follow suit, as was described in the general method of solving the Hartree-Fock equation until convergence is achieved.