CHAPTER 3

METHODOLOGY

The present chapter shall deals with the procedures of solving the Hartree-Fock equations. In the first sub-section (3.1), the resulting eigenvalues and eigenfunctions obtained by solving the Hamiltonian with a deformed harmonic oscillator potential are briefly discussed. The basis parameters which are related to the deformed harmonic oscillator basis states are then introduced. These parameters will be optimised in the course of performing the calculation which will then be described. Section 3.2 will detail the calculation of the local densities from the eigenfunctions which are solutions to the deformed harmonic oscillator potential. The next section (3.3) will give the expression of the local densities as well as the scalar functions which are needed for the calculation of the Hartree-Fock equations which are written in terms of the well known Hermite and associated Laguerre polynomials. Subsequently, section 3.4 will describe the calculation of the matrix elements of the Hartree-Fock equations while section 3.5 presents the calculation of the matrix elements of Coulomb interaction starting from a Gaussian interaction. Finally, we shall conclude the present chapter with some notes on the pairing strength and pairing window of the BCS approach in Section 3.6.

3.1. OPTIMIZATION OF BASIS PARAMETERS

3.1.1. Solution to the deformed harmonic oscillator

As aforementioned, one needs an ansatz for the density in order to solve the Hartree-Fock equations. The densities can be calculated by approximating the one-body potential to be a deformed harmonic oscillator potential since most heavy nuclei tend to have a deformed shape except for some magic nuclei and around. By solving the static Schrodinger equation for the harmonic oscillator Hamiltonian, one would get the eigenvalues and their corresponding eigenfunctions necessary for the calculation of the local densities. The deformed potential in a Cartesian coordinate is written as:

$$V(x,y,z) = \frac{1}{2}m\omega_{\perp}^{2}x^{2} + \frac{1}{2}m\omega_{\perp}^{2}y^{2} + \frac{1}{2}m\omega_{z}^{2}z^{2} \tag{1}$$

which assumes that the nucleus has an axial symmetry along the z-direction. One can then transform the expression of V from Cartesian coordinates into cylindrical coordinates by introducing the radial part of the position as:

$$r^{2} = x^{2} + y^{2} \tag{2}$$

The potential is then written in the form of:

$$V(r,z) = \frac{1}{2}m\omega_{\perp}^{2}r^{2} + \frac{1}{2}m\omega_{z}^{2}z^{2} \tag{3}$$

Solving the static Schrodinger equation in a three dimensional space using the harmonic oscillator potential, one would obtain the solution for the total energy as:

$$E = \hbar\omega_{\perp}(n_{\perp} + 1) + \hbar\omega_{z}\left(n_{z} + \frac{1}{2}\right) \tag{4}$$

with $n_{\perp} = 2n_{r} + |\Lambda|$, Λ being the third component of the angular momentum. The label $n_{r}\ and\ n_{z}$ refers to the nodes in the radial and z- directions. The eigenfunction of the harmonic oscillator (see Vautherin (1973)):

$$\Psi_{n_r n_z \Lambda \Sigma}(r, z, \varphi) = \psi_{n_r}^{\Lambda}(r)\psi_{n_z}(z)\frac{e^{i\Lambda\varphi}}{\sqrt{2\pi}}\chi_{\Sigma}(\varphi) \tag{5}$$

is written as a separable function in the radial and z- direction. For the z- direction, the wavefunction is written in terms of Hermite polynomials, $H_{n_z}(\zeta)$:

$$\psi_{n_z}(z) = N_{n_z}\beta_z^{1/2}e^{-\zeta^2/2}H_{n_z}(\zeta) \tag{6}$$

while the radial part on the other hand is written in terms of associated Laguerre polynomial $L_{n_r}^{\Lambda}(\varpi)$ as:

$$\psi_{n_r}^{\Lambda}(r) = N_{n_r}^{\Lambda}\beta_{\perp}\sqrt{2}\varpi^{\Lambda/2}e^{-\varpi/2}L_{n_r}^{\Lambda}(\varpi) \tag{7}$$

The symbol ζ and ϖ are the "stretched" coordinates associated with the z-axis and radial parts given by the relation:

$$\zeta = z\beta_z \qquad\qquad \varpi = r^2\beta_{\perp}^2 \tag{8}$$

and $\beta_{\perp}$ and β_z are the oscillator constants defined by:

$$\beta_{\perp} = \left(\frac{m\omega_{\perp}}{\hbar}\right)^{\frac{1}{2}} \qquad , \ \beta_z = \left(\frac{m\omega_z}{\hbar}\right)^{\frac{1}{2}} \tag{9}$$

The normalization constants are given as:

$$N_{n_z} = \left(\frac{1}{\sqrt{\pi}2^{n_z}\, n_z!}\right)^{1/2} , N_{n_r}^{\Lambda} = \left(\frac{n_r!}{(n_r+\Lambda)!}\right)^{1/2} \tag{10}$$

3.1.2. Parameter β_0 and q

Having obtained the harmonic oscillator eigenfunction, one could then expand the neutron (or proton) single particle states in terms of this oscillator states such that:

$$\Phi_m(\vec{r},\sigma) = \sum_\alpha x_\alpha^m \Psi_\alpha(\vec{r},\sigma) \tag{11}$$

where α represents the set of quantum numbers, $\{n_r, n_z, \Lambda, \Sigma\}$ of the harmonic oscillator states. In principle, the expansion is carried out for the sum over all α. However, in performing the Hartree-Fock calculation, such expansion on the oscillator state is obviously truncated so that the sum is only taken up to a certain total number of nodes, N_0 (in the spherical case). An energy cut-off is imposed onto the total energy, E, so that (Flocard *et al.*, 1973):

$$\hbar\omega_\perp(n_\perp + 1) + \hbar\omega_z\left(n_z + \frac{1}{2}\right) \leq \hbar\omega_0(N_0 + 2) \tag{12}$$

with ω_0 corresponding to the angular frequency of a spherical nucleus and its relation to the other angular frequencies by:

$$\omega_0^3 = \omega_\perp^2\omega_z \tag{13}$$

with its corresponding oscillator parameter being:

$$\beta_0 = \left(\frac{m\omega_0}{\hbar}\right)^{\frac{1}{2}} \tag{14}$$

In performing the variational calculation, one needs to optimise the parameter β_0 for a given basis size, N_0. Optimization is made by varying and finding the value of the oscillator parameter which gives the lowest (most stable) total energy. As discussed earlier, when solving approximately (as in the Hartree Fock approach) the static Schrodinger equation by using the variational method, one obtains quite generally an energy eigenvalue that is higher than the real ground state energy. Therefore, a lower value of the total energy is always a better approximation to the ground state energy of the nucleus.

Another parameter which needs to be optimised is the deformation parameter, q given by (Flocard *et al.*, 1973):

$$q \equiv \frac{\omega_\perp}{\omega_z} = \frac{a_z}{a_\perp} \tag{15}$$

The symbol a_z and $a_\perp$ refers to the semi axes of the nucleus in the z- and radial direction respectively. As the name suggest, the deformation parameter gives an indication of the deviation of the nuclear shape from spherical point. For a spherical shape, the value of q is 1. An oblate shape has q<1 while for prolate, q > 1. Similar to the oscillator constant, one also needs to find the optimal value of the deformation parameter which gives the lowest total energy. The method described by Flocard *et al.* (1973) is used for the optimization of the parameter q. For an ellipsoidal liquid drop, the deformation parameter is related to the quadrupole moment by:

$$Q = \frac{2}{5} A r_0^2 q^{-2/3} (q^2 - 1)$$

with $r_0 = 1.2049A^{-1/3}$ fm. Using the curve of Q(q), one can then approximate the optimal value of the deformation parameter for a given quadrupole moment.

For calculations involving different types of nuclei, one first determines a sufficient basis size, N_0 by fixing the parameters β_0 and q for a particular nuclear shape while varying N_0. Figure 3.1 shows the ground state total energy obtained with different basis sizes for ^{208}Pb at spherical shape (q=1) and by fixing β_0=0.40. One can see a general trend of a decreasing total energy with the inclusion of larger basis size. By enlarging the basis size, one actually has a larger basis "area" in which to search for and thus increases the chances of obtaining a total energy similar or closer to the real ground state. In principle, one would prefer to work with a large basis size since it will give a more accurate result. However, performing such calculation requires extensive computational time especially if one were to work on very heavy nucleus. Moreover, in the present study, we are only interested with the variation of the energy e.g. deformation. Therefore, it would be sufficient to perform the calculation whereby the truncation effect is small compared to the order of magnitude of the results being considered. In Figure 3.1, the energy difference between N_0=12 and N_0=14 is much smaller as compared with what is obtained with the N_0=10 and N_0=12 calculation. Thus, further calculations will be carried out with N_0=12.

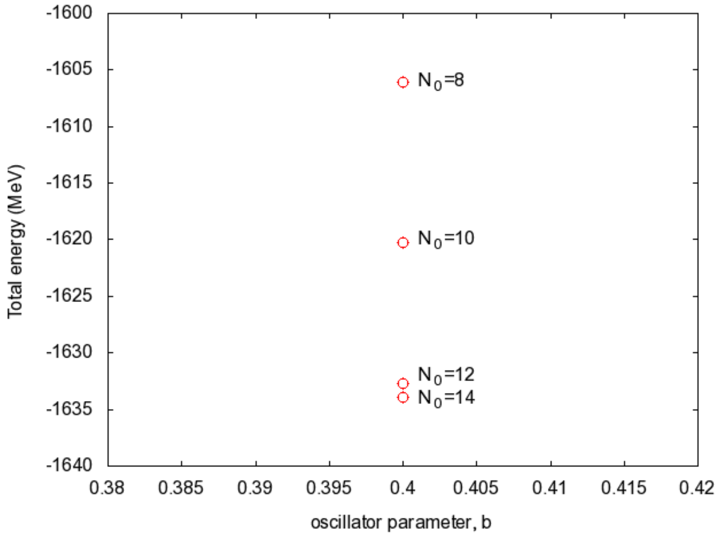

Figure 3.1: Optimization of basis size, N_0 with a fixed value of β_0.

After fixing the basis size, one then fix the parameter q to be 1 (when one is dealing with a spherical shape nucleus) while varying the value of parameter β_0. One then strives to obtain the minimal energy as a variation of β_0. One then takes for the optimal value of β_0 the one corresponding to the minimal total energy. Figure 3.2 shows an example for the optimization process of parameter β_0 for ^{208}Pb with N_0=12 (more details on optimization of β_0 and q in Flocard *et al.* (1973)).

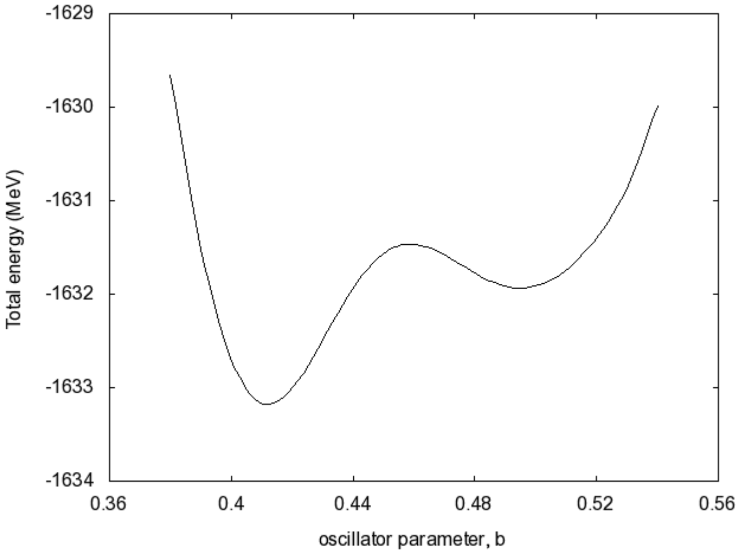

Figure 3.2: Optimization of oscillator parameter, β_0 by fixing N_0=12 and q=1.

3.2. Calculation of the local densities from the wavefunctions

Let us calculate the three local densities which will be needed to determine the one-body potential. These local densities are given in equations (91) to (93) of Chapter 2. Assuming that an even-even nucleus possesses an axial symmetry along the z- axis then the third component of the angular momentum, L_z is a good quantum number. Let Ω_m be the eigenvalue of the operator J_z for the state m. One then writes the neutron (or proton) single particle wavefunction in the cylindrical coordinate and spin coordinate, σ in the form of (Vautherin, 1973):

$$\Phi_m(\vec{r},\sigma,) = \Phi_m^+(r,z)e^{i\Lambda^-\varphi}\chi_{+1/2}(\sigma) + \Phi_m^-(r,z)e^{i\Lambda^+\varphi}\chi_{-1/2}(\sigma) \qquad (16)$$

with:

$$\Lambda^\pm = \Omega_m \pm \frac{1}{2} \qquad (17)$$

For the wavefunction in the spin coordinate (called spinor $\chi_{\pm\frac{1}{2}}$), the quantum number $+\frac{1}{2}$ and $-\frac{1}{2}$ represent a spin up and spin down nucleon state respectively. As can be seen, the wavefunction on the right hand side is sub-divided into two parts corresponding to the two spin quantum number values. As such, one can drop the summation over the spin state in the initial form of the equation for the nucleon density so that the neutron (or proton) density is now written in a more explicit form:

$$\rho(r,z) = \sum_m [|\Phi_m^+(r,z)|^2 + |\Phi_m^-(r,z)|^2] \qquad (18)$$

By writing the gradient operator in cylindrical coordinate:

$$\nabla_r = \frac{\partial}{\partial r} \quad , \quad \nabla_z = \frac{\partial}{\partial z} \quad , \quad \nabla_\varphi = \frac{1}{r}\frac{\partial}{\partial\varphi} = \frac{1}{r}\frac{i\hat{L}_z}{\hbar} \qquad (19)$$

one then have the expression for the kinetic energy density term as:

$$\tau(r,z) = \sum_m \Big(\left|\nabla_{\mathrm{r}}\Phi_m^+(r,z)\right|^2 + \left|\nabla_{\mathrm{r}}\Phi_m^-(r,z)\right|^2 + \frac{1}{r^2}\,|\,\Lambda^-\,\Phi_m^+(r,z)|^2$$

$$+\tfrac{1}{r^2}\,|\,\Lambda^+\,\Phi_m^-(r,z)|^2 + \left|\nabla_{\mathrm{z}}\Phi_m^+(r,z)\right|^2 + \left|\nabla_{\mathrm{z}}\Phi_m^-(r,z)\right|^2\Big) \tag{20}$$

The divergence of the spin-orbit density, div$\vec{J}$ can be obtained from the definition of the spin orbit density such that:

$$\mathrm{div}\vec{J} = (-i)\textstyle\sum_{m,\sigma,q} \vec{\nabla}\Phi_m^*(\vec{r},\sigma)\cdot\left(\vec{\nabla}\times\vec{\sigma}\right)\Phi_i(\vec{r},\sigma) \tag{21}$$

with $\vec{\sigma}$ being the spin operator. By writing the operator $\left(\vec{\nabla}\times\vec{\sigma}\right)$ as (Vautherin, 1973):

$$(-i)\left(\vec{\nabla}\times\vec{\sigma}\right)_r = \sigma_z\tfrac{\hat{L}_z}{r} + \tfrac{1}{2}\left(\sigma_+e^{-i\varphi} - \sigma_-e^{+i\varphi}\right)\nabla_z \tag{22}$$

$$(-i)\left(\vec{\nabla}\times\vec{\sigma}\right)_z = -\tfrac{1}{2}\sigma_+e^{-i\varphi}\left(\nabla_r + \tfrac{\hat{L}_z}{r}\right) + \tfrac{1}{2}\sigma_-e^{+i\varphi}\left(\nabla_r - \tfrac{\hat{L}_z}{r}\right) \tag{23}$$

$$\left(\vec{\nabla}\times\vec{\sigma}\right)_\varphi = \tfrac{1}{2}\left(\sigma_+e^{-i\varphi} - \sigma_-e^{+i\varphi}\right)\nabla_z - \sigma_z\nabla_r \tag{24}$$

and using the gradient operator in cylindrical coordinate as in equation (19), the divergence of the spin-orbit density can be written as:

$$\mathrm{div}\vec{J}(r,z) = 2\sum_m \big(\nabla_r\Phi_m^+(r,z)\nabla_z\Phi_m^-(r,z) - \nabla_r\Phi_m^-(r,z)\nabla_z + (r,z)$$

$$+\frac{\Lambda^-}{r}\Phi_m^+(r,z)[\nabla_r\Phi_m^+(r,z) - \nabla_z\Phi_m^-(r,z)]$$

$$-\tfrac{\Lambda^+}{r}\Phi_m^-(r,z)[\nabla_z\Phi_m^+(r,z) + \nabla_r\Phi_m^-(r,z)]\Big) \tag{25}$$

It is well known (Kramers degeneracy) that the time reversed state, $\Phi_{\bar{m}}$ of the single particle state Φ_m has the same single particle energy eigenvalue if one were to solve the Hartree-Fock equation with a time even HF Hamiltonian which is the case for an even-even nucleus. For such a nucleus, the Slater determinant is time-reversal invariant and thus the Hartree-Fock Hamiltonian also possesses the time reversal property. Following this time reversal invariance property, one can then calculate local densities for only the positive values of the third component of the total angular momentum, Ω_m and then multiply when summing over all single particle states the calculation results by 2 to account for the negative values of Ω_m.

3.3. Calculation of the scalar functions entering the Hartree-Fock equation

For the purpose of calculating the average one-body potential, U whose expression was given in equation (73) of Chapter 2, one would need to first calculate some scalar functions namely the nucleon density, kinetic energy density, div$\vec{J}(r,z)$ and $\nabla^2\rho(r,z)$ in coordinate space as the evaluation of the average potential is done in coordinate space as well. In order to calculate the first three functions, one would need the expression for $\Phi_m^{\pm}, \nabla_r\Phi_m^{\pm}$ and $\nabla_z\Phi_m^{\pm}$. The expression for $\Phi_m^{\pm}$ can be obtained directly from the expansion of the single particle states onto the harmonic oscillator wavefunction with x_α^m as the expansion coefficient (Vautherin, 1973):

$$\Phi_m^{\pm} = \left[\frac{\beta_z\beta_\perp^2 e^{-(\zeta^2+\varpi)}}{\pi}\right]^{1/2} \sum_\alpha x_\alpha^m \delta_{\Sigma,\pm\frac{1}{2}} \delta_{\Lambda,\Lambda^\mp} N_{n_z} N_{n_r}^\Lambda \varpi^{\Lambda/2} H_{n_z}(\zeta) L_{n_r}^\Lambda(\varpi) \qquad (26)$$

For the other two functions, one shall use the relations:

$$\nabla_r \psi_{n_r}^\Lambda(r) = N_{n_r}^\Lambda \beta_\perp^2 \sqrt{2}\varpi^{(\Lambda-1)/2} e^{-\varpi/2} \tilde{L}_{n_r}^\Lambda(\varpi) \qquad (27)$$

$$\nabla_z \psi_{n_z}(z) = N_{n_z} \beta_z^{3/2} e^{-\zeta^2/2} \widetilde{H}_{n_z}(\zeta) \tag{28}$$

In the equations above, the symbol $\tilde{L}_{n_r}^{\Lambda}(\varpi)$ and $\widetilde{H}_{n_z}(\zeta)$ of the associated Laguerre and Hermite polynomial are given by:

$$\widetilde{H}_{n_z}(\zeta) = \zeta H_{n_z}(\zeta) - H_{n_z+1}(\zeta) \tag{29}$$

$$\tilde{L}_{n_r}^{\Lambda}(\varpi) = 2(n_r + 1) L_{n_r}^{\Lambda}(\varpi) - (2n_r + \Lambda + 2 - \varpi) L_{n_r}^{\Lambda}(\varpi) \tag{30}$$

These two relations can be derived by using the general expression for the two considered types of polynomials. For the associated Laguerre polynomial, the general expressions are (Erdelyi, 1953):

$$(n_r + 1) L_{n_r+1}^{\Lambda}(\varpi) = (2n_r + \Lambda + 1 - \varpi) L_{n_r}^{\Lambda}(\varpi) - (n_r + \Lambda) L_{n_r-1}^{\Lambda}(\varpi) \tag{31}$$

$$\varpi \frac{dL_{n_r}^{\Lambda}(\varpi)}{d\varpi} = n_r L_{n_r}^{\Lambda}(\varpi) - (n_r + \Lambda) L_{n_r-1}^{\Lambda}(\varpi) \tag{32}$$

while the relations for Hermite polynomial are:

$$H_{n_z+1}(\zeta) = 2\zeta H_{n_z}(\zeta) - 2n_z H_{n_z-1}(\zeta) \tag{33}$$

$$\frac{dH_{n_z}(\zeta)}{d\zeta} = 2n_z H_{n_z-1}(\zeta) \tag{34}$$

One can then used the relations given above to obtain the divergence of the wavefunction in the radial and z- direction as given below:

$$\nabla_r \Phi_m^{\pm} = \left[\frac{\beta_z \beta_\perp^4 e^{-(\zeta^2+\varpi)}}{\pi}\right]^{1/2} \sum_\alpha x_\alpha^m \delta_{\Sigma,\pm\frac{1}{2}} \delta_{\Lambda,\Lambda^{\mp}} N_{n_z} N_{n_r}^{\Lambda} \varpi^{(\Lambda-1)/2} H_{n_z}(\zeta) L_{n_r}^{\Lambda}(\varpi) \tag{35}$$

$$\nabla_z \Phi_m^{\pm} = \left[\frac{\beta_z^3 \beta_\perp^2 e^{-(\zeta^2+\varpi)}}{\pi}\right]^{1/2} \sum_\alpha x_\alpha^m \delta_{\Sigma,\pm\frac{1}{2}} \delta_{\Lambda,\Lambda^{\mp}} N_{n_z} N_{n_r}^{\Lambda} \varpi^{\Lambda/2} \widetilde{H}_{n_z}(\zeta) L_{n_r}^{\Lambda}(\varpi) \tag{36}$$

Finally, the function $\nabla^2 \rho(r,z)$ can be evaluated using the relation:

$$\begin{aligned}\nabla^2 \rho(r,z) &= 2\tau(r,z) + 2\sum_m (\Phi_m^* \nabla^2 \Phi_m) \\ &= 2\tau(r,z) + 4\sum_m \left\{\Phi_m^+(r,z)\left[\nabla^2 - \frac{(\Lambda^-)^2}{r^2}\right]\Phi_m^+(r,z)\right. \\ &\quad \left. + \Phi_m^-(r,z)\left[\nabla^2 - \frac{(\Lambda^+)^2}{r^2}\right]\Phi_m^-(r,z)\right\}\end{aligned} \tag{37}$$

The operator $\left[\nabla^2 - \frac{(\Lambda^{\pm})^2}{r^2}\right]$ is to act as (Vautherin, 1973):

$$\begin{aligned}\left[\nabla^2 - \frac{(\Lambda^-)^2}{r^2}\right]\Phi_m^+(r,z) &= \left[\frac{\beta_z \beta_\perp^2 e^{-(\zeta^2+\varpi)}}{\pi}\right]^{1/2} \sum_\alpha x_\alpha^m \delta_{\Sigma,\pm\frac{1}{2}} \delta_{\Lambda,\Lambda^{\mp}} N_{n_z} N_{n_r}^{\Lambda} \\ &\quad \times \left[\beta_z^2 \zeta^2 + \beta_\perp^2 \varpi - 2\beta_z^2\left(n_z + \frac{1}{2}\right)\right. \\ &\quad \left. - 2\beta_z^2(2n_r + |\Lambda| + 1)\right] \varpi^{\Lambda/2} H_{n_z}(\zeta) L_{n_r}^{\Lambda}(\varpi)\end{aligned} \tag{38}$$

Using these relations as well as the notation for the density matrix whereby taking into account the occupation probability, V_m^2 of the single particle states:

$$\rho_{\alpha\beta} = 2\sum_{m>0} V_m^2 \left(x_\beta^m\right)^* (x_\alpha^m) \tag{39}$$

one can then obtain the final expression for all the four functions discussed thus far:

$$\rho(r,z) = \frac{\beta_z \beta_\perp^2 e^{-(\zeta^2+\varpi)}}{\pi} \sum_{\alpha\beta} \rho_{\alpha\beta} \delta_{\Sigma,\Sigma'} N_{n_z} N_{n_z'} N_{n_r}^{\Lambda} N_{n_r'}^{\Lambda'} \varpi^{\Lambda} H_{n_z}(\zeta) H_{n_z'}(\zeta) L_{n_r}^{\Lambda}(\varpi) L_{n_r'}^{\Lambda'}(\varpi) \tag{40}$$

$$\begin{aligned} \tau(r,z) = {} & \frac{\beta_z \beta_\perp^2 e^{-(\zeta^2+\varpi)}}{\pi} \sum_{\alpha\beta} \rho_{\alpha\beta} \delta_{\Sigma,\Sigma'} N_{n_z} N_{n_z'} N_{n_r}^{\Lambda} N_{n_r'}^{\Lambda'} \varpi^{\Lambda-1} \\ & \times \Big[\varpi b_z^2 \widetilde{H}_{n_z}(\zeta) \widetilde{H}_{n_z'}(\zeta) L_{n_r}^{\Lambda}(\varpi) L_{n_r'}^{\Lambda'}(\varpi) \\ & + \beta_\perp^2 H_{n_z}(\zeta) H_{n_z'}(\zeta) \left[\tilde{L}_{n_r}^{\Lambda}(\varpi) \tilde{L}_{n_r'}^{\Lambda'}(\varpi) + \Lambda\Lambda' L_{n_r}^{\Lambda}(\varpi) L_{n_r'}^{\Lambda'}(\varpi) \right] \Big] \end{aligned} \tag{41}$$

$$\begin{aligned} \nabla^2 \rho(r,z) = {} & 2\tau(r,z) + 2 \frac{\beta_z \beta_\perp^2 e^{-(\zeta^2+\varpi)}}{\pi} \sum_{\alpha\beta} \rho_{\alpha\beta} \delta_{\Sigma,\Sigma'} N_{n_z} N_{n_z'} N_{n_r}^{\Lambda} N_{n_r'}^{\Lambda'} \varpi^{\Lambda} \\ & \times \left[\beta_z^2 \zeta^2 + \beta_\perp^2 \varpi - 2\beta_z^2 \left(n_z + \frac{1}{2} \right) - 2\beta_\perp^2 (2n_r + |\Lambda| + 1) \right] \\ & \times H_{n_z}(\zeta) H_{n_z'}(\zeta) L_{n_r}^{\Lambda}(\varpi) L_{n_r'}^{\Lambda'}(\varpi) \end{aligned} \tag{42}$$

$$\begin{aligned} \mathrm{div}\vec{J}(r,z) = {} & 2 \frac{\beta_z \beta_\perp^2 e^{-(\zeta^2+\varpi)}}{\pi} \sum_{\alpha\beta} \rho_{\alpha\beta}\, \varpi^{\Lambda+\Lambda'-1}\, N_{n_z} N_{n_z'} N_{n_r}^{\Lambda} N_{n_r'}^{\Lambda'} \\ & \times \Big[(\Sigma - \Sigma') H_{n_z}(\zeta) \widetilde{H}_{n_z'}(\zeta) \tilde{L}_{n_r}^{\Lambda}(\varpi) L_{n_r'}^{\Lambda'}(\varpi) \\ & - |\Sigma - \Sigma'| \Lambda H_{n_z}(\zeta) \widetilde{H}_{n_z'}(\zeta) L_{n_r}^{\Lambda}(\varpi) L_{n_r'}^{\Lambda'}(\varpi) \\ & + 2\delta_{\Sigma,\Sigma'} \frac{\beta_\perp}{\beta_z} \Lambda\Sigma H_{n_z}(\zeta) H_{n_z'}(\zeta) L_{n_r}^{\Lambda}(\varpi) \tilde{L}_{n_r'}^{\Lambda'}(\varpi) \varpi^{-1/2} \Big] \end{aligned} \tag{43}$$

3.4. Calculation of the matrix elements in Hartree-Fock equations

Having obtained the expressions for the single particle wavefunctions and consequently the three local densities, one can then solve the Hartree-Fock equation by calculating the matrix elements of the single particle Hamiltonian, H_{SP} given by:

$$H_{SP} = -\vec{\nabla}\frac{\hbar^2}{2m_q^*}\vec{\nabla} + U_q(\vec{r}) + \vec{W}_q(-i)\big(\vec{\nabla} \times \vec{\sigma}\big) \tag{44}$$

The terms on the left hand side correspond to the single particle kinetic energy term, one-body potential term and the spin-orbit term respectively and they in turn, depends on the Skyrme parameters as well as the three local densities (see Chapter 2). To obtain the single particle energy, e_m, one shall take the expectation value of the single particle Hamiltonian with respect to the single particle states which are expanded on the deformed harmonic oscillator basis state. The expectation value of the single particle Hamiltonian, H_{SP} in the deformed harmonic oscillator basis state, α (with $\alpha \equiv \{n_r, n_z, \Lambda, \Sigma\}$) can be written as:

$$\textstyle\sum_{\alpha\beta}\langle\alpha|H_{SP}|\beta\rangle\, x_\alpha^{m*} x_\beta^m = \sum_\alpha e_m\, |x_\alpha^m|^2 \tag{45}$$

with:

$$\langle\alpha|H_{SP}|\beta\rangle = \left\langle\alpha\middle|-\vec{\nabla}\frac{\hbar^2}{2m_q^*}\vec{\nabla} + U_q(\vec{r}) + \vec{W}_q(-i)\big(\vec{\nabla} \times \vec{\sigma}\big)\middle|\beta\right\rangle \tag{46}$$

The first term on the right hand side being a kind of kinetic energy term can be written after integration by parts as:

$$\left\langle\alpha\middle|-\vec{\nabla}\frac{\hbar^2}{2m_q^*}\vec{\nabla}\middle|\beta\right\rangle = \textstyle\sum_\sigma \int d^3\vec{r}\, \frac{\hbar^2}{2m_q^*(r,z)} \nabla\Psi_\alpha^*(\vec{r},\sigma)\nabla\Psi_\beta(\vec{r},\sigma) \tag{47}$$

where $\Psi_\beta(\vec{r},\sigma) = \langle(\vec{r},\sigma)|\beta\rangle$ is the axially deformed harmonic oscillator wavefunction. By writing the gradient operator in cylindrical coordinate and using the expression of the harmonic oscillator wavefunctions given in equation (6) and (7), the expectation value of the kinetic energy term was shown to be (Vautherin, 1973):

$$\begin{aligned}\left\langle\alpha\left|-\vec{\nabla}\frac{\hbar^2}{2m_q^*}\vec{\nabla}\right|\beta\right\rangle = {} & \delta_{\Lambda\Lambda'}\delta_{\Sigma\Sigma'}N_{n_z}N_{n_z'}N_{n_r}^{\Lambda}N_{n_r'}^{\Lambda'}\int_0^\infty d\varpi\,\varpi^{\Lambda-1}\,e^{-\varpi}\int_{-\infty}^{\infty}e^{-\zeta^2}d\,\zeta \\ & \times\left\{\beta_z^2\widetilde{H}_{n_z}(\zeta)\widetilde{H}_{n_z'}(\zeta)L_{n_r}^{\Lambda}(\varpi)L_{n_r'}^{\Lambda'}(\varpi)\,\varpi+\beta_\perp^2H_{n_z}(\zeta)H_{n_z'}(\zeta)\right. \\ & \left.\times\left[\tilde{L}_{n_r}^{\Lambda}(\varpi)\tilde{L}_{n_r'}^{\Lambda'}(\varpi)+\Lambda\Lambda' L_{n_r}^{\Lambda}(\varpi)L_{n_r'}^{\Lambda'}(\varpi)\right]\right\}\frac{\hbar^2}{2m_q^*\left(\beta_\perp^{-1}\varpi^{1/2},\beta_z^{-1}\zeta\right)}\end{aligned}\tag{48}$$

The relations for $\widetilde{H}_{n_z}(\zeta)$ and $\tilde{L}_{n_r}^{\Lambda}(\varpi)$ are given in equations (29) and (30) while the oscillator constants in the perpendicular and z-direction are given in equation (9). The matrix element of the one-body central is written as (see Vautherin (1973)):

$$\begin{aligned}\langle\alpha|U|\beta\rangle = {} & \delta_{\Lambda\Lambda'}\delta_{\Sigma\Sigma'}N_{n_z}N_{n_z'}N_{n_r}^{\Lambda}N_{n_r'}^{\Lambda'}\int_0^\infty d\varpi\,\varpi^{\Lambda}\,e^{-\varpi} \\ & \times\int_{-\infty}^{\infty}e^{-\zeta^2}d\,\zeta\;H_{n_z}(\zeta)H_{n_z'}(\zeta)L_{n_r}^{\Lambda}(\varpi)L_{n_r'}^{\Lambda'}(\varpi)U\left(\beta_\perp^{-1}\varpi^{1/2},\beta_z^{-1}\zeta\right)\end{aligned}\tag{49}$$

while the spin-orbit term is:

$$\begin{aligned}\left\langle\alpha\left|\overrightarrow{W}_q(-i)\left(\vec{\nabla}\times\vec{\sigma}\right)\right|\beta\right\rangle = {} & N_{n_z}N_{n_z'}N_{n_r}^{\Lambda}N_{n_r'}^{\Lambda'}\int_{-\infty}^{\infty}e^{-\zeta^2}d\,\zeta\;\int_0^\infty e^{-\varpi}\varpi^{(\Lambda+\Lambda'-2)/2}d\varpi \\ & \times\{-2\delta_{\Sigma\Sigma'}\delta_{\Lambda\Lambda'}\Lambda\Sigma\beta_\perp^2H_{n_z}(\zeta)H_{n_z'}(\zeta)\left[\tilde{L}_{n_r}^{\Lambda}(\varpi)L_{n_r'}^{\Lambda'}(\varpi)\right. \\ & \left.+L_{n_r}^{\Lambda}(\varpi)\tilde{L}_{n_r'}^{\Lambda'}(\varpi)\right]+(1-\delta_{\Sigma\Sigma'})\beta_\perp\beta_z\varpi^{1/2} \\ & \times\left\{\widetilde{H}_{n_z}(\zeta)H_{n_z'}(\zeta)L_{n_r}^{\Lambda}(\varpi)\left[(\Lambda'-\Lambda)\tilde{L}_{n_r'}^{\Lambda'}(\varpi)+\Lambda' L_{n_r'}^{\Lambda'}(\varpi)\right]\right. \\ & \left.+\widetilde{H}_{n_z}(\zeta)H_{n_z'}(\zeta)L_{n_r'}^{\Lambda'}(\varpi)\left[(\Lambda'-\Lambda)\tilde{L}_{n_r}^{\Lambda}(\varpi)+\Lambda L_{n_r}^{\Lambda}\right]\right\}\} \\ & \times W\left(\beta_\perp^{-1}\varpi^{1/2},\beta_z^{-1}\zeta\right)\end{aligned}\tag{50}$$

Numerical calculation of the integration in equations (48) to (50) are carried out using the Gauss-Hermite and Gauss-Laguerre quadrature formulas. The Gauss-Hermite quadrature formula for an integration of a function $e^{-\zeta^2} f(\zeta)$ is given as (see e.g. Abramowitz and Stegun (1972)):

$$\int_{-\infty}^{\infty} e^{-\zeta^2} f(\zeta)\, dx \approx \sum_{i=1}^{n} \omega_i\, f(\zeta_i) \tag{51}$$

where ζ_i is the i^{th} zeros of the Hermite polynomial, $H_n(\zeta_i)$ and ω_i refers to its associated weight given by the relation:

$$\omega_i = \frac{2^{(n-1)} n! \sqrt{\pi}}{n^2 [H_{n-1}(\zeta_i)]^2} \tag{52}$$

The index n represents the number of points used to approximate the integration. The calculation for the present study uses 50 Gauss-Hermite points.

On the other hand, the formula for the integration of a function $e^{-\varpi} f(\varpi)$ using the Gauss-Laguerre quadrature is given as (see e.g. Abramowitz and Stegun (1972)):

$$\int_{0}^{\infty} e^{-\varpi} f(\varpi) \approx \sum_{i=1}^{n} \eta_i\, f(\varpi_i) \tag{53}$$

where ϖ_i is the i^{th} zeros of the associated Laguerre polynomial, $L_n^{\Lambda}(\varpi_i)$ while its corresponding weight is denoted here by η_{i} with the relation:

$$\eta_i = \frac{(n!)^2 \varpi_i}{(n+1)^2 \left[L_{n+1}^{\Lambda}(\varpi_i)\right]^2} \tag{54}$$

The index n is similar to the Gauss-Hermite case, referring to the number of integration points which is taken to be 16 in present calculations.

3.5. Calculation of Coulomb matrix elements

In an earlier work, Quentin proposed to calculate analytically the matrix elements of Coulomb interaction starting from Gaussian matrix elements (Quentin, 1972). The matrix elements were evaluated in a deformed basis state which consists of the eigenvectors of an axially deformed harmonic oscillator Hamiltonian which is indeed the one used in the present study. In the discussion below, we shall briefly look at final expression of the Gaussian matrix element derived in Quentin (1972) and relate the Coulomb interaction and the Gaussian interaction. Having established the relation between the two interactions, one could then obtain the matrix elements of the former interaction in terms of the latter. Finally, the recursion relations of an integral necessary to evaluate the Coulomb matrix elements are presented.

3.5.1. Matrix element of Gaussian interaction

For a Gaussian interaction given by:

$$V_{12} = \frac{1}{\sigma^3} e^{-r^2/\sigma^2} \tag{55}$$

Quentin showed that the total matrix element of a Gaussian interaction can be written as (Quentin, 1972):

$$\left\langle 12 \left| \frac{e^{-r^2/\sigma^2}}{\sigma^3} \right| 34 \right\rangle = \beta_0^3 \left[\sum_n f^n \sum_p C(n, n', p)\, A(p) \left(\frac{1}{\sqrt{1+\beta_z^2 \sigma^2}} \right)^{p+1} \right] \left(\sum_{a,b} g^{a,b}\, W_{a,b,a',b'}^{\beta_\perp, \sigma} \right) \tag{56}$$

whereby $\beta_0 = \sqrt{\frac{m\omega_0}{\hbar}}$ is the spherical harmonic oscillator constant with $\omega_0^3 = \omega_\perp^2\omega_z$. The symbol $\omega_\perp$ and ω_z denote the angular frequency in the perpendicular plane and z-direction respectively. The integers on the left hand side represent the set of quantum numbers $\left\{n_{z_\eta}, \alpha_\eta, \beta_\eta\right\}$ of the nucleon state, η with $\eta = 1,2,3,4$. The quantum number n_z denotes the number of nodes in the z- direction while α and β are related to the number of nodes in the perpendicular direction, $n_\perp$ and the third component of the angular momentum, Λ by:

$$\alpha = \frac{n_\perp + \Lambda}{2} \qquad \beta = \frac{n_\perp - \Lambda}{2} \tag{57}$$

The function f and g are given as:

$$f^n \equiv f^n(n_1, n_2, n_3, n_4) = \langle n_1 n_2 | nN \rangle \langle n_3 n_4 | n'N \rangle \tag{58}$$

$$g^{a,b} = g^{a,b}(\alpha_1, \beta_1, \alpha_2, \beta_2, \alpha_3, \beta_3, \alpha_4, \beta_4) = \langle \alpha_1 \alpha_2 | aA \rangle \langle \beta_1 \beta_2 | bB \rangle \langle \alpha_3 \alpha_4 | a'A \rangle \langle \beta_3 \beta_4 | b'B \rangle \tag{59}$$

The brackets on the right hand side of both equations (58) and (59) are called the Moshinsky coeffiecients with the particle states denoted by the quantum numbers for example n_1, n_2 (or α_1, α_2 and β_1, β_2) are being written in coordinate $\vec{r}_1$ and $\vec{r}_2$ respectively while the symbol n, N (or a, A and b, B) denotes particle states in the relative coordinate, $\vec{r}$ and "center of mass coordinate", $\vec{R}$:

$$\vec{r} = \frac{\vec{r}_1 - \vec{r}_2}{\sqrt{2}} \quad , \quad \vec{R} = \frac{\vec{r}_1 + \vec{r}_2}{\sqrt{2}} \tag{60}$$

The Moshinsky coefficients, $\langle n_1 n_2 | nN \rangle$, $\langle \alpha_1 \alpha_2 | aA \rangle$ and $\langle \beta_1 \beta_2 | bB \rangle$ are calculated by the relation below (which is written for the $\langle n_1 n_2 | nN \rangle$ case but nevertheless the same for the other two transformation brackets with a change of notation) (see e.g. Quentin (1972)):

$$\langle n_1 n_2 | nN \rangle = \delta_{n_1+n_2,n+N} \sqrt{\frac{n_1! n_2! n! N!}{2^{n_1+n_2}}} \sum_{l=\max(0,n_2-N)}^{min(n_2,n)} \frac{(-)^l}{(n_2-l)!(N-n_2+l)!l!(n-l)!} \tag{61}$$

The coefficients A(n), C(n,n',p) and $W^{\beta_\perp,\sigma}_{a,b,a',b'}$ are given as:

$$A(n) = \delta_{n,even} \frac{(-)^{n/2}\sqrt{n!}}{2^{n/2}\left(\frac{n}{2}\right)!} \tag{62}$$

$$C(n,n',p) = \frac{\sqrt{n!\, n'! p!}}{\left[\frac{n+n'-p}{2}\right]! \left[\frac{n'+p-n}{2}\right]! \left[\frac{p+n-n'}{2}\right]!} \tag{63}$$

$$W^{\beta_\perp,\sigma}_{a,b,a',b'}$$

$$= \delta_{a-b,a'-b'} \frac{(\beta_\perp \sigma)^{2|a-b|}}{\left(1+\beta_z^2\sigma^2\right)^{(a+a'+b+b')/2}} \frac{\left[\left(a+a'+b+b'\right)/2\right]!}{\sqrt{a!a'!b!b'!}} \sum_{k=0}^{\min(b,b')} (\beta_z^4 \sigma^4)^k \frac{C_b^k C_{b'}^k}{C^k_{(a+a'+b+b')/2}} \tag{64}$$

in which C_b^k is the binomial expansion coefficient while $\beta_\perp$ and β_z are the oscillator constants with the relation $\beta_i = \sqrt{\frac{m\omega_i}{\hbar}} \qquad i = z, \perp.$

3.5.2. Gaussian function and relation to the Coulomb interaction

The Yukawa interaction can be written in an integral representation in terms of the Gaussian interaction by:

$$\frac{e^{-\mu|r_1-r_2|}}{|\vec{r}_1-\vec{r}_2|} = \sqrt{\frac{2}{\pi}} \int_0^\infty e^{-\mu^2\sigma^2/2} \frac{1}{\sigma^3} e^{-r^2/\sigma^2}\, \sigma\, d\sigma \tag{65}$$

The Coulomb interaction in $\mu = 0$ limit of the Yukawa interaction so that one has:

$$\frac{1}{|\vec{r}_1-\vec{r}_2|} = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \frac{1}{\sigma^3} e^{-r^2/\sigma^2} \ \sigma \, d\sigma \tag{66}$$

3.5.3. Matrix element of Coulomb interaction from a Gaussian interaction

Taking the expectation value of the Coulomb interaction with respect to the particle states, we have:

$$\left\langle 12 \middle| \frac{1}{|\vec{r}_1-\vec{r}_2|} \middle| 34 \right\rangle = \sqrt{\frac{2}{\pi}} \int_0^{\infty} \ \left\langle 12 \middle| \frac{1}{\sigma^3} e^{-r^2/\sigma^2} \middle| 34 \right\rangle \sigma \, d\sigma \tag{67}$$

The term inside the bracket on the right hand side is exactly the expression shown in equation (56). Inserting the expression into equation (67) above and after some rearrangement of the terms, one can then write the expression above in terms of an integral I, such that:

$$\left\langle 12 \middle| \frac{1}{|\vec{r}_1-\vec{r}_2|} \middle| 34 \right\rangle = \sqrt{\frac{2}{\pi}} \beta_0^3 \sum_n f^n \sum_p C(n, n', p) \, A(p) \sum_{a,b} g^{a,b} \, \delta_{a-b,a'-b'}$$

$$\frac{[(a+a'+b+b')/2]!}{\sqrt{a!a'!b!b'!}} \sum_{k=0}^{\min(b,b')} \frac{C_b^k C_{b'}^k}{C_{(a+a'+b+b')/2}^k} I^{\beta_z,\beta_\perp}_{\frac{p}{2},|a-b|,k,(a+a'+b+b'+2+2k)/2} \tag{68}$$

where the integral I was defined as:

$$I^{\beta_z,\beta_\perp}_{q,l,m,n} = \int_0^{\infty} \sigma \, d\sigma \ \frac{\left(\beta_z^2\sigma^2\right)^l \left(\beta_z^2\sigma^2-1\right)^m}{\left(1+\beta_z^2\sigma^2\right)^n \sqrt{1+\beta_z^2\sigma^2}^{\,2q+1}} \tag{69}$$

with restrictions on the integers q, l, m and n to be positive numbers and $l + m \leq n - 1$. By introducing the deformation parameter denoted as $\alpha = \frac{\omega_z}{\omega_\perp}$, the integral I can then be written as:

$$I_{q,l,m,n}^{\beta_z,\beta_\perp} = \frac{\alpha^{n-l-m}(-)^{m+l}}{\beta_z^2} \sum_{i,j} C_l^i C_m^j (-)^{i+j} (1+\alpha)^{m-j} \int_1^\infty \frac{u^{2(i+j-q)}}{(u^2+\alpha-1)^n} du \tag{70}$$

3.5.4. Calculation of the J integral from recurrence relations

To obtain the value for the integral I, one will need to evaluate the terms inside integral on the right hand side of equation (70). This is done by taking:

$$\int_1^\infty \frac{u^{2(i+j-q)}}{(u^2+\alpha-1)^n} du = \delta^{2(i+j-q-n)+1} J_{i+j-q,n}^{\varepsilon} \tag{71}$$

with:

$$J_{m,n}^{\varepsilon}(\delta) = \int_{1/\delta}^\infty \frac{u^{2m}}{(u^2-\varepsilon)^n} du \tag{72}$$

There are two types of deformations to be considered in evaluating this integral. There are the prolate shape (α<1) and oblate shape (α>1). At the same time, we have the relation, $\alpha - 1 = -\varepsilon\delta^2$ so that for a prolate shape, $\varepsilon = 1$ while for an oblate shape, $\varepsilon = -1$. The following recursion relations for the integral J may be used. They are given for different range of m values as (Quentin, 1972):

$$m > 0; \quad J_{m,n}^{\varepsilon}(\delta) = \frac{1}{2n-2m-1} \frac{\delta^{2n-2m-1}}{(1-\varepsilon\delta^2)^{n-1}} - \varepsilon \frac{2m-1}{2n-2m-1} J_{m-1,n}^{\varepsilon}(\delta) \tag{73}$$

$$m < 0; \quad J_{m,n}^{\varepsilon}(\delta) = \frac{\varepsilon}{2m+1} \frac{\delta^{2n-2m-3}}{(1-\varepsilon\delta^2)^{n-1}} - \varepsilon \frac{2n-2m-3}{2m+1} J_{m+1,n}^{\varepsilon}(\delta) \tag{74}$$

$$m = 0; \quad J_{0,n}^{\varepsilon}(\delta) = \frac{\varepsilon}{2n-2}\frac{\delta^{2n-3}}{(1-\varepsilon\delta^2)^{n-1}} - \varepsilon\frac{2n-3}{2n-2}J_{0,n-1}^{\varepsilon}(\delta) \tag{75}$$

The numerical stability of these recurrence relations has to be checked. In some cases (Bloas, 2010) one prefers instead to use some direct integration after some relevant changes of integration variables.

3.6. Pairing strengths and the pairing window

For each charge state q, the pairing matrix elements are given in terms of an adjustable parameter G_q by (Bonneau, Quentin and Samsoen, 2004):

$$\langle i\bar{i}|V|j\bar{j}\rangle_q = -\frac{G_q}{11+N_q}\ (MeV) \tag{76}$$

where G_n and G_p is the pairing strength parameter for neutrons and protons respectively while N_q is the number of nucleons of charge q within the pairing single particle active space. For the present study, the pairing active space (or pairing window) is taken from the lowest single particle energy state up to some states above the Fermi level λ, defined as $\lambda + X$ where X is an adjustable value. Instead of a sharp cut-off for energy levels outside the pairing window, a diffuse cut-off of the order of 0.2 MeV is used in the present work (see e.g. Bender, Heenen and Reinhard (2003)).