CHAPTER III

HARTREE-FOCK FORMALISM AND CENTRE-OF-MASS MOTION

III.0 Introduction

The basic idea of the Hartree-Fock (HF) formalism is to obtain an average potential in which every nucleon moves independently of each other. This average field is generated by the interaction of a nucleon with all other nucleons. This average potential provides connection with the one-body potential used in the shell-model. HF formalism is applied to nuclear problems to obtain approximate ground state and excited state wave functions of nuclei, which are single Slater determinants.

It is well-known that 2s-1d and 1p shell nuclei show rotational spectra, though not so pronounced as in heavy deformed ones. These states can be interpreted in terms of rotating deformed intrinsic states of the nuclei. The HF formalism provides a means to study deformations in nuclei[2]. HF calculations assuming spherical symmetry obviously can not give any information about the deformation in nuclei. Deformed HF calculations on the other hand involving axial symmetry or ellipsoidal symmetry give rise to deformed intrinsic HF solutions. Solutions with axial symmetry describe the shapes of the nuclei as spheroidal ones and the projection of good angular momentum states from intrinsic

states gives rise to collective rotational spectra in nuclei. The single particle orbitals obtained with HF calculations involving axial symmetry in fact correspond to the orbitals obtained in the deformed shell model of Nilsson.[5]

The first deformed HF calculations were reported by Kelson[3] to explain the collective rotational spectra of some 2s-1d shell nuclei. HF formalism has been successfully applied(Refs: 1-4 and 10-12) to study the problems involving nuclear structure when the pairing forces between the nucleons are not important. If the energy gap between the lowest unoccupied and the highest occupied single particle states is large (as is the case for A=4n nuclei), the pairing is not important. For the nuclei we have undertaken to study, i.e., the nuclei in the 1p shell and the 2s-1d shell; pairing is not important and so the HF formalism can be successfully employed.

We shall briefly review the HF formalism in this chapter. We shall then study the implications of the centre-of-mass motion in the HF theory. In this chapter, we shall restrict ourselves only to density independent effective interactions. We shall employ Sussex[6] and the density independent Skyrme variant SV[7]. We shall study the nuclei ^{8}Li, ^{8}Be, ^{8}B, ^{12}C, ^{16}O and ^{20}Ne. We shall be concerned only with the intrinsic properties of the nuclei in this chapter. We shall study the intrinsic properties

and the spectroscopic properties employing density dependent forces in later chapters.

III.1 Hartree-Fock Formalism

The Hamiltonian can be written as

$$H = \sum_{\alpha\beta} \langle\alpha|t|\beta\rangle\, a_\alpha^\dagger a_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} \langle\alpha\gamma|v|\beta\delta\rangle\, a_\alpha^\dagger a_\gamma^\dagger a_\delta a_\beta \qquad \text{III(1)}$$

where t is the kinetic energy operator and V denotes the two-body interaction.

Here $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots$ etc. denote the basis states $|n_\alpha\ l_\alpha\ j_\alpha\ m_\alpha, \tau_\alpha\rangle$ etc; n_α is the radial quantum number, l_α and j_α are orbital and total angular momenta respectively, m_α is the projection on symmetry axis of j_α and τ_α is the isospin projection quantum number distinguishing between a proton and a neutron for a single nucleon wave-function. $a_\alpha^+ (a_\alpha)$ is the creation (annihilation) operator of the single nucleon state $|\alpha\rangle$. These operators obey the following anticommutation relations since we are dealing with Fermions;

$$[a_\alpha, a_\beta^\dagger]_+ = a_\alpha a_\beta^\dagger + a_\beta a_\alpha^\dagger = \delta_{\alpha\beta}$$

$$[a_\alpha^\dagger, a_\beta^\dagger]_+ = [a_\alpha, a_\beta]_+ = 0 \qquad \text{III(2)}$$

Now consider a unitary transformation C on the basis operators as shown below:

$$a_i^+ = \sum_\alpha C_\alpha^i a_\alpha^+$$
$$a_i = \sum_\alpha C_\alpha^{i*} a_\alpha \qquad \text{III(3)}$$

We now construct an A particle state

$$|\phi\rangle = \prod_{i=1}^{A} a_i^+ |0\rangle \qquad \text{III(4)}$$

so that

$$E = \langle\phi|H|\phi\rangle \qquad \text{III(5)}$$

is a minimum for any variation of the unitary transformation C. It follows that the creation (annihilation) operators $a_i^+(a_i)$ of the "deformed" basis obey the same anticommutation relations as in III(2), i.e.

$$[a_i, a_j^+]_+ = a_i a_j^+ + a_j^+ a_i = \delta_{ij}$$
$$[a_i^+, a_j^+]_+ = [a_i, a_j]_+ = 0$$

This implies that

$$\langle\phi|\phi\rangle = 1$$

The Hamiltonian H can be written in the new basis as,

$$H = \sum_{ij} \langle i|t|j\rangle a_i^\dagger a_j + \frac{1}{2} \sum_{ijkl} \langle ik|V|jl\rangle a_i^\dagger a_k^\dagger a_l a_j \qquad \text{III(6)}$$

The kinetic energy and the potential energy matrix elements can be expressed as,

$$\langle i|t|j\rangle = \sum_{\alpha\beta} \langle\alpha|t|\beta\rangle \, C_\alpha^{i*} C_\beta^{j} \qquad \text{III(7a)}$$

$$\langle ik|V|jl\rangle = \sum_{\alpha\beta\gamma\delta} \langle\alpha\gamma|V|\beta\delta\rangle C_\alpha^{i*} C_\gamma^{k*} C_\beta^{j} C_\delta^{l} \qquad \text{III(7b)}$$

The total energy for a nucleus with A particles is given by

$$\langle \phi|H|\phi\rangle = \sum_{i=1}^{A} \langle i|t|i\rangle + \frac{1}{2} \sum_{ij}^{A} \langle ij|\tilde{V}|ij\rangle \qquad \text{III(8)}$$

where tilde denotes the antisymmetrized matrix element of the two-body interaction,

$$\langle ij|\tilde{v}|ij\rangle = \langle ij|v|ij\rangle - \langle ij|v|ji\rangle \qquad \text{III(8a)}$$

The HF approximation consists in putting the variation of III(8) with the constraints:

$$[a_i, a_i^+]_+ = 1 \text{ i.e. } \sum_\alpha C_\alpha^{i*} C_\alpha^i = 1 \quad \text{for all i,}$$

equal to zero, which means that,

$$\frac{\partial}{\partial C_\alpha^{i*}}\left[\langle\phi|H|\phi\rangle - \sum_{i=1}^{A} \epsilon_i \sum_\alpha C_\alpha^{i*} C_\alpha^i\right] = 0 \qquad \text{III(9)}$$

where ϵ_i are the Lagrangian parameters. This procedure leads us to the following matrix diagonalization problem;

$$\sum_\beta \langle\alpha|h|\beta\rangle C_\beta^i = \epsilon_i C_\alpha^i \qquad \text{III(10a)}$$

where h is the HF Hamiltonian defined as,

$$\langle\alpha|h|\beta\rangle = \langle\alpha|t|\beta\rangle + \sum_{j\,occ}^{A} \langle\alpha j|\tilde{v}|\beta j\rangle$$

$$= \langle\alpha|t|\beta\rangle + \sum_{\gamma\delta}\langle\alpha\gamma|\tilde{v}|\beta\delta\rangle\,\rho_{\delta\gamma} \qquad \text{III(10b)}$$

where

$$\rho_{\delta\gamma} = \sum_{j\,occ}^{A} C_{\gamma}^{j*} C_{\delta}^{j} \qquad \text{III(11)}$$

The unitary transformation C diagonalizes the HF Hamiltonian h which itself depends on this transformation. Therefore the HF equations III(10a) and III(10b) must be solved self-consistently i.e. by the method of **iterations** . Initially a guess for the transformation C is made, i.e. for the wave function and HF Hamiltonian $\langle\alpha|h|\beta\rangle$ is set up and diagonalized. The new eigenfunctions define a new transformation C and this is used to obtain a new HF Hamiltonian which is diagonalized. This procedure continues till the eigenfunctions between two consecutive iterations are the same, i.e. when the self-consistency between the single particle orbits and the single particle potential defined by III(10a) and III(10b) is achieved.

The second term of the equation III(10b), viz:

$$\sum_{\gamma\delta} \langle\alpha\gamma|\tilde{v}|\beta\delta\rangle \rho_{\delta\gamma}.$$

gives the average or the self-consistent field produced which corresponds to the shell theory potential. The eigenvalues ϵ_i are the single particle energies of the HF orbitals $|i\rangle$, i.e.

$$h|i\rangle = \epsilon_i |i\rangle \qquad \text{III(12)}$$

In terms of HF single particle energies, the total energy E can be expressed as,

$$E = \sum_{i=1}^{A} \langle i|t|i\rangle + \frac{1}{2} \sum_{ij} \langle ij|\tilde{v}|ij\rangle$$

$$= \frac{1}{2} \sum_{i=1}^{A} [\langle i|t|i\rangle + \epsilon_i] \qquad \text{III(13)}$$

In our calculations, we shall assume axial symmetry throughout. The deformed orbital $|i\rangle$ can therefore be expressed as,

$$|i\rangle = \sum_{n_\alpha l_\alpha j_\alpha} c^{i}_{n_\alpha l_\alpha j_\alpha} |n_\alpha l_\alpha j_\alpha, m_i \tau_i\rangle$$

When it does not cause confusion, we shall drop the quantum numbers m_i and τ_i.

III.1.1 Alternative expression for HF equations.

The Hartree-Fock equations III(10a) and III(10b) can be expressed in terms of h and the one-body density operator ρ.

The density matrix ρ is defined as

$$\rho_{ij} = \langle | a_j^+ a_i | \rangle \qquad \text{III(14)}$$

where $|\ \rangle$ denotes the physical vacuum. For an orthonormal set of wave functions $|i\rangle$ we have

$$\rho_{ij} = 0 \quad \text{for} \quad i \neq j$$
$$\rho_{ii} = 0 \quad \text{for} \quad \epsilon_i > \epsilon_f \qquad \text{III(15)}$$
$$= 1 \quad \text{for} \quad \epsilon_i < \epsilon_f$$

From this definition, the necessary conditions followed by ρ are

$$\rho = \rho^+ \quad \text{i.e.} \quad \rho \text{ is Hermitian} \qquad \text{III(16a)}$$

$$\rho^2 = \rho \qquad \text{III(16b)}$$

$$Tr(\rho) = \sum_i \langle | a_i^+ a_i | \rangle$$
$$= N = \text{number of particles.} \qquad \text{III(16c)}$$

The fact that ρ and h can be diagonalized simultaneously as seen from the equations III(10a) and III(15) can be expressed as

$$[h, \rho]_- = 0 \qquad \text{III(17)}$$

with of course $\rho^2 = \rho$.

III.1.2 Single particle separation energies.

The energy required to remove a particle from the l-th orbital from a nucleus with A particles is defined as the separation energy for that orbital. In the absence of the corrections arising due to the centre-of-mass motion, this is

the HF single particle energy ϵ_l of the l-th orbital.

$$\epsilon^{(l)}_{s.p.} = E^{A} - E^{A-1}_{(l)} \qquad \text{III(18)}$$

where $E^{A-1}_{(l)}$ denotes the binding energy of the residual nucleus after the removal of a nucleon from the l-th orbital in the parent nucleus with A nucleons.

$$\epsilon^{(l)}_{s.p.} = \sum_{i=1}^{A} \langle i|t|i\rangle + \frac{1}{2}\sum_{ij}^{A} \langle ij|\tilde{v}|ij\rangle$$

$$- \sum_{\substack{i=1 \\ i\neq l}}^{A-1} \langle i|t|i\rangle - \frac{1}{2}\sum_{\substack{ij \\ i,j\neq l}}^{A-1} \langle ij|\tilde{v}|ij\rangle$$

$$= \langle l|t|l\rangle + \sum_{j=1}^{A} \langle lj|\tilde{v}|lj\rangle$$

$$\text{i.e.} \quad \epsilon^{(l)}_{s.p.} = \epsilon_l \qquad \text{III(18a)}$$

which is the HF single particle energy for the l-th orbital. Thus, the separation energy for a particular orbital is given by the HF single particle energy for that orbital. This is known as the Koopman's theorem[8].

III.2 Centre-of-mass motion and single particle separation energies.

A nucleus is invariant with respect to the translation of

its centre-of-mass and hence a plane wave $\exp\left[i \, (\vec{P}.\vec{R}) / \hbar \right]$ should describe the correct dependence of the nuclear wave function on the centre-of-mass. Here, $\vec{P} = \sum_{i=1}^{A} \vec{p}_i$ and $\vec{R} = (1/A) \sum_{i=1}^{A} \vec{r}_i$. The independent particle model of a finite nucleus, however, leads to a wave function which generally does not have the translational invariance and may not separate into a product of wave functions describing the centre-of-mass motion (c.m.m.) and the internal motion. Unless the wave function obtained in the independent particle model separates into centre-of-mass wave function and internal wave function, there is no unique way to obtain a translationally invariant wave function. Moreover, the Hamiltonian depends on the centre-of-mass through the kinetic energy. Both the simplicity and the success of the independent particle model compel one to account for the spurious effects due to c.m.m. in an indirect manner. One method is the use of operators which do not depend on the centre-of-mass while evaluating expectation values with the model wave functions. Better still, one may obtain the independent particle wave function through a variational principle using internal operators only[9]. For example, one may perform a Hartree-Fock variational calculation using a Hamiltonian from which c.m.m. is deleted. Such calculations have been carried out and reported in literature[10-12]. However, the Hamiltonian in this case can be written in two forms and an interpretation of the HF solutions and HF single particle energies has been quite ambiguous in the past.

We show that in calculating the single particle separation energies, one should use the c.m.m. corrected Hamiltonian for both the initial and the final states and that this energy is invariant to the form of the Hamiltonian, unlike that obtained by the straightforward application of Koopman's theorem. Also it is shown that the same variational HF state results, irrespective of the form of the Hamiltonian, as should be the case[13].

III.2.1 c.m.m. and two forms of the Hamiltonian.

The Hamiltonian for A nucleons with the c.m.m. subtracted is given by

$$H = \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j}^{A} v_{ij} - \frac{\left(\sum_{i=1}^{A} \vec{p}_i\right)^2}{2mA} \qquad \text{III(19)}$$

neglecting the neutron-proton mass difference. This Hamiltonian can be put in two alternative forms:

$$H(A) = \sum_{i=1}^{A} \left(1 - \frac{1}{A}\right) \frac{p_i^2}{2m} + \sum_{i<j}^{A} \left(v_{ij} - \frac{\vec{p}_i \cdot \vec{p}_j}{mA}\right) \qquad \text{III(20)}$$

or

$$H(A) = \sum_{i<j}^{A} \left(v_{ij} + \frac{(\vec{p}_i - \vec{p}_j)^2}{2mA} \right)$$

III(21)

where the last form III(21) contains only a two-body interaction.

The HF Hamiltonians $h^{(1)}$ and $h^{(2)}$ for the forms III(20) and III(21) are given by

$$h^{(1)} = \sum_{\alpha\beta}' \left[\langle \alpha | \left(1 - \frac{1}{A}\right) \frac{p^2}{2m} | \beta \rangle + \sum_{\gamma\delta} \langle \alpha\gamma | \widetilde{v_{12} - \frac{\vec{p}_1 \cdot \vec{p}_2}{mA}} | \beta\delta \rangle \rho_{\gamma\delta} \right] a_\alpha^\dagger a_\beta$$

$$h^{(2)} = \sum_{\alpha\beta}' \left[\langle \alpha\gamma | \widetilde{v_{12} + \frac{(\vec{p}_1 - \vec{p}_2)^2}{2mA}} | \beta\delta \rangle \rho_{\gamma\delta} \right] a_\alpha^\dagger a_\beta \qquad \text{III(22)}$$

III(23)

where tilde denotes antisymmetrization. It is obvious that $h^{(1)}$ and $h^{(2)}$ are quite different, but, we shall see that the H.F equation $[h^{(2)}, \rho] = 0$ implies $[h^{(1)}, \rho] = 0$ and vice versa. $h^{(2)}$ can be easily expressed in terms of $h^{(1)}$ as

$$h^{(2)} = h^{(1)} + \frac{1}{A}(t - (t\rho + \rho t)) + \frac{T}{A}$$

III(24)

where $t = p^2/2m$ is an operator and T is a c-number equal to the expectation of t. Now consider the commutator with the density operator ρ,

$$[h^{(2)}, \rho] = [h^{(1)}, \rho] + \frac{1}{A}[t, \rho] - \frac{1}{A}[t\rho + \rho t, \rho]$$

$$= [h^{(1)}, \rho] + \frac{1}{A}[t, \rho - \rho^2]$$

$$= [h^{(1)}, \rho]$$

since $\rho^2 = \rho$ III(25).

This shows that we should obtain the same determinant with either of the Hamiltonian forms III(22) or III(23). If ρ commutes with $h^{(2)}$, it also commutes with $h^{(1)}$ and vice versa and thus the HF solution obtained is invariant to the form of the Hamiltonian used, although the HF single particle energy eigenvalues may be different in both cases.

III.2.2 Single particle energies and separation energies.

The HF single particle energy eigenvalues obtained with the HF Hamiltonian forms $h^{(1)}$ and $h^{(2)}$ can be expressed in terms of each other in a diagonal representation.for either Hamiltonian. It can be shown easily that

$$\epsilon_i^{(2)} = \epsilon_i^{(1)} + \frac{1}{A}[-t_{ii}] + \frac{T}{A} \quad \text{for i occupied} \qquad \text{III(26a)}$$

and

$$\epsilon_i^{(2)} = \epsilon_i^{(1)} + \frac{1}{A}[-t_{ii}] + \frac{T}{A} \quad \text{for i not occupied} \qquad \text{III(26b)}$$

The total HF energy is same in both cases:

$$E = \frac{1}{2} \sum_{i_{occ}} \epsilon_i^{(2)}$$

$$= \frac{1}{2} \sum_{i_{occ}} \left(\epsilon_i^{(1)} + t_{ii}\left(1 - \frac{1}{A}\right) \right) \qquad \text{III(27)}$$

The transformation from one Hamiltonian form to another without affecting the physical state seems to change the single particle separation energies as given by Koopman's theorem rather drastically ($\epsilon_i^{(2)}$ to $\epsilon_i^{(1)}$ as can be seen from eqn. III(18a)). This paradox[13] is easily removed if one notices that the c.m.m. correction is A dependent and that one should use the c.m.m. corrected Hamiltonian for the residual (A-1) particle

system also. That is, A should be treated as a number operator. Then one obtains identical single particle separation energies (ϵ s.p.) with either form of the Hamiltonian:

$$\epsilon^{(i)}_{s.p.} = \epsilon^{(1)}_i + \frac{1}{A-1}\left\langle \frac{p^2}{2mA} \right\rangle_{A-1} \qquad \text{III(28a)}$$

$$= \epsilon^{(2)}_i - \frac{1}{A-1}\sum_{(k<j)_{occ}}^{A-1} \langle kj | \frac{(\vec{p}_1 - \vec{p}_2)^2}{2mA} | kj \rangle \qquad \text{III(28b)}$$

where $\vec{P}$ is the total momentum and the expectation values are evaluated with respect to the residual nucleus after the sudden removal of a nucleon from orbital $|i\rangle$. It should be noted that the expression obtained above for the single particle separation energies $\epsilon^{(i)}_{s.p.}$ differs from that given by Kerman et al.[10] who arbitrarily subtract the average kinetic energy contribution for the whole nucleus from HF single particle energies $\epsilon^{(2)}$ to obtain single particle separation energies.

III.2.3 Calculation for ^{16}O using the two forms of the Hamiltonian.

We performed HF calculations for the nucleus ^{16}O with both the forms of Hamiltonian III(22) and III(23) to check that the separation energy and the variational determinantal

state of a nucleus are independent of the form of the Hamiltonian used. In Table III.1 we present the results with both forms of the Hamiltonian, giving identical results.

The calculations are performed in the space of first four major shells. We used the Sussex matrix elements with the harmonic oscillator parameter b = 1.5 fm. The Coulomb repulsion between the protons is explicitly taken into account.

The results for ^{16}O for the single particle separation energies with the c.m.m. correction tend to be more repulsive for deep lying orbitals and give slightly better agreement with the trend of the experimental data[14] compared to those without the c.m.m. correction. In Table III.2 we give the HF energy and the r.m.s. radius for the ^{16}O nucleus without and with the centre-of-mass correction. It can be seen that the c.m.m. contributes as much as 14 MeV to the binding energy giving slightly smaller r.m.s. radius.

We have thus shown that the two Hamiltonian forms III(20) and III(21) are equivalent in obtaining HF states and c.m.m. corrected single particle separation energies provided that the c.m.m. correction is applied to both the target and the residual nuclei treating A as the number operator and that the variational determinantal state of a nucleus is independent of the form of the Hamiltonian used.

III.3 HF calculations with density independent Skyrme Interaction

We shall restrict ourselves to the density independent set SV of Skyrme interaction obtained by Beiner et al.[7] and compare HF results with Sussex interaction for some 1p shell nuclei. We report the results for the nuclei ^{8}Li, ^{8}Be, ^{8}B, ^{12}C and ^{16}O. We also have chosen one member of the 1d-2s shell viz. ^{20}Ne, a well-beaten nucleus. The calculations are performed in the configuration space of first four major shells including Coulomb and c.m.m. corrections. The c.m.m. is treated as given in the eq.III(21), i.e. the Hamiltonian does not contain one-body part. The contribution of these corrections to the nuclear spectra was found to be negligible, although they may contribute several MeV to the intrinsic ground state energies. Since our aim is to study the spectroscopic properties of the nuclei, these effects have not been included in some cases in order to make projection calculations less complicated.

III.3.1 Sensitivity of the calculation on the oscillator parameter b.

Our calculations do not include configurations beyond the fourth major shell. This truncation of the configuration space makes the HF calculations severely dependent on the oscillator parameter b. If the configuration space is quite large the calculations would be insensitive to the size parameter b.

This is particularly true in the case of Skyrme interaction. The saturation would be achieved through the optimization of b. This optimized value of b is then the proper b to be used in the calculation of spectroscopic properties. For every nucleus we calculated the optimized b value. For the nuclei studied, the b value ranges from 1.6 fm to 1.9 fm. Sussex interaction does not show such a severe b-dependence for the 1p shell nuclei in the configuration space of four major shells[15]. The calculations for 1p shell nuclei with Sussex interaction were performed with b=1.5 fm while for ^{20}Ne, b=1.7 fm was used.

III.3.2 Results and Discussion.

The optimized b value for the nuclei ^{8}Li, ^{8}Be and ^{8}B was found to be 1.7 fm for the Skyrme interaction variant SV. For ^{12}C and ^{16}O it was found to be 1.6 fm. The truncation effects are strikingly seen in the case of ^{20}Ne for which the optimum b was found to be 1.9 fm. This value of b is rather large than the value generally used (1.7 fm), but, this is how this nucleus saturates. For HF calculations with Sussex interaction for ^{20}Ne, b=1.7 fm was used while for other nuclei, b=1.5 fm was used.

We display the results of HF calculations with the density independent Skyrme variant SV and the Sussex interaction in Tables III.3A and III.3B respectively. It can be seen that SV gives much better binding energies than does Sussex which

highly underbinds these nuclei. It also can be seen that the r.m.s. radii obtained with SV are slightly larger compared to the ones obtained with Sussex interaction providing better agreement with experimental values.

The energies obtained with SV, though better than the ones obtained with Sussex interaction, are less than the experimental ones. This could be due to the fact that the parameters in the Skyrme variants SII to SIV of Beiner et al.[7] are fitted for nuclei ^{16}O and above. Another reason could be that the oscillator basis used in our calculations may not be the proper basis to be used. In our calculations it was assumed that the Skyrme variants which reproduce the bulk properties of nuclei ^{16}O and above should not prove to be too unphysical for the nuclei lighter than ^{16}O.

For ^{8}Li and ^{8}B, we obtain two HF solutions with K=1 and K=2 which lie close in energy. Here, K denotes the projection of total angular momentum J on the symmetry axis taken to be the Z-axis. Because of the axial symmetry, $J_z|\phi_K\rangle = K|\phi_K\rangle$, where $|\phi_K\rangle$ is the HF determinant. We display the two solutions with the interaction SV in Tables III.4A and III.4B for ^{8}B only. In Tables III.5A and III.5B we display the corresponding solutions with Sussex interaction for comparison. For ^{8}Be, ^{12}C, ^{16}O and ^{20}Ne, only one solution with K=0 is obtained. We give HF orbitals for these nuclei in Tables III.6 through III.9 only for SV.

It can be seen that the gap i.e. the difference between single particle energies between the lowest unoccupied and the highest occupied orbitals is quite large and so the HF formalism is quite valid for these nuclei.

Since we would like to perform HF and spectroscopic calculations employing density dependent Skyrme interactions, we do not elaborate here more on the HF intrinsic properties using density independent effective forces. We take up the topic of performing HF calculations employing density dependent Skyrme interactions in the next chapter.

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Table III.8 HF orbitals for ^{16}O with Skyrme variant SV without c.m.m. and Coulomb corrections.

Table III.9 HF orbitals for ^{20}Ne with Skyrme variant SV without c.m.m. and Coulomb corrections.

TABLE III.1

HF Results for ^{16}O

	lj	without c.m.m. correction n=0	without c.m.m. correction n=1	$\epsilon^{(0)}$ MeV	with c.m.m. correction n=0	with c.m.m. correction n=1	$\epsilon^{(1)}$ MeV	$\epsilon^{(2)}$ MeV	$\epsilon_{s.p.}$ MeV	$\epsilon_{s.p.}$ expt[14] MeV
Protons	$s_{1/2}$	0.9989	0.0473	-51.8372	0.9991	0.0420	-52.002	-31.289	-50.967	-34±3.5
	$p_{3/2}$	0.99998	0.0057	-21.8683	0.9993	0.0383	-23.364	-3.258	-22.470	-18±2.5
	$p_{1/2}$	0.9988	-0.04925	-13.777	0.9998	-0.0179	-14.766	5.431	-13.878	-13±2
Neutrons	$s_{1/2}$	0.9984	0.0566	-55.917	0.9987	0.0511	-56.121	-35.420	-55.083	--
	$p_{3/2}$	0.9998	0.0183	-25.752	0.9987	0.05096	-27.308	-7.225	-26.414	-21.81
	$p_{1/2}$	0.9994	-0.0356	-17.549	0.99999	-0.0038	-18.596	1.577	-17.708	-15.65

The mixing amplitudes for the occupied orbitals are listed along with the HF single particles energies $\epsilon^{(0)}$(without c.m.m.correction), $\epsilon^{(1)}$, $\epsilon^{(2)}$(with c.m.m.correction using the two Hamiltonian forms) and the physical separation energies $\epsilon_{s.p.}$. The experimental values are given in the last column. n denotes the principal quantum number.

Table.III.2

HF energy and r.m.s. radius for the nuclues ^{16}O (a) without and (b) with c.m.m. correction with Sussex interaction. Coulomb repulsion between protons has been included in both (a) and (b).

	E_{HF} (MeV)	r.m.s.radius (fm)
(a)	-66.87	2.2426
(b)	-80.67	2.2060

Table III.3A

HF results with Skyrme Interaction: Variant SV.

Nucleus	K	b fm	E_{HF} MeV	Q_{HF} fm^2	RMS fm	B.E.(Expt.)[16] MeV
^{8}Li	2	1.7	-34.25	23.44	2.4474	41.28
	1	1.7	-34.38	24.75	2.4588	
^{8}Be	0	1.7	-44.99	45.33	2.5621	56.50
$*^{8}Be$	0	1.7	-36.91	44.21	2.5804	
^{8}B	2	1.7	-30.82	23.82	2.4596	37.74
	1	1.7	-30.96	25.09	2.4707	
^{12}C	0	1.6	-79.26	-33.33	2.5578	92.16
$*^{12}C$	0	1.6	-76.22	-32.50	2.5632	
$*^{16}O$	0	1.6	-126.68	0.0	2.6322	127.62
$*^{20}Ne$	0	1.9	-151.52	68.17	2.8835	160.65

* denotes that c.m.m. and Coulomb corrections have not been included.

Table III.3B

HF results with Sussex Interaction.

Nucleus	K	b fm	E_{HF} MeV	Q_{HF} fm^2	RMS fm	B.E(Expt.)[16] MeV
^{8}Li	2	1.5	-5.48	21.55	2.2393	41.28
	1	1.5	-4.50	21.18	2.2504	
^{8}Be	0	1.5	-17.02	37.00	2.2905	56.50
^{8}B	2	1.5	-1.75	21.88	2.2546	37.74
	1	1.5	-0.7942	21.15	2.2654	
^{12}C	0	1.5	-38.58	-27.16	2.2382	92.16
^{16}O	0	1.5	-80.67	0.0	2.2060	127.62
$*^{20}Ne$	0	1.7	-102.35	58.55	2.5392	160.65

* denotes that c.m.m. and Coulomb corrections have not been included.

Explanation for the Tables

HF orbitals have been tabulated in the following way. The first column denoting 'range' gives the components of a particular orbital. For example (1-4) would denote the following components in the order

$^{1}d_{5/2}\ 1/2$, $^{1}d_{3/2}\ 1/2$, $^{1}s_{1/2}\ 1/2$ and $^{2}s_{1/2}\ 1/2$

These components are tabulated in Appendix A. Second coulumn denotes projection of J on Z - axis m specifying the orbital and parity. Third and fourth columns give the HF single particle energy and the separation energy for the orbital respectively. Remaining columns give the components of the HF orbital. TL denotes time-like and TR denotes time-reversed orbitals.

For even-even time-reversal invariant nuclei both Proton and Neutron time-like orbitals are given when c.m.m. and Coulomb corrections are applied; otherwise only proton time-like orbitals are given. In the absence of the c.m.m. and Coulomb corrections, separation energy $\epsilon_{s.p.}$ and the HF single particle energy ϵ are the same.

* denotes the lowest unoccupied orbital.

Table III.4A

HF orbitals for the nucleus ^{8}B ; K= 2

Interaction: SV with c.m.m.and Coulomb corrections(b=1.7fm)

E_{HF}= -30.82 MeV Q_{HF}= 23.82 fm^2 RMS = 2.4596 fm.

	Range	m^{π}	ϵ MeV	ϵ s.p. MeV	HF orbitals (Protons)					
T L	1 - 4	$1/2^+$	-20.05	-31.29	0.081189	-0.078486	0.992152	0.053695		
	8 -13	$1/2^-$	0.81	-9.97	0.072369	-0.035789	0.898346	-0.058166	-0.422293	0.068853
	14-17	$-3/2^-$	10.23	-0.45	0.074984	0.080608	0.991803	-0.064853		
	8 -13*	$1/2^-$	20.58	9.96	0.047948	0.045155	0.415220	-0.123382	0.864552	-0.246130
T R	1 - 4	$-1/2^+$	-14.71	-25.80	0.069480	0.094313	0.991580	0.055184		
	8 -13	$-1/2^-$	4.23	-6.58	0.078264	0.053004	0.939524	-0.083304	0.311051	-0.068312
	14-17*	$3/2^-$	11.77	1.53	0.066262	-0.045936	0.990371	-0.112536		
					HF orbitals (Neutrons)					
T L	1-4	$1/2^+$	-25.12	-36.43	0.080929	-0.074261	0.991443	0.070538		
	8-13*	$1/2^-$	0.32	-9.99	0.081186	-0.044533	0.892564	-0.097070	-0.422347	0.083391
T R	1-4	$-1/2^+$	-19.52	-30.73	0.056132	0.081705	0.992382	0.073152		
	8-13	$-1/2^-$	2.47	-8.33	0.060686	0.034273	0.946116	-0.081785	0.295496	-0.077455
	14-17*	$3/2^-$	9.07	-1.14	0.082194	-0.047750	0.989837	-0.105768		

For explanation see page 64

Table III.4B

HF orbitals for the nucleus ^{8}B :K=1

Interaction: SV with c.m.m. and Coulomb corrections (b=1.7fm)

E_{HF}= -30.96 MeV Q_{HF}= 25.09 fm^2 RMS = 2.4707 fm.

	Range	m^{π}	ϵ_{MeV}	$\epsilon_{s.p.}$ MeV	HF orbitals (Protons)					
	1-4	$1/2^+$	-19.10	-30.26	0.069483	-0.080791	0.992921	0.052464		
T	8-13	$1/2^-$	1.94	-8.79	0.065628	-0.033686	0.895288	-0.075474	-0.425593	0.078683
L	14-17	$3/2^-$	10.20	-0.40	0.089664	0.078847	0.990389	-0.069807		
	8-13*	$1/2^-$	19.91	9.40	0.075736	0.058162	0.417288	-0.124872	0.863417	-0.235941
	1-4	$-1/2^+$	-15.31	-26.32	0.092972	0.101144	0.989423	0.046546		
T	8-13	$-1/2^-$	2.44	-8.25	0.090233	0.061334	0.924156	-0.067132	0.353717	-0.066394
R	14-17*	$3/2^-$	11.95	1.79	0.062730	-0.053358	0.989960	-0.114874		
					HF orbitals (Neutrons)					
T	1-4	$1/2^+$	-19.34	-30.50	0.058576	-0.075403	0.993772	0.057453		
L	8-13	$1/2^-$	2.13	-8.63	0.058190	-0.028903	0.917978	-0.090809	-0.371356	0.83321
	14-17*	$3/2^-$	8.08	-1.92	0.087357	0.060626	0.992008	-0.067916		
T	1-4	$-1/2^+$	-24.88	-36.09	0.089348	0.088609	0.989162	0.075653		
R	8-13*	$-1/2^-$	0.06	-10.14	0.086685	0.055672	0.896013	-0.092591	0.412956	-0.086259

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Table III.5A

HF orbitals for the nucleus ^{8}B: K=2

Interaction: Sussex with c.m.m.and Coulomb corrections(b=1.5 fm)

E_{HF}= -1.75 MeV Q_{HF}= 21.88 fm^2 RMS = 2.2546 fm

	Range	m^{π}	ϵ MeV	ϵ s.p. MeV	HF orbitals (Protons)					
T L	1-4	$1/2^+$	-8.28	-21.74	0.107115	-0.104951	0.988488	-0.020091		
	8-13	$1/2^-$	8.75	-4.09	0.073632	-0.028744	0.858757	-0.108594	-0.486849	0.086448
	14-17	$-3/2^-$	14.93	4.10	0.079933	0.063506	0.981415	-0.162487		
	8-13*	$1/2^-$	24.98	12.47	0.044612	0.038770	0.474054	-0.148280	0.829765	-0.247549
T R	1-4	$-1/2^+$	-6.41	-19.615	0.091289	0.094607	0.991280	0.008870		
	8-13	$-1/2^-$	9.52	-3.26	0.078355	0.075415	0.883171	-0.099993	0.438991	-0.073956
	14-17*	$3/2^-$	21.12	8.78	0.059431	-0.049838	0.972038	-0.221642		
					HF orbitals (Neutrons)					
T L	1-4	$1/2^+$	-16.13	-29.63	0.109532	-0.089377	0.989883	0.012075		
	8-13*	$1/2^-$	6.25	-5.86	0.082514	-0.047344	0.850845	-0.103687	-0.499027	0.085037
T R	1-4	$-1/2^+$	-12.67	-26.10	0.102145	0.104736	0.989206	-0.008224		
	8-13	$-1/2^-$	4.79	-7.98	0.071662	0.059907	0.871177	-0.090942	0.468016	-0.070820
	14-17*	$3/2^-$	16.85	4.62	0.076503	-0.036140	0.978880	-0.186105		

For explanation see page 64

TABLE III.5B

HF orbitals for the nucleus ^{8}B; K=1

Interaction: Sussex with c.m.m. and Coulomb corrections (b=1.5fm)

E_{HF} = -0.79 MeV Q_{HF} = 21.52 fm^2 RMS = 2.2654 fm

	Range	m^{π}	ϵ MeV	ϵ s.p. MeV	HF orbitals (Protons)					
	1-4	$1/2^+$	-8.58	-21.83	0.090409	-0.090904	0.991730	0.005880		
T	8-13	$1/2^-$	8.09	-4.58	0.064638	-0.060726	0.854600	-0.096463	-0.493840	0.092782
	14-17	$-3/2^-$	17.80	5.04	0.071079	0.066601	0.976371	-0.192905		
L	8-13*	$1/2^-$	25.012	12.63	0.063740	0.039181	0.478961	-0.176613	0.820857	-0.244947
	1-4	$-1/2^+$	-6.10	-19.24	0.105984	0.107926	0.988283	-0.020381		
T	8-13	$-1/2^-$	10.18	-2.51	0.083569	0.038935	0.890564	-0.117702	0.424301	-0.067157
R	14-17*	$3/2^-$	20.06	7.94	0.066259	-0.046014	0.976779	-0.198487		
					HF orbitals (Neutrons)					
	1-4	$1/2^+$	-10.44	-23.76	0.101402	-0.086984	0.990900	-0.016389		
T	8-13	$1/2^-$	5.73	-6.93	0.068578	-0.031697	0.872771	-0.096531	-0.465734	0.079591
L	14-17*	$-3/2^-$	14.25	2.28	0.075067	0.070713	0.982628	-0.154292		
	1-4	$-1/2^+$	-18.27	-31.61	0.109646	0.105311	0.988258	0.015293		
T										
F	3-13*	$-1/2^-$	5.28	-6.67	0.083215	0.068634	0.849737	-0.103542	0.499330	-0.079118

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TABLE III.6

HF orbitals with nucleus ^{8}Be: K=0

Interaction: SV with c.m.m. and Coulomb corrections (b=1.7 fm)

E_{HF} = -44.99 MeV Q_{HF} = 45.33 fm^2 RMS = 2.5621 fm.

	Range	m^{π}	ϵ MeV	ϵ s.p. MeV	HF orbitals (Protons)				
T	1-4	$1/2^+$	-17.86	-28.56	0.150931	-0.159067	0.975632	0.007699	
L	8-13	$1/2^-$	-3.07	-13.34	0.120408	-0.085135	0.856420	-0.095487	-0.475485	0.097949
	14-17*	$-3/2^-$	13.35	3.73	0.137996	0.111383	0.975315	-0.131571	
					HF orbitals (Neutrons)				
T	1-4	$1/2^+$	-19.50	-30.19	0.149445	-0.158285	0.975908	0.014659	
L	8-13	$1/2^-$	-4.57	-14.83	0.120579	-0.085508	0.857387	-0.089005	-0.475592	0.094478
	14-17*	$-3/2^-$	11.53	1.94	0.138221	0.112008	0.976725	-0.119817	

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TABLE III.7

HF orbitals for the nucleus ^{12}C; K=0

Interaction: SV without c.m.m. and Coulomb corrections (b=1.6 fm)

E_{HF} = -76.22 MeV Q_{HF} = -32.50 fm^2 RMS = 2.5637 fm

	Range	m^{π}	ϵ MeV	HF orbitals (Protons)					
T	1-4	$1/2^+$	-46.46	-0.067653	0.084570	0.993961	-0.017692		
	14-17	$-3/2^-$	-19.77	-0.060626	-0.059580	0.982514	-0.165652		
L	8-13	$1/2^-$	-17.36	-0.069182	-0.017887	0.787940	-0.095356	0.589090	-0.133881
	8-13*	$1/2^-$	-5.34	0.070762	-0.072792	-0.0588384	0.122476	0.775339	-0.165366

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Table III.8

HF orbitals for the nucleus ^{16}O; K=0

Interaction: SV without c.m.m. and Coulomb corrections(b=1.6 fm)

E_{HF}= -126.68 MeV Q_{HF}= 0.0 fm^2 RMS = 2.6322 fm

	Range	m^{π}	ϵ MeV	HF orbitals (Protons)					
T	1-4	$1/2^+$	-56.36	0.000003	-0.000003	0.999065	-0.043241		
	8-13	$1/2^-$	-25.22	0.000003	-0.000001	0.988189	-0.153239	-0.000029	-0.000006
L	14-17	$3/2^-$	-25.22	0.000002	0.000002	0.988189	-0.153237		
	8-13	$1/2^-$	-17.46	-0.000000	0.000002	0.000029	-0.000006	0.981664	-0.190619
	1-4*	$1/2^+$	0.53	1.000000	0.0	0.0	0.0		

For explanation see page 64

Table III.9

HF orbitals for the nucleus ^{20}Ne:K=0
Interaction: SV without c.m.m. and Coulomb corrections(b=1.9 fm)
E_{HF}= -151.52 MeV Q_{HF}= 68.17 fm^2 RMS=2.8835 fm

Range	m^{π}	ϵ MeV	HF orbitals (protons)					
1-4	$1/2^+$	-61.24	0.063596	-0.058514	0.986011	0.142524		
T 8-13	$1/2^-$	-34.25	0.082125	-0.069794	0.914329	0.077065	-0.382605	-0.007795
14-17	$3/2^-$	-27.30	0.062171	0.043950	0.990637	0.113315		
L 8-13	$1/2^-$	-20.87	0.018607	0.068493	0.385344	0.033420	0.918096	0.049534
1-4	$1/2^+$	-11.28	0.872564	-0.267140	-0.013045	-0.408775		
5-6*	$3/2^+$	-7.54	0.981241	0.192787				

For explanation see page 64