CHAPTER IV

DENSITY DEPENDENT SKYRME INTERACTION IN THE HARTREE-FOCK FORMALISM

IV.0 Introduction

The usual phenomenological interactionsused often in the Hartree-Fock calculations require a strong exchange component to ensure saturation. The effective interactions derived from Brueckner's calculations$^{1-5)}$ in nuclear matter acquire in addition to a strong exchange component a strong density dependence. In addition to the strong density dependence, the interactions of Negele$^{1)}$ and Banerjee and Sprung$^{2)}$ also give a starting energy dependence. Their saturation properties would be lost without the density dependence. In such calculations, the effective interaction is first derived in lowest order from a relative two-body force and the higher order corrections to it are parametrized, since the Brueckner's theory of nuclear matter leads to a defect of the order of 4 MeV for the binding energy per particle. Rather than calculating higher order terms in Brueckner's theory, a phenomenological correction is added to compensate for this defect in binding energy. In any case, all these interactions lead to a significant density dependence of the interaction. Most of these interactions give a satisfactory description of the radii, binding energies and single particle energies of doubly-closed shell nuclei. From these calculations it is seen that to describe saturating properties of nuclear forces (especially arising from tensor force and the repulsive core) the effective potential must be made to depend on density$^{6,7)}$. In fact, this is the way in which the saturation is achieved. The attraction between two nucleons decreases as the density increases.

Another class of calculations leaves out any consideration of the realistic force and the effective interaction is parametrized as a whole. In any case a parametrization is required to improve upon the realistic interaction. Such phenomenological interactions can give a good insight into the study of various properties of nuclei. Density independent effective interactions$^{8-11)}$ usually do not explain either the nuclear radii or the binding energies or the spectroscopic properties. Density dependent forces on the other hand, generally provide a good description of nuclear radii and binding energies.

As was shown in the Chapter II, the density dependence of the G-matrix arises naturally due to the exclusion principle. The effective interaction depends very much on the presence of the other nucleons because the other nucleons prevent them from scattering into the states which they occupy. This makes G a complicated function. Therefore a simplifying assumption made for G is that the effect of other nucleons is accounted for by representing G as a density dependent function of the two nucleon co-ordinates. In a finite nucleus where the density is not constant, the local density approximation is used. In this approximation the interaction between two nucleons at the positions $\vec{r}_1$ and $\vec{r}_2$ is assumed to take place in a medium the density of which is equal to the density of matter at the centre-of-mass position $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ of the two interacting nucleons.

Among the various density dependent effective interactions are Moszkowski's modified δ -interaction[12)] and the interaction which has become quite popular of late the Skyrme interaction[13)] advocated by Vautherin and Brink[14)]. **There** have ben numerous calculations using Skyrme interaction now available in literature[14-16)] for the bulk properties of the nuclei. The Hamiltonian density for nuclear system described by a Slater determinant can be expressed as an algebraic function of the nuclear and kinetic energy densities. This is possible because of the simple structure of the Skyrme interaction. In this energy density formalism, the Hartree-Fock equations reduce to ordinary differential equations which can be solved numerically by usual iteration procedure.

The Skyrme interaction is described in detail in Chapter II. The three-body contact force in it is equivalent to a two-body density dependent interaction for HF calculations of even-even nuclei and is partly responsible for the saturation property of the force.

The Skyrme interaction is characterized by only a few parameters, still many different sets of these parameters[14,16] have been obtained which more or less fit the binding energies and r.m.s. radii for nuclei all over periodic table. In spite of this phenomenal success achieved with Skyrme interactions in reproducing the bulk properties of the nuclei, there has been little effort in calculating spectroscopic properties such as energy spectra[17,18], transition rates, etc.using such interactions. This could be due to the difficulties posed by the three-body contact interaction simulating a density dependent two-body interaction. The three-body interaction in Skyrme force as stated in Chapter II, overbinds odd-mass and odd-odd nuclei and produces unstable spin-aligned HF ground states in nuclear matter and even-even nuclei. Hence the two-body density dependent interaction is preferred to three-body contact interaction.

Since the 'equivalent' two-body density dependent force is rotationally non-invariant for deformed nuclei, for density is no more a scalar function of position in space, it is unsuitable for a rigorous spectroscopic calculation requiring good angular momentum eigenstates which is the object of the present study. We shall propose in this chapter a modification of the Skyrme interaction that enables us to perform spectroscopic calculations[19] by employing a scalar density dependence averaged over the whole band of states contained in the variational intrinsic state. Such an interaction will be equivalent to the usual Skyrme force in spherically symmetric nuclei, thus maintaining the agreement for bulk properties obtained all over the periodic table.

In the following sections we shall define the scalar band averaged density to be used in the calculations and outline the procedure to perform density dependent HF calculations. We shall restrict ourselves to the intrinsic properties of some even-even, N=Z time-reversal invariant nuclear systems only. The problem of projecting out good angular momentum states from the HF solutions will be taken up in the next chapter. We shall also compare our results with other available calculations.

IV.1 Definition of Band Averaged Density.

In the Skyrme interaction, the density appearing in the two-body density dependent part needs to be evaluated at the centre-of-mass of two interacting nucleons. The interaction between two nucleons at the positions $\vec{r}_1$ and $\vec{r}_2$ is assumed to take place in a medium the density of which is equal to the density of matter at the centre-of-mass position $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$. However, for a contact force such as Skyrme interaction this coincides with density at the position of either of the two interacting nucleons.

For time-reversal invariant HF calculations of even-even nuclei, the two-body density dependent force in Skyrme interaction is given by,

$$V_{12} = (t_3/6)\ (1+P_\sigma)\ \delta\,(\vec{r}_1-\vec{r}_2)\,\rho\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right) \qquad \text{IV(1)}$$

The density $\rho\ (\vec{r})$ is defined as,

$$\rho\,(\vec{r}) = \sum_{i=1}^{A} \langle \vec{r}\,|\,\phi_i\rangle\langle\phi_i\,|\,\vec{r}\rangle \qquad \text{IV(2)}$$

The density ρ for an axially deformed, time reversal invariant even-even nucleus can be expanded in terms of its multipole components as follows:

$$\rho\,(\vec{r}) = \sum_{L} \rho_L\,(\vec{r})$$

$$L = 0,2,4\ldots\ldots \qquad \text{IV(3)}$$

It is easily seen that the scalar part of density (ρ_0) can be expressed as the average of scalar densities of the states projected onto the space of good angular momentum:

$$\rho_0\,(\vec{r}) = \sum_{J} |a_J|^2\ \rho_0^{J}\,(\vec{r}) \qquad \text{IV(4a)}$$

where $\rho_{o}^{J}(\vec{r}) = \frac{1}{2J+1} \sum_{M} \langle JM | \rho_{op} | JM \rangle$ IV(4b)

$$\rho_{op} = \sum_{i=1}^{A} \delta(\vec{r}_i - \vec{r}) \qquad \text{IV(4c)}$$

In IV(4a), $|a_J|^2$ is the probability of the state with angular momentum J contained in the deformed intrinsic state.

We suggest a modification in the interaction[19] (eq.IV(1)) such that the deformed density $\rho(\vec{r})$ is replaced by the "band averaged" scalar density $\rho_o(\vec{r})$ (eq.IV(4a)) . We replace V_{12} by V'_{12} and write

$$V'_{12} = (t_3/6)(1+P_\sigma)\,\delta(\vec{r}_1 - \vec{r}_2)\,\rho_o\left(\frac{\vec{r}_1 + \vec{r}_2}{2}\right)$$

IV(5)

The interaction V'_{12} would retain the rotational invariance and at the same time would not disturb the agreement for the bulk properties for spherical nuclei. It is straightforward to obtain the expression for $\rho_o(\vec{r})$ to be used in the HF calculations.

$$\rho(\vec{r}) = \sum_{i=1}^{A} \langle \vec{r} | \phi i \rangle \langle \phi i | \vec{r} \rangle$$

$$= \sum_{i=1}^{A} \sum_{\alpha\beta} c_{\alpha}^{i*} c_{\beta}^{i} \langle \vec{r} | \beta, m_i \tau_i \rangle \langle \alpha, m_i \tau_i | \vec{r} \rangle$$

IV(6)

where $\alpha \equiv n_\alpha l_\alpha j_\alpha$

Eqn.IV(6) could be written as:

$$\rho(\vec{r}) = \sum_{i=1}^{A} \sum_{\alpha\beta} C_\alpha^{i*} C_\beta^{i} (-1)^{j_\alpha - m_i} \cdot \sum_J C \begin{pmatrix} j_\alpha & j_\beta & J \\ -m_i & m_i & 0 \end{pmatrix} \langle \vec{r} | \psi^J(\alpha,\beta,\tau_i) \rangle$$

IV(7)

where

$$\langle \vec{r} | \psi^J(\alpha,\beta,\tau_i) \rangle \equiv \sum_{m_\alpha m_\beta} (-1)^{j_\alpha - m_\alpha} \cdot C \begin{pmatrix} j_\alpha & j_\beta & J \\ -m_\alpha & m_\beta & M \end{pmatrix} \langle \vec{r} | \beta\, m_\beta, \tau_i \rangle \cdot \langle \alpha\, m_\alpha \tau_i | \vec{r} \rangle$$

Zeroth multipole of density can be obtained by setting J=0. It is then trivial to show that IV(7) reduces to

$$\rho_0(\vec{r}) = \sum_{i=1}^{A} \sum_{\alpha\beta} C^{i*}_{n_\alpha l_\alpha j_\alpha} C^{i}_{n_\beta l_\alpha j_\alpha} \frac{1}{(2j_\alpha+1)} \sum_{m_\alpha} \langle \vec{r} | n_\beta l_\alpha j_\alpha m_\alpha, \tau_i \rangle \cdot \langle n_\alpha l_\alpha j_\alpha m_\alpha, \tau_i | \vec{r} \rangle$$

IV(8)

IV(8) is then the expression to be used in the HF calculations for the "band averaged scalar density". Introduction of this band averaged scalar density now makes the Hamiltonian rotationally invariant and spectroscopic calculations are made completely feasible. Employing the scalar density defined in IV(8) we shall briefly review the density dependent Hartree-Fock formalism in the following section.

IV.2 Density dependent Hartree-Fock theory

We shall closely follow the treatment given in section III.1 to discuss the HF formalism with density dependent Skyrme forces. We shall denote by v_{12} all the terms of Skyrme interaction which are independent of density. V'_{12}, as defined in the eqn.IV(5), denotes the two-body density dependent term in which the deformed density $\rho(\vec{r})$ has been replaced by the band averaged scalar density $\rho_0(\vec{r})$. In the 'deformed' basis defined by eqn.III(3), the Hamiltonian can be written as,

$$H = \sum_{ij} \langle i | t | j \rangle a_i^{+} a_j + \frac{1}{2} \sum_{ijkl} \langle ik | v_{12} + V'_{12} | jl \rangle a_i^{+} a_k^{+} a_l a_j \qquad \text{IV(9)}$$

Because of axial symmetry, the deformed orbital $| i \rangle$ can be expressed in terms of the basis states as,

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

$$\equiv \sum_{\alpha} C^{i}_{\alpha} | \alpha , m_i \tau_i \rangle$$

where C is the unitary transformation on the basis states defined in the eqn.III(3). When it does not cause confusion we shall drop the quantum numbers m_i and τ_i. Denoting by $|\phi\rangle$ the A particle state,

$$|\phi\rangle = \prod_{i=1}^{A} a_i^{+} |0\rangle$$

we have, the total energy for the nucleus with A nucleons

$$\begin{aligned} E &= \langle \phi | H | \phi \rangle \\ &= \sum_{i=1}^{A} \langle i | t | i \rangle + \frac{1}{2} \sum_{ij}^{A} \langle ij | \tilde{v}_{12} + \tilde{V}'_{12} | ij \rangle \end{aligned}$$

IV(10)

where tilde denotes the antisymmetrized matrix element defined in eqn.III(8a).

As given in eqn.III(9), the HF approximation requires for all α's,

$$\frac{\partial}{\partial c_\alpha^{i*}} \left[\langle \phi | H | \phi \rangle - \sum_{i=1}^{A} \epsilon_i \sum_{\alpha} c_\alpha^{i*} c_\alpha^{i} \right] = 0$$

i.e.,

$$\frac{\partial}{\partial c_\alpha^{i*}} \left[\sum_{i=1}^{A} \langle i | t | i \rangle + \sum_{ij}^{A} \langle ij | \tilde{v}_{12} + \tilde{V}'_{12} | ij \rangle - \sum_{i=1}^{A} \epsilon_i \sum_{\alpha} c_\alpha^{i*} c_\alpha^{i} \right] = 0$$

IV(11)

This leads to the following equation,

$$\sum_{\beta}\Big[\langle\alpha|t|\beta\rangle+\sum_{j=1}^{A}\langle\alpha j|\tilde{v}_{12}+\tilde{V}'_{12}|\beta j\rangle\Big]C^{i}_{\beta}$$

$$+\frac{1}{2}\sum_{ij}^{A}\langle ij|\frac{\partial V'_{12}(\rho_0)}{\partial\rho_0}\cdot\frac{\partial\rho_0}{\partial C^{i*}_{\alpha}}(1-P_M P_\sigma P_\tau)|ij\rangle$$

$$=\epsilon_i C^{i}_{\alpha} \qquad \text{IV(12)}$$

where $(1-P_M P_\sigma P_\tau)$ is the antisymmetrization operator. The diffrentiation with respect to C^{i*}_{α} of the density dependent term gives rise to the two terms shown in IV(12). This is due to the density dependence of the interaction V'_{12}. It is shown in appendix B, that after some algebra, one has

$$\frac{1}{2}\sum_{ij}^{A}\langle ij|\frac{\partial V'_{12}}{\partial\rho_0}\cdot\frac{\partial\rho_0}{\partial C^{i*}_{\alpha}}(1-P_M P_\sigma P_\tau)|ij\rangle$$

$$=\sum_{\beta}\frac{t_3}{4}C^{i}_{\beta}\langle\alpha|(\rho_p\rho_n)_0|\beta\rangle \qquad \text{IV(13)}$$

for an even-even time-reversal invariant nucleus.

ρ p(n) is the density of the protons (neutrons) and $(\rho_p\rho_n)_0$ is the zeroth multipole of the product $(\rho_p\rho_n)$. It is to be noted that the term in IV(12) which arises purely out of density dependence reduces to a one-body terms as given in IV(13). If we start with a spherical density ρ_0, only the zeroth multipole of the product $(\rho_p \rho_n)$ contributes. This is shown in the appendix C. The expression for the m.e. $\langle\alpha|(\rho_p\rho_n)_0|\beta\rangle$ is given in appendix D.

Following the treatment given in chapter III, one can easily see that the Hartree-Fock equations now can be written from eqn. IV(12) as,

$$\sum_{\beta} \langle\alpha|h|\beta\rangle C^{i}_{\beta} = C^{i}_{\alpha}\,\epsilon_i \qquad \text{IV(14a)}$$

$$\begin{aligned}\langle\alpha|h|\beta\rangle = {} & \langle\alpha|\frac{p^2}{2m}|\beta\rangle \\ & + \sum_{i\,occ}^{A} \sum_{\gamma\delta} \langle\alpha\gamma|\tilde{v}_{12} + \tilde{V}'_{12}|\beta\delta\rangle C^{i*}_{\gamma} C^{i}_{\delta} \\ & + (t_3/4)\langle\alpha|(\rho_p\rho_n)_0|\beta\rangle\end{aligned} \qquad \text{IV(14b)}$$

The solution of eqns.IV(14a) and IV(14b) involves the problem of double self-consistency between the interaction matrix elements and the HF wave function. One starts with a trial wave function and calculates two-body scalar density matrix elements $\langle\alpha\gamma|\tilde{V}'_{12}|\beta\delta\rangle$ and the one-body density matrix elements $\langle\alpha|(\rho_p\rho_n)_0|\beta\rangle$ and sets up the Hamiltonian matrix $\langle\alpha|h|\beta\rangle$, eqn.IV(14b). Its diagonalization gives a new set of eigenvalues and eigenfunctions. With this new wave function, again new two-body scalar density matrix elements are evaluated and the Hamiltonian matrix set up and diagonalized. This procedure is continued until two successive wave functions and the sets of two-body matrix elements calculated are the same, i.e. when both interaction matrix elements and the HF solution are mutually self-consistent. It is clear from this procedure that the density dependent HF calculations are an order of magnitude more difficult than the density independent ones.

IV.2.1 Rearrangement energy

For density independent forces, the total energy E of a nucleus can be expressed as

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

For Skyrme interaction, there is an additional term arising out of the density dependence of the interaction. The expression III(13) is replaced by

$$E = \frac{1}{2} \sum_{i=1}^{A} \left[\langle i | t | i \rangle + \epsilon_i \right] + E_R \qquad \text{IV(15)}$$

where E_R is called the "rearrangement energy" and is given by

$$E_R = \frac{-t_3}{8} \sum_{i=1}^{A} \langle i | \rho_p \rho_n | i \rangle \qquad \text{IV(16a)}$$

In our modified version of Skyrme interaction, only the zeroth multipole of the product $\rho_p \rho_n$ contributes and the expression becomes ,

$$E_R = \frac{-t_3}{8} \sum_{i=1}^{A} \langle i | (\rho_p \rho_n)_0 | i \rangle \qquad \text{IV(16b)}$$

From the expression IV(16b) for the rearrangement energy E_R, it can be seen that this quantity is always negative. In fact, this would be the case for any form of density dependence of interaction. Thus the total energy in density dependent HF theory is always lower than the ordinary HF theory would lead us to expect from the <u>given</u> single particle energy eigenvalues.

Due to the relation III(13) for total binding energy for density independent forces in HF approximation, it is well-known that it is not possible to fit the radius, single particle energies and total binding energies using a single density independent force[14,23]. For Skyrme force, however, the relation III(13) is replaced by IV(15). The rearrangement energy term E_R which arises purely due to the density dependence of the interaction is then responsible in obtaining good agreement for binding energies of nuclei with experiment.

IV.2.2 <u>HF single particle energies and separation energies</u>.

We shall show in this section that when we consider the two-body density dependent version of the force in Skyrme interaction rather than the three-body contact force, the

Koopman's theorem 21) no longer holds assuming that the single particle wave functions of the A and A-1 systems are identical. Koopman's theorem strictly holds when the three-body contact interaction **is** used as shown by Vautherin and Brink 14).

Koopman's theorem is known to hold for density independent two-body interaction only in the absence of centre-of-mass motion (c.m.m.) as shown in chapter III. In this section, we shall not consider c.m.m. to make the discussion simple and concentrate only on the density dependent part of the interaction.

We recall that we are working in the band averaged density formalism described in sections IV.1 and IV.2. Hence $\rho_0(\vec{r})$, $(\rho_p\rho_n)_0$ etc. denote the zeroth multipoles.

The contribution $\epsilon^{(3)}_{(K)}$ to the HF single particle energy $\epsilon_{(K)}$ for the orbital K from eqns. IV(14a) and IV(14b) due to the density dependent part is given by ,

$$\epsilon^{(3)}_{(K)} = \sum_{j}^{A} \langle Kj \,|\, \frac{t_3}{6}(1+P_\sigma)\rho_0\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\delta(\vec{r}_1-\vec{r}_2)\,|\,\widetilde{Kj}\rangle$$

$$+ \frac{t_3}{4}\langle K \,|\, (\rho_p\rho_n)_0 \,|\, K\rangle$$

IV(17)

Since we consider only even-even time-reversal invariant nuclei, it can be shown that IV(17) reduces to,

$$\epsilon^{(3)}_{(K)} = \frac{t_3}{4} \langle K | (\rho_0^A)^2 - (\rho_0^{q_K})^2 | K \rangle$$

IV(18)

where (ρ_0^A) denotes the band averaged density for the nucleus with A particles. q_K denotes whether the orbital K is a proton or a neutron orbital. Consider it to be a neutron orbital. Then,

$$\epsilon^{(3)}_{(K)} = \frac{t_3}{4} \langle K | (\rho_0^A)^2 - (\rho_0^N)^2 | K \rangle$$

IV(19)

ρ_0^N is the zeroth multipole of density of neutrons. This expression for HF single particle energies is identical with the one given by Vautherin and Brink$^{14)}$.

We shall now calculate the contribution to separation energy due to the density dependent part of Skyrme interaction, $\epsilon^{(3)}_{s.p.}(K)$ required to remove the nucleon from Kth orbital. We have by definition,

$$\epsilon^{(3)}_{s.p.}(K) = E^{A} - E^{A-1}$$

$$= \frac{1}{2}\sum_{ij}^{A} \langle ij | \frac{t_3}{6}(1+P_\sigma)\,\rho_0^{A}\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\delta(\vec{r}_1-\vec{r}_2)\,|\widetilde{ij}\rangle$$

$$-\frac{1}{2}\sum_{\substack{ij\\ i,j\neq K}}^{A-1} \langle ij | \frac{t_3}{6}(1+P_\sigma)\,\rho_0^{A-1}\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\delta(\vec{r}_1-\vec{r}_2)\,|\widetilde{ij}\rangle \qquad \text{IV(20)}$$

ρ_0^{A} and ρ_0^{A-1} denote the band averaged densities for nuclei with (A) and (A-1) nucleons respectively. We assume here that the orbitals of the residual nucleus with (A-1) nucleons do not change after sudden removal of the particle from the orbital K. With this assumption IV(20) can be written as

$$\epsilon^{(3)}_{s.p.}(K) = \frac{1}{2}\sum_{ij}^{A} \langle ij | \frac{t_3}{6}(1+P_\sigma)\,\phi_K^{*}\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right) \cdot \phi_K\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\delta(\vec{r}_1-\vec{r}_2)\,|\widetilde{ij}\rangle$$

$$+\sum_{j}^{A} \langle Kj | \frac{t_3}{6}(1+P_\sigma)\,\rho_0^{A-1}\left(\frac{\vec{r}_1+\vec{r}_2}{2}\right)\delta(\vec{r}_1-\vec{r}_2)\,|\widetilde{Kj}\rangle \qquad \text{IV(21)}$$

Considering K to be neutron orbital, it is easy to show that IV(21) reduces to,

$$\epsilon^{(3)}_{s.p.}(K) = \frac{t_3}{4}\langle K|\left(\rho_0^{A}\right)^2-\left(\rho_0^{N}\right)^2|K\rangle$$

$$-\frac{t_3}{4}\langle K|\,\rho_0^{P}\,\phi_K^{*}\,\phi_K\,|K\rangle \qquad \text{IV(22)}$$

i.e.

$$\epsilon^{(3)}_{s.p.}(\kappa) = \epsilon^{(3)}_{\kappa} - \frac{t_3}{4} \langle \kappa | \rho_0^{p} \phi^*_{\kappa} \phi_{\kappa} | \kappa \rangle \qquad \text{IV(23)}$$

We thus see that the separation energies differ from HF single particle energies by an amount given by the second term in IV(23) and so the Koopman's theorem no longer holds when a two-body density dependent interaction is used.

It should be noted that our expression for HF single particle energies is identical with that of Vautherin and Brink and so with their separation energies since they use three-body contact force. Our expression for separation energies, however, is different. Three-body contact force and two-body density dependent force are equivalent only for the even-even time-reversal invariant systems.

As we saw in **chapter** III, the Koopman's theorem is not valid when c.m.m. is incorporated in HF calculations and the particle number A is to be treated as a number operator. We see that when the interaction itself depends on the particle number, the Koopman's theorem will not be valid. The total density of a system depends on the total number of particles A in the system and so the Koopman's theorem will not be valid for density dependent interactions. The effect of 2nd term in IV(23), however, is expected to be small, approximately by a factor (1/A) and so $\epsilon^{(3)}_{s.p.}(K)$ and $\epsilon^{(3)}(K)$ would be quite close especially when the number of nucleons is quite large. Hence single particle energies would be quite close to the actual separation energies when density dependent forces are used.

IV.3 HF calculations with the band averaged Skyrme interaction.

As remarked in the section IV.2, the solution of HF equations in the density dependent HF theory involves the problem of double self-consistency between the interaction matrix elements and the HF wave functions. Following the procedure outlined there, the calculations were carried out for the nuclei ^{8}Be, ^{12}C, ^{16}O and ^{20}Ne using the scalar band averaged density dependent Skyrme interaction.

The interaction set chosen was the variant SIV of Beiner et al$^{16)}$. This set will be denoted as BASIV in our band averaged formalism. The set SIV has a rather weak-density dependence compared to other sets. This set was chosen since because of its weak density dependence, the convergence is very rapid. Other sets because of their large density dependence, pose the problem of numerical instability of the HF solution and hence that of its convergence. The corrections arising due to the centre-of-mass motion and Coulomb repulsion have not been included in order to make the projection calculations simpler and also because it was found that the contribution of these corrections to the energy spectrum is quite insignificant$^{20)}$.

We display the results of the HF calculations with the interaction BASIV in tables IV.1 through IV.5 for the nuclei ^{8}Be, ^{12}C, ^{16}O and ^{20}Ne. Only the proton time-like orbitals are given. It is seen that the interaction BASIV provides a much better agreement for the binding energies of these nuclei compared to the variant SV and the Sussex interaction (Tables III.3A and III.3B). It should be noted that the interaction BASIV lifts up the deep lying orbitals as compared to SV which is in accordance with the calculations reported by Beiner et al$^{16)}$. The r.m.s. radii given by BASIV compare well with those given by SV. It can be seen that the HF gaps obtained with BASIV are consistently larger than the ones obtained with SV. One can conclude that, in general, the interaction BASIV provides a better description of the intrinsic properties of nuclei.

IV.4 Summary

In this chapter, we have proposed a modification of the Skyrme interaction by replacing the intrinsic density by the "band averaged" scalar density. This makes the Hamiltonian rotationally invariant and projection of good angular momentum states from the intrinsic HF solution is made possible. We derived HF equations using density dependent Skyrme interaction and saw that when density dependent interaction is used, Koopman's theorem does not hold because the interaction depends upon the total number of particles in the system. We saw that the interaction BASIV provides a good description of the nuclei studied compared to the interactions SV and Sussex. We shall take up the topic of projecting good angular momentum states from the HF intrinsic state in order to study the collective properties of nuclei in the next chapter.

References

1. J.W. Negele, Phys. Rev. C1 (1970) 1260.
2. P.K. Banerjee and D.W.L. Sprung, Nucl. Phys. A168 (1971) 273.
3. P. Siemens, Nucl. Phys. A141 (1970) 225.
4. J. Nemeth and D. Vautherin, Phys. Lett. 32B (1970) 561.
5. J. Zofka and G. Ripka, Nucl. Phys. A168 (1971) 65.
6. H.A. Bethe, Ann. Rev. Nucl. Sc. 21 (1971) 93.
7. G. Ripka, Lectures given at the 14th International Meeting of Physicists "Fast Neutron and the Study of Nuclear Structure" at Duiloronear Split, Yogoslavia, Sept. 8-20, 1969.
8. D.M. Brink and E. Boeker, Nucl. Phys. 91 (1967) 1.
9. A.B. Volkov, Nucl. Phys. 74 (1965) 33.
10. C.W. Nestor, K.T.R. Davies, S.J. Krieger and M. Baranger Nucl. Phys. A113 (1968) 14.
11. G. Saunier and J.M. Pearson, Phys. Rev. C1 (1970) 1353.
12. S.A. Moszkowski, Phys.Rev. C2 (1970) 402.
13. T.H.R. Skyrme, Phil.Mag. 1 (1956) 1043;
    Nucl.Phys. 9 (1959) 615.
14. D. Vautherin and D.M. Brink, Phys. Rev. C5(1972) 626.
15. D. Vautherin, Phys. Rev. C7 (1973) 296.
16. M. Beiner, H. Flocard, Nguen Van Giai and P. Quentin, Nucl.Phys. A238 (1975) 29.

17. K.H. Passler and U. Mosel, Nucl. Phys. A257 (1976) 242.

18. G.F. Bertsch and S.F. Tsai, Phys. Rep.18, No.2 (1975) 125.

19. S.B. Khadkikar and V.B. Kamble, Phys. Lett. 64B(1976) 131.

20. V.B. Kamble, S.B. Khadkikar and D.R. Kulkarni, Proceedings of the Nuclear Physics and Solid State Physics Symposium, Bombay. Vol.17B (1974) 204.

21. T. Koopmans, Physica 1 (1934) 104.

22. A.H. Wapstra and N.B. Gove, Nuclear Data Tables, 9(1971) 265.

23. A.K. Kerman, in Cargese Lectures in Physics, edited by M. Levy (Gordon and Breach, New York, 1968), Vol.II.

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Table IV.1

HF properties of nuclei with interaction BASIV.

Nucleus	b fm	E_{HF} MeV	Q_{HF} fm^2	RMS fm	Re.En. MeV	Expt.[22) MeV
^{8}Be	1.7	-42.94	47.19	2.5386	-6.44	-56.50
^{12}C	1.6	-81.70	-36.31	2.5583	-15.96	-92.2
^{16}O	1.6	-125.99	0.0	2.6395	-26.36	-127.62
^{20}Ne	1.9	-156.69	74.77	2.9009	-32.64	-160.65

Table IV.2

HF orbitals for the nucleus ^{8}Be with Interaction BASIV (b = 1.7 fm).

E_{HF}= -42.94 MeV Q_{HF}= 47.19 fm^2 RMS= 2.5386 fm.

Range	m^π	ϵ MeV	HF orbitals					
1-4	$1/2^+$	-29.41	0.176311	-0.183866	0.963942	-0.076962		
8-13	$1/2^-$	-17.44	0.149012	-0.105569	0.838093	-0.145709	-0.477385	0.122972
14-17*	$-3/2^-$	-3.38	0.186543	0.145929	0.960512	-0.146022		

For explanation see page 64.

Table IV.3

HF orbitals for the nucleus ^{12}C with Interaction BASIV
(b = 1.6 fm)

E_{HF} = -81.70 MeV Q_{HF} = -36.31 fm^2 RMS = 2.5583 fm.

Range	m^{π}	ϵ_{MeV}	HF orbitals					
1-4	$1/2^+$	-41.23	-0.092928	0.110477	0.988882	-0.035645		
14-17	$-3/2^-$	-20.09	-0.087076	-0.079816	0.981256	-0.152263		
8-13	$1/2^-$	-17.72	-0.096997	-0.033852	0.770395	-0.074295	0.611660	-0.127627
$8\text{-}13^*$	$1/2^-$	-4.00	0.106977	-0.104996	-0.603995	0.132727	0.756463	-0.151221

For explanation see page 64.

Table IV.4

HF orbitals for the nucleus ^{16}O with Interaction BASIV
(b = 1.6 fm)
$E_{HF} = -125.99$ MeV $Q_{HF} = 0.0$ fm^2 RMS = 2.6395 fm.

Range	m^{π}	ϵ MeV	HF orbitals					
1-4	$1/2^+$	-48.05	0.0	0.0	0.998000	-0.063221		
8-13	$1/2^-$	-23.28	0.0	0.0	0.988050	-0.154137	0.0	0.0
14-17	$-3/2^-$	-23.28	0.0	0.0	0.988050	-0.154137		
8-13	$1/2^-$	-15.72	0.0	0.0	0.0	0.0	0.981649	-0.190697
7-7*	$5/2^+$	-1.61	1.0					

For explanation see page 64.

Table IV.5

HF orbitals for the nucleus ^{20}Ne wtih Interaction BASIV
(b=1.9 fm)

E_{HF} = -156.69 MeV Q_{HF} = 74.77 fm^2 RMS = 2.9009 fm.

Range	m^{π}	ϵ MeV	HF orbitals					
1-4	$1/2^+$	-52.09	0.094156	-0.083123	0.986204	0.107826		
8-13	$1/2^-$	-32.84	0.112374	-0.090761	0.900803	0.067988	-0.403796	-0.003668
14-17	$3/2^-$	-24.53	0.087974	0.060413	0.988387	0.108174		
8-13	$1/2^-$	-18.23	0.034781	0.092603	0.408981	0.029128	0.905766	0.041083
1-4	$1/2^+$	-12.98	0.859362	-0.280068	-0.059325	-0.423721		
5-6	$3/2^+$	-8.42	0.976684	0.214682				

For explanation see page 64.