CHAPTER I
INTRODUCTION

The nucleus is a system of finite number of fermions interacting through strong, short range forces. The number of nucleons in a given nucleus may be anywhere from a few to a few hundred. The internucleon force besides being strong and short ranged is also complex in nature having central, spin-orbit and tensor components and perhaps has also many-body character. Yet another aspect of this complicated force is its strong repulsive character at very short distances. It is not surprising then that one observes a rich and wide-ranging variety of phenomena in nuclei. From the theoretical viewpoint the understanding of and predicting the behaviour of a nucleus forms a fascinating, though at times difficult, study. The problem here is that of calculating all the properties of a finite many-body system of fermions interacting through a complicated, as yet not fully understood force. More precisely, on the one hand one has the problem of dealing with the complicated nuclear force whose exact nature is not known and on the other, the problem of solving the finite many-body Schroedinger equation. We are concerned in this thesis with approaches to the approximate solution of the latter problem.
The independent particle model (IPM) provides the simplest of all the approaches towards an approximate solution of the nuclear many-body Schrödinger equation. The IPM approach consists in taking the strongly interacting many-particle system to be a system of non-interacting particles moving in an average field. Depending upon how this average field is constructed there are many forms of IPM. A widely-used IPM is the Hartree-Fock (HF) method in which the average field generated is a self-consistent field giving minimum energy for the system. This HF self-consistent field idea is at the back of all the present-day microscopic theories of nuclear structure. These sophisticated theories start from HF as a first approximation and attempt in different ways to include the residual interaction which is ignored in the HF picture. This thesis is concerned with the 'goodness' of wave function and operators obtained by the HF method.

The approximate wave function used for nucleons in the IPM is a Slater determinant which is an antisymmetrized product of independent particle wave functions. In the last ten years or so, such a determinant has very often been obtained by the HF method in which one finds the determinant having the lowest energy. It is generally accepted that the HF approximation describes many nuclear properties,
including the ground state energy well. In particular some of the single-particle properties (expectation values of one-body operators in the HF state) show spectacular agreement with experiments. In spite of the agreement one finds with the experiment it is not clear how 'good' the HF wave function is. To be more precise, one does not know how well this approximate wave function compares with the "exact" solution of the Hamiltonian in the model space. Often one also does not know how the calculated properties would change with improvement in the wave function. It seems justified therefore not to strive for "very good" agreement between the HF results and the experimental ones without a proper investigation of corrections to the HF. In view of this, we make a modest beginning in chapter II of systematically studying these questions. A more detailed discussion of some measures for testing approximate wave functions and the related variational principles is given in the same chapter.

Consider the HF solution for the nuclear system and evaluate its variance $\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2$. The width $\sigma$ provides us with a measure of departure of the approximate wave function from the "exact" solution for the system. Of course this quantity by itself does not tell us how important the "correlation" effects are for the nuclear properties.
One way of learning about these is to improve the wave function by the use of perturbation theory. We have therefore evaluated the correction to the HF wave function and the HF energy in perturbation theory. This is described in chapter II. The width may also be used as a measure for comparing two approximate wave functions. For example, given the widths of two determinantal states, one can say that the one with the smaller width is closer to the "exact" solution of the system. In the same chapter we also discuss how the width of the HF state changes with a change in the size of the vector spaces. We also examine the changes in the ground state energy with this truncation and see how the width is related to the total energy spectrum span of the nuclear system.

Besides studying the HF solution we also examine in chapter III an alternative variational procedure suggested earlier[^6] to obtain determinantal states. In this we minimize the variance $\sigma^2$ for the system rather than the energy. It should be clear that the energy of the new determinant $\Psi_\sigma$ will be higher than that of $\Psi_{HF}$ but its width will be smaller. If we therefore use the width as a measure of "goodness" of a wave function then the state $\Psi_\sigma$ is an improvement over $\Psi_{HF}$. Moreover, if we carry out perturbation theory corrections for $\Psi_\sigma$ and $\Psi_{HF}$ we expect
smaller 2ph correction for $\psi_\sigma$ than for $\psi_{HF}$. This is because in the determination of $\psi_\sigma$ we are already including some excitations to intermediate 2ph states. Of course as far as the energy criterion is concerned the HF solution is superior to the corresponding solution obtained by minimizing $\sigma^2$.

The numerical calculation in chapter III are carried out for light "spherical" nuclei within the space of three and four harmonic oscillator shells. Three different effective interactions have been used. It should be pointed out that the calculations we have carried out are meant for "internal" comparison of the two variational methods and for illustrating the various points. It is not our aim to compare the results of our calculations with experimental quantities.

In chapter IV we extend our study of goodness of approximate wave functions to the class of deformed HF wave functions. Results for widths of N=Z even even nuclei calculated in the 0d-1s major shell using two different realistic two-body interactions are given. We also describe a schematic interaction in 0d-1s shell and give results for this interaction.

Another major topic dealt with in this thesis is concerned with the properties of fermion operators and
spaces. This is described in chapter V. Our main object here is to study the efficiency with which the two-body interaction is converted into an effective one-body operator by the HF "machinery". This efficiency factor indicates in a global sense how good is the HF single-particle basis. If a large part of the two-body interaction gets converted into a one-body like operator under HF then we can say that the Hamiltonian behaves essentially like a (0+1)-body operator and that the s.p. basis generated by the HF procedure is on the whole a good basis. One can also use this criterion for goodness of s.p. basis to seek the best s.p. basis which would be the one which optimizes this contribution from two-body term to an effective one-body term. The formulation and investigation of these and other related questions involve the use of a mathematical framework in which one carries out orthogonal decomposition of operators. Further, one needs measures for the sizes of operators so that one can study their behaviour in many particle spaces. The framework we use here for the classification of operators is that provided by unitary groups in spectroscopic spaces. As a measure for the size of an operator we make use of the Euclidean norm of an operator 7.

We all know that for the most part of the current microscopic theories of nuclear structure are attempts to solve
the finite many-body problem in truncated spaces defined by a finite number \( N \) of single-particle states. With the consideration of unitary transformations in these finite spaces the unitary group in \( N \)-dimensions \( U(N) \) automatically enters into the discussion forming a starting point for all further group theoretic discussions of nuclear structure. Thus the unitary group \( U(N) \) and also its family of subgroups provide a natural and convenient mathematical framework for the study of the structure of fermion operators and spaces and also for investigating other physically relevant questions about them. We use this framework here to study the goodness of HF s.p. basis. The relevant groups here are the unitary group \( U(N) \) and its family of direct sum subgroups \( U(m) \oplus U(N-m) \) where \( N \) is the total number of s.p. states and \( m \) is the number of particles. The subgroup we discuss here is the one generated by the HF procedure in which one decomposes via a variational procedure the \( N \) s.p. states into \( m \) occupied and \( (N-m) \) unoccupied ones. We decompose the interaction into its irreducible representations under both the \( U(N) \) and \( U(m) \oplus U(N-m) \) groups using the standard techniques for the unitary group decomposition of a general fermion operator. We describe these techniques in detail \(^8\text{-}^{10}\). Further we need proper measures for the sizes of operators and their symmetry parts to study their relative importance. The measure we
consider here is the Euclidean norm of an operator. We derive an expression for the square of the norm of total (0+1)-unitary rank part of the interaction when decomposed under the group $U(m) + U(N-m)$. In terms of this norm and also the norms of various irreducible parts of $H$ under $U(N)$ we define a ratio $R$ which serves as a global measure for the goodness of the HF s.p.basis. This ratio tells us how much of the two-body interaction has been converted into an effective one-body operator when a HF calculation is done. We present the results of norms of various parts of the interaction decomposed under $U(N)$ and $U(m) + U(N-m)$ along with a discussion of them for $N=Z$ even even nuclei in $0f-1p$ and $0d-1s$ shells using realistic two-body interactions. We also evaluate the efficiency ratio $R$ for these nuclei.

Finally in Chapter VI we present a summary of the entire work and also some suggestions for future research.
REFERENCES FOR CHAPTER I