CHAPTER VI

SUMMARY AND FUTURE PROSPECTS

To sum up, we have studied in this thesis two distinct topics. The first topic deals with the goodness of Hartree-Fock states and also with the variational method based on the minimization of energy variance for obtaining Slater determinants. In the second topic we have studied the decomposition of fermion operators under unitary groups and the norms of these operators in spectroscopic spaces.

In the first place, we have studied the goodness of HF states by evaluating their widths. The width of a state provides us with a measure of the departure of the state from an exact eigenstate of the nuclear system in the model space. We have evaluated the widths of HF states of some light spherical nuclei using realistic two-body interactions. We find that the HF states have large widths which implies that the HF single Slater determinantal description is inadequate.

Besides studying the goodness of HF states we have also investigated in detail a new variational method wherein we minimize the energy variance of a Slater determinant.
instead of its energy as is done in the conventional HF method. We have derived the equations for determining the self-consistent set of single particle orbits using the new variational procedure. We have applied this method to some light spherical nuclei. We find that the new procedure yields determinants which are close to the HF determinants. We have also calculated perturbation theory corrections for both kinds of determinants viz, the HF and the minimum variance determinant to estimate the correlation effects. A comparative study of the properties of the Slater determinants obtained from the two variational procedures has also been made. Further, we have also studied the goodness of deformed HF states of some $N=Z$ even even nuclei in the $0d-1s$ major shell.

The second major topic dealt with in this thesis is about the structure of fermion operators and spaces. We have studied here the question to what extent the HF procedure converts the two-body interaction into an effective one-body operator. For this purpose we require two things. First, we need a proper classification scheme for operators in which we can carry out an orthogonal decomposition of them. Secondly, we need proper measures or norms for the sizes of operators so that we can study their behaviour in spectroscopic spaces and also make a
comparative study of them. In our study we have used the group theoretic classification for operators the relevant groups being unitary groups in spectroscopic spaces. More precisely, we have here a set of $N$ single-particle states in which $m$ particles are distributed. We have classified the two-body interaction according to the irreducible symmetries of the unitary group $U(N)$ and its direct sum subgroup $U(m) + U(N-m)$. The subgroup here is the one generated by the HF decomposition of s.p. space into $m$ occupied and $(N-m)$ unoccupied states. We have studied here the question to what extent the irreducible tensor part of the two-body interaction $H(2)$ under $U(N)$ is converted into an effective one-body operator under the subgroup $U(m) + U(N-m)$ supplied by the HF procedure. As already said, for our purpose we need also suitable norms for the sizes of operators in $m$ particle spaces. We have used here the Euclidean norm as a proper measure for the size of an operator. We have derived a polynomial expression for the square of the norm of the effective one-body operator which results when the two-body interaction is classified under the subgroup generated by the HF procedure. Next a quantity called conversion ratio is defined in terms of norms of different symmetry parts of the interaction decomposed according to $U(N)$ and
This ratio tells us to what extent the two-body interaction has been converted into an effective one-body operator when a HF calculation is done. It further indicates in a global sense how good is the HF single-particle basis. This ratio has been evaluated for the HF solutions of some N=Z even even nuclei both in 0f-1p and 0d-1s shells using realistic two-body interactions. Our studies reveal that this conversion is quite small which implies that a large part of the two-body interaction is still irreducible under the subgroup generated by the HF procedure and that the HF s.p. basis is not a good universal basis.

Finally a few suggestions for future investigations which emerge from these studies may be indicated here:

(a) Our study of widths has shown that single Slater determinantal description of exact eigenstates of the Hamiltonian is inadequate. One way of improving the determinantal energy and wave function is to correct them in perturbation theory by including 1ph and 2ph correlations as we did in Chapter III. A better approach which is nonperturbative is through an elementary application of Lanczos algorithm. This involves the evaluation of moments of the Hamiltonian \( H \) in the determinantal state \( \Psi \). If we restrict
ourselves to the model space consisting of 0ph, 1ph and 2ph states then we can reduce the energy eigenvalue problem to the diagonalization of a 2x2 matrix whose elements are given in terms of the first three moments of the Hamiltonian in the state $|\Psi\rangle$. This method provides an exact solution of the system in the model space.

(b) The energy variance minimization method described in this thesis may be modified to include constraints. If one can minimize the energy variance of a determinant at a given energy then one has the best s.p. basis (in the sense of minimum width) at that energy. This will be helpful in the study of level densities etc.

(c) As already mentioned in Chapter III, it will be interesting to investigate whether the expectation values $\langle \Phi | \hat{P}^p | \Psi \rangle$ (p > 2) where $|\Psi\rangle$ is a Slater determinant, also become minimum the neighbourhood of the HF minimum.

(d) The expression for the square of the norm of effective one-body operator which we have derived in Chapter V can be easily extended for the general case by including all those terms which were zero