Chapter 1

INTRODUCTION

The ultimate aim of nuclear physics is to understand the properties of nuclei in terms of those of their constituents – the nucleons – and the interactions among them. However, the nature of the internucleon forces is still far from being precisely known. Even if it were, it would still be extremely difficult to obtain an exact description of the behaviour of a nucleus starting from that of the individual nucleons, due to the nucleus being a many-body system. Any meaningful theoretical treatment of the nucleus must somehow limit the degrees of freedom available to the nucleons. This requirement makes imperative the construction of nuclear models in which only a few degrees of freedom are excited. Efforts are made, as far as possible, at compensating the effect of the neglected degrees of freedom, by renormalizing the actual operators acting on the system to obtain 'effective' model operators.

The shell-model has, by far, been the most successful model in correlating the vast amount of information available about the structure of nuclei in various regions of the periodic table. The basic assumption of this model is that the major effect of the internucleon forces can be absorbed in a common single-particle potential for all the nucleons.
and the remainder can be accounted for by a two-body residual interaction among the nucleons. The common potential gives rise to a set of allowed orbits for the nucleons. The shell-model problem, in all its generality, involves the diagonalization of the nuclear hamiltonian in the infinite dimensional Hilbert space spanned by all possible configurations arising from the distribution of the nucleons in the allowed single-particle orbits. This task is prohibitively difficult. However, the situation is saved by the fact that those configurations which are widely separated in energy, are not expected to intermix appreciably. Thus, in practice, in a specific shell-theory calculation, only a few of the single-particle orbits are considered 'active' and are available for being occupied by the valence nucleons outside an inert closed-shell core. Multiparticle basis states are formed by distributing the valence nucleons among the available single-particle orbits and an 'effective' hamiltonian is diagonalized in this basis. The resulting eigenvalues are associated with the energies of various states of the nucleus and the corresponding eigenvectors are the wavefunctions of these states. These wavefunctions may be further used, together with a set of effective operators, to calculate other quantities of interest, such as, the spectroscopic factors, multipole moments of nuclear states and the probabilities of electromagnetic transitions between various nuclear states.
The starting point in a shell-theory calculation is the choice of a suitable model space and an effective hamiltonian to be used in this space. In general, the effective interaction must take into account not only the parts of the true nucleon-nucleon force not accounted for by the average field, but must also compensate for the neglected interaction and degrees of freedom of the core nucleons. Thus suitable effective hamiltonians are not expected to be related, in a simple manner, to the free nucleon-nucleon interaction and may, in principle, consist of many-body operators. In practice, however, we require the effective hamiltonian to contain \((0+1+2)\)-body terms only. The designing of effective interactions has been proceeding along two main lines:

1. Derivation of the effective interaction from the free nucleon-nucleon interaction (Reaction Matrix Approach)

   This approach was first employed by Kuo and Brown [1] to design an effective interaction for use in the s-d shell. Since then this method has found wide application in shell-model calculations (For reviews of the applications of this method and the underlying perturbation theories see references [2-10]). However, calculations of this type are very complicated and the matrix elements are usually evaluated by taking the first few terms in an infinite perturbation series. Several questions regarding the convergence of the series are still unanswered.
2. Deduction of the effective interaction from a fit of the shell-model quantities (energies, transition rates etc.) to the experimental observations

In one version of this method, the effective interaction between nucleons is assumed to be given by a phenomenological force consisting of a central part, a spin-orbit term, a tensor force, and, possibly, a quadratic spin-orbit term. The strengths and ranges etc. of the various terms are then adjusted to obtain an optimum fit to the experimental data. Typical calculations of this type are reported in references [11-17].

In another version of this method, pioneered by Talmi and collaborators [18-24], the shell-model matrix elements of the effective interaction themselves are treated as adjustable parameters, without specifying the algebraic form of the interaction. This approach is essentially limited to small model spaces; otherwise the number of parameters and thus the number of pieces of experimental data required to fix all the matrix elements will be prohibitively large.

In a third variation of this method, one proceeds by collecting experimental data on nuclei with two valence nucleons only. Assuming simple pure configurations for such cases, the matrix elements of the effective interaction may be directly deduced from the experimental spectra. Schiffer and co-workers [25-27] have analysed a large amount of experimental data on two-particle nuclei. They have also studied the question of finding a general or universal form for the
effective interaction which is able to reproduce the matrix elements obtained directly from the experimental data.

All these procedures of determining the effective interactions have their merits and demerits and we shall not go into their details. We shall, however, briefly discuss how a weighted average of the shell-model matrix elements of the effective interaction may be obtained in a straightforward manner from the experimental data on single-particle transfer reactions. Bansal's generalized energy-weighted monopole sum-rule [28] relates the centroid of the states of the residual nucleus excited in a single-particle transfer reaction, to the occupancies of various orbits in the target state and the average effective interaction matrix elements. We have used this relationship to obtain the average interaction matrix elements in the region of light- and medium-mass nuclei. The results are presented in the Appendix. These average matrix elements provide useful constraints on the nature of the detailed two-body interaction.

Turning now to the choice of the shell-model vector spaces, the past experience is that for nuclei away from a closed shell, it is usually adequate to include orbits belonging to a single major shell, while for nuclei near the closed shells, two or more major shells may often be required. In either case, the desired model space may be too large for the calculations to be carried out. Even when a large calculation is possible, all the detailed information it produces is not really useful
because, generally we are interested in the low-lying states of nuclear systems. It is, therefore, very much desirable to devise effective methods for the truncation of shell-model vector spaces. Several truncation techniques have been used in literature [29-31]. In order to offset the effects of truncation, it becomes necessary to 'renormalize' the effective Hamiltonian designed for the untruncated space. If the truncation effects are small, there is ample evidence [24] that one can construct simple (i.e., one- and two-body, mass independent) renormalized effective interactions for the truncated space. If the truncation effects are large, one must use [30] complicated many-body effective interactions. The determination of the renormalized interaction is, in itself, a tedious job and no really well-defined procedure is available for it.

The aim of the present investigation is to study the efficacy of Weak-Coupling Approximations for cutting down the size of shell-model problems without appreciably affecting the predictions of the untruncated calculations. These approximations are possible extensions of the weak-coupling procedure used by Arima and his co-workers [32] and involve no renormalization of the effective interaction. Our main concern throughout has been to reproduce the results of untruncated shell-model calculations for the low-lying states of nuclei and our weak-coupling approximations are designed specifically for this purpose. The general outline of the procedure is as follows:
Quite often we encounter shell-model problems where the dimensionalities of the Hamiltonian matrices in the desired model space are too large to be handled. We divide the model space into two parts which are expected to retain some degree of individuality within the complete model space and for which separate exact shell-theory calculations can be managed. The relevant parts of the Hamiltonian are exactly diagonalized in the two subspaces. Depending upon the nature of the states we wish to study in the complete system, we choose certain sets of low-lying states of the two subsystems and form product wavefunctions taking one eigenvector at a time from each of the two subspaces. These product wavefunctions span a part of the complete model space for the larger system, and we hope that these have large overlaps with the low-lying eigenstates of the complete Hamiltonian in the larger space. We do not expect these to be directly the good eigenstates of the larger system as would be the case for extreme weak-coupling. Instead, we treat the product wavefunctions as providing us a good basis for calculating the eigenstates in the larger space. By limiting the number of states, from each of the subspaces, to be used for forming this basis, we can keep the dimensionalities of matrices, for the larger system, under control.

The two subspaces, involved in the weak-coupling calculation, may be completely inequivalent, that is, having no single-particle orbit in common, or these may be partially or totally equivalent, that is, having a few or all of the single-
particle orbits common to both. The weak-coupling calculation is relatively easier in the first case because the orthonormality of the wavefunctions in the inequivalent subspaces automatically ensures the orthonormality of the coupled wavefunctions in the complete space. In the second case where the two subspaces have some single-particle orbit(s) in common, the job of antisymmetrization and orthogonalization of the product wavefunctions is much more complex.

The problem of weak-coupling in the case involving equivalent subspaces is dealt with in Chapter 3. One such calculation has been reported earlier by Wong and Zuker [33] for some nuclei in the s-d shell. Our method of calculation is essentially similar to the one used by these authors, but for the sake of completeness, we discuss it in full detail and apply it to calculate the energy spectra of some Nickel-isotopes.

As mentioned earlier, the necessary treatment of antisymmetrization and orthogonalization of the wavefunctions limits the usefulness of weak-coupling calculations involving equivalent subspaces. In the case of inequivalent subspaces, the calculation is much more straightforward. A weak-coupling model for inequivalent subspaces involved in the study of particle-hole states, has been developed by Ellis and England [34]. These authors work with the wavefunctions etc. in a configuration space representation. In Chapter 5, we reformulate the model in a second-quantized representation.
which is more suited to such type of calculations. In that chapter we also give a simple formula for the matrix elements of the residual interaction hamiltonian involved in the calculation of two-particle - one hole states in a nucleus with just one nucleon outside a closed core; with this, we study the even-parity states in $^{41}\text{Ca}$ and $^{41}\text{Sc}$.

Only a few shell-model calculations have been reported in literature for the spectroscopy of heavy nuclei since the dimensionalities of hamiltonian matrices in the desired model spaces become prohibitively large. It is here that the weak-coupling calculations can really prove to be useful. Because of the large neutron excess in heavy nuclei, the active protons and neutrons are usually filling different shells. As suggested by McGrory [35], it is convenient to work in the neutron-proton formalism and divide the model space into a proton space and a neutron space. The proton-proton and the neutron-neutron parts of the interaction are treated exactly and the proton- and neutron-subsystem are then weakly coupled to describe the complete system. Even for nuclei which have active protons and neutrons filling the same shells, it is possible to break up the complete shell-model space into a proton space and a neutron space which are treated as inequivalent. However, the coupled states in this case will not, in general, have good isospin ($T$). It is possible, of course, to form good-$T$ states from those in the n-p formalism but we may have to work in a vector space larger than what would be
required in an isospin formalism. In the present work, we shall restrict ourselves to the case where the active protons and neutrons are in different shells, so that the isospin is a redundant quantum number. The calculational procedure is discussed in detail in Chapter 4. The applications include the study of the energy spectra and electromagnetic transitions in various isotopes of Yttrium, Zirconium and Molybdenum.

Our calculational procedure is based upon the Second Quantized Tensorial Techniques developed by French [36,37]. In Chapter 2, we briefly review the essential features of the formalism and present some basic results that we use later. The representation of the shell-model hamiltonian and electromagnetic transition operators in terms of second-quantized spherical tensors is also discussed.
References to Chapter 1
