CHAPTER I

INTRODUCTION

1. Nuclear Shell Model

Theoretical studies of the structure and properties of nuclei have been made for several years now, within the framework of the independent particle model or the nuclear shell model. The idea of the shell model with the introduction of a strong spin-orbit term was resurrected by Mayer and by Jensen et al, and it has had immense success in interpreting experimental results. The basic postulate of the shell model is that the complex interactions between the nucleons in a nucleus (about which we have very little precise information) may be largely replaced by an overall effective potential field V acting on each nucleon independently. There are already available several excellent reviews on the subject,[1,2] and we may briefly sketch some of the important aspects of the shell model which will be relevant for our subsequent discussions.

The solution of the Schrodinger equation for a nucleon moving in the potential V gives a complete set of orthonormal eigenfunctions, characterised by a set of quantum numbers, and the energy eigenvalues. We now consider the A ($= N + Z$) nucleons of the nucleus to occupy a set of these single particle eigenstates. Such a set of A occupied eigenstates will be

called a configuration. The total nuclear wavefunction in the simplest approximation is the properly anti-symmetrised product (Slater determinant) of the occupied eigenstates.

From an empirical analysis of the nuclear properties such as binding energies, ground state spins and parities, reduced widths of the low lying energy levels etc., we can obtain a rough picture of the single particle energy level scheme. We require that the potential V should, to a reasonable approximation, reproduce this empirical pattern. In all explicit shell model calculations, detailed properties of V do not enter at all. In such explicit calculations, the single particle energy levels, or rather the relative energies of the levels involved, are chosen as given by the experiments. Similarly the single particle wavefunctions are generally chosen to be those of a simple harmonic oscillator with a range parameter suitably related to the nuclear radius. This choice of the wavefunction is primarily dictated by ease in subsequent shell model calculations, and is partly justified by the argument that a harmonic oscillator potential with an appropriate spin-orbit term provides a fairly adequate explanation of the observed single particle level schemes. It should be possible to derive more detailed properties of V by empirical analysis of nuclear properties. Although this appears not to have been done systematically, we note that the inclusion of the spin-orbit term was dictated by the empirical pattern of the magic numbers; or the

observation of large quadrupole moments and transitions for many nuclei indicated that at least for some nuclei the single particle potential must deviate from spherical symmetry[3]. Other features of the potential V have become clear from recent theoretical analysis[4] of the foundations of the shell model. It has been shown from the equality of the binding energy per nucleon in the nucleus that the potential V must have a velocity dependence, so that it has a depth of about 70 MeV for the most tightly bound nucleons and about 35 MeV for the most weakly bound ones[5]. One may also surmise that the shape of the nuclear potential should roughly follow the nuclear density distribution, which can be well described in terms of a Woods-Saxon shape[6],

$$\left[1 + \exp(r-R)/b\right]^{-1}$$

Thus the harmonic oscillator is only an approximation, and it is well known that the use of the harmonic oscillator wavefunctions gives rise to incorrect binding energy results.

The other important concept underlying the shell model is that of the configuration space. We have defined the configuration as a set of particle states occupied by individual nucleons. A state of a given configuration is obtained by suitably coupling the angular momenta, spins and isotopic spins of individual nucleons to obtain the total angular momentum etc. Of course, the overall nuclear wavefunction must be made fully antisymmetric in all the

nucleons. In general, a given nuclear state may then be obtained by superposition of the suitable states of one or more configurations. In the lowest approximation the configuration space chosen is one dimensional i.e. only one configuration is assumed to describe the nuclear state satisfactorily. Various specialised versions of shell model are obtained depending upon the choice of the configuration space. For studying some detailed properties of the nuclear states it may be necessary to extend the configuration space to many dimensions, i.e. consider superposition or mixing of many configurations. In general the configuration space chosen depends upon the nature of the problem, the relative importance of the nearby configurations, and the ease of computation. It has been customary in shell model to include only the few energetically lowest configurations, and diagonalise the Hamiltonian matrix constructed in this limited space. The analysis of Brueckner and others[4] has provided an understanding of the validity of this procedure.

We may point out that in the model as described hitherto, there is considerable degeneracy in energy of nuclear states, i.e. there will exist several states with different spins J, but all degenerate in energy. For example, if we describe the nucleus O^{18} by the simple choice, viz., configuration $(d_{5/2})^2$, it will have three states with total angular momentum $J = 0, 2,$ and 4. Energetically, all the three states are degenerate, since they arise from the same configuration. Such degeneracies

are, however, not experimentally observed. To account for the observed splitting of these states, the shell model now introduces interactions between the nucleons; in other words correlations amongst the nucleons (which were till now considered independent), but only as small perturbations. It should be remarked that some correlations are already imposed by the action of the Pauli principle, and should be distinguished from these additional correlations which are now introduced empirically. The choice of these perturbing interactions has also been largely dictated by the ease of computation. Intuitively, one may characterise these inter-nucleon forces as residual effective interactions after the single particle potential V is extracted from the exact many body problem. In absence of apriori knowledge of these interactions, it has been customary to choose them in the variational spirit with a number of free parameters to be determined by comparison with the experimental results.

These nuclear interactions which we shall call effective interactions (they have also been referred to as psuedo potentials) are considered rather weak, so that the Hamiltonian matrix can be evaluated in Born approximation (first order perturbation theory) and the configuration mixing introduced (in particular high configurations) is small. They are generally chosen as central two-body forces of the form

$$V_{12} = V_0\left[A_0 + A_1 M + A_2 B + A_3 MB\right] f(r_{12}) \qquad (1.1)$$

where M, B are the space and spin exchange operators (Majorana and Bartlett) and A_K are constants. The function $f(r_{12})$ of the distance between the two nucleons is chosen of the Gaussian or Yukawa shape, although a square-well or a δ-function are also occasionally used. Some calculations have also been made with inclusion of tensor or two-body spin-orbit forces. We should also add that, generally, more than two-body forces are neglected, and there are some phenomenological calculations which show that this seems to be a reasonably good approximation[7]. In general, then, we would have a very large number of arbitrary parameters in the interaction, and unless enough experimental data is available, or a systematic investigation can be made, or unless there is additional justification for choice of some of the parameters, it would be difficult to attach much physical significance to such empirical nuclear interactions. It does not appear to us that a satisfactory investigation on the nature of V_{12}, its uniqueness in a particular case, or for a group of nuclei, or a variation of its parameters as we go from one nucleus to another has been reported. Perhaps there has not been enough experimental data.

Even with the rather stringent limitation of only two-body central interactions, we find that most of the authors have chosen different interactions mostly as a matter of expediency. Table 1 lists some of the interactions reported in the literature; the list though not exhaustive, is representative. Listed are strengths of

Table 1

The relative strengths of the interactions, P_{ij}, in states with $i = 2T + 1$ and $j = 2S + 1$. P_{13} denotes the strength of interaction in $T = 0$, $S = 1$ state and is normalised to unity.

Author \ P_{ij}	P_{33}	P_{11}	P_{31}	P_{13}	Reference
Rosenfeld	-0.34	-1.78	0.60	1.0	8
Inglis	-0.60	-1.00	0.60	1.0	8
Soper	0.15	0.00	0.46	1.0	9
Meshkov & Ufford	0.20	-0.20	0.60	1.0	10
Talmi & Unna	-0.39	-0.37	0.51	1.0	11
Barker	0.38	0.81	0.50	1.0	12
Elliott & Flowers	-0.26	0.50	0.70	1.0	13
Peaslee	0.00	0.56	0.34	1.0	14
Pandya & Shah	1.10	0.78	0.43	1.0	15

the interaction in various spin and isotopic spin states of two nucleons, for example P_{31} denotes the strength of the interaction in $T = 1$, $S = 0$ state (singlet even). These are related to A_k of equation (1.1) by

$$\begin{aligned} P_{13} &= A_o + A_1 + A_2 + A_3 = 1 \quad \text{(normalisation condition)} \\ P_{11} &= A_o - A_1 - A_2 + A_3 \\ P_{31} &= A_o + A_1 - A_2 - A_3 \\ P_{33} &= A_o - A_1 + A_2 - A_3 \end{aligned} \tag{1.2}$$

It has been generally found that the effective two-body interaction appears to have a rather long range - of the order of the nuclear size - compared to the range of the free nucleon-nucleon interactions. Table 1 shows that there seems to be little agreement on the exchange nature of the interaction. These effective interactions do not appear to be of the Serber type. In particular, the forces in the odd states seem to be much less well determined, compared to the even states, for P_{31} appears to have a rather well defined value of ≈ 0.55.

A major aim of the work reported in this thesis is to attempt a systematic study as far as possible of the nature of the effective nuclear forces. The investigations of Brueckner et al previously mentioned have given considerable insight in the general qualitative nature of the effective interactions. In the next section we outline some of the ideas of the Brueckner theory, and then make

additional remarks on the problem of the effective nuclear interactions.

2. Brueckner Theory

The nuclear shell model as described in the previous section is an empirical model. It is based on an assumption that the nucleons in a nucleus move independently of each other in a common potential well; in other words, the Hartree-Fock procedure of atomic spectroscopy can also be applied to study nuclear spectra. The work initiated by Brueckner et al and carried on, extended and expanded by many investigators has now enabled us to understand why the shell model procedure has been so successful and has actually provided a more rigorous and somewhat modified Hartree-Fock procedure for application to nuclei.

2a. Realistic two-body potential

Any theoretical study of the nuclear structure starting from the first principles necessarily needs a complete knowledge of the nucleon-nucleon forces. A satisfactory procedure would be to obtain firstly from a theory of elementary particles the nature of the nucleon-nucleon forces, and then to proceed to solve the Schrödinger equation for the many-body problem with these interactions. However, at present, it is not even possible to derive the nucleon-nucleon forces rigorously from Meson theory. Our present knowledge of nuclear

forces is derived in a semi-phenomenological manner from a study of two nucleon systems such as the deuteron and the nucleon-nucleon scattering experiments. Two-nucleon potentials can be chosen to fit the experimental data and static as well as velocity-dependent or non-local forces have been used. Although non-local potentials have been explored by several authors, the static potentials, particularly those associated with the names of Gammel-Thaler and Signell-Marshak appear to be more popular. It is now known that the interactions are strong, short ranged, have a hard repulsive core (which may be simulated by a non-local, non-singular potential) and are spin- and isotopic-spin-dependent. The potentials have central, tensor and spin-orbit terms and taking our cue from meson theory, they are given Yukawa shapes, i.e.

$$V = \infty \qquad r < r_c$$
$$= V_0 \left[\exp(-\mu r)\right] / \mu r \qquad r > r_c .$$

The strength and range (V_0 and μ) in various states (TS) can be specified, although not always unambiguously. The forces in T = 0 states are not precisely or unambiguously determined. We give in table 2 a set of parameters obtained by Gammel and Thaler[16]. These parameters have been used for nuclear spectroscopy calculations by Banerjee and Dutta Roy[17]. (For other sets of potentials also used in nuclear calculations see N. Meshkov[18] and Dawson, Talmi and Walecka[19].

Table 2

Parameters of the Gammel-Thaler potentials.
The potentials have the Yukawa shape $V_0[\exp(-\mu r)]/\mu r$ outside an infinite repulsive core of radius 0.4 fm[16].

State	Strength V_0 (MeV)	Inverse range μ $(fm)^{-1}$
Singlet even	-434	1.45
Triplet odd		
Central	-14	1.00
Tensor	22	0.80
Spin-orbit	-7315	3.70
Singlet odd	130	1.00
Triplet even		
Central	-877.4	2.091
Tensor	-159.4	1.045
Spin-orbit	-5000	3.70

Two points should be made. Firstly, although the role of non-local potentials is not yet clearly established, there seems to be an increasing awareness of their importance in view of the fact that they are non-singular and easy to handle in applying to calculations of nuclear structure. Secondly, one should remember that the analysis of two-nucleon systems only gives knowledge of nucleon-nucleon forces "on the energy shell". Matrix elements of the interaction "off the energy shell" can only be studied from more-than-two-body systems, such as H^3, He^3 or scattering of nucleons by deuterons etc. There is further the problem of possible existence of three-body or many-body forces[20,21] and the best that can be said is that at present there seems to be no definite phenomenological evidence in favour of their existence.

2b. Reaction Matrix

We have now to consider the nucleus as an assembly of a large number of nucleons (A) interacting via the strong, short-ranged interactions described above. The total Hamiltonian is given by

$$H = \sum_{i=1}^{A} T_i + \sum_{i<j} V_{ij} \qquad (2.1)$$

where T_i = kinetic energy of the i^{th} nucleon and V_{ij} the two-body interaction potential. The energy of the system can be calculated from the Schrödinger equation

$$H\Psi = E\Psi \tag{2.2}$$

The conventional Hartree-Fock procedure cannot be followed to obtain a solution of the above equation, when the Hamiltonian contains strong (and infinite in static case) forces. The achievement of the Brueckner theory is to provide a modified prescription for the evaluation of the energy of the state. This can be described as follows:

Introduce a single particle potential V_i operating on each nucleon i. Then a single particle wave equation can be written:

$$\left(T_\ell + V_\ell\right)\phi_\ell = \left(-\frac{\hbar^2}{2m}\nabla_\ell^2 + V_\ell\right)\phi_\ell = E_\ell\phi_\ell \,. \tag{2.3}$$

With the solutions ϕ_ℓ and the single particle energies E_ℓ of the above equation, we construct a "reaction matrix" or a K - matrix,

$$(\ell m|K|rs) = (\ell m|V_{ij}|rs) + \sum_{pq} (\ell m|V_{ij}|pq)\frac{Q}{\Delta E_{pq}}(pq|K|rs) \tag{2.4}$$

where the matrix elements in the space of the single particle states ϕ_ℓ etc. are denoted by the well known bracket notation, and ΔE_{pq} is the excitation energy of the two particle state (pq)

$$\Delta E_{pq} = E_\ell + E_m - E_p - E_q \,. \tag{2.5}$$

The projection operator Q takes care of the exclusion principle, and is zero for all states for which $\Delta E_{pq} = 0$ or approximately zero - as we discuss later, and $Q = 1$ otherwise. Thus K matrix is obtained from the solution of the above integral equation. Next, a self-consistency requirement is imposed by condition that the single particle potential should be given by

$$(l|V|m) = \sum_n \left\{ (ln|K|mn) - (ln|K|nm) \right\} . \quad (2.6)$$

Thus the potential V obtained from the above equation should be identical with the potential with which we started in the equation (2.3), $V_l = (l|V|l)$. When the self-consistency requirement is satisfied, one may obtain the so-called energy shift,

$$\epsilon_{lm} = (lm|K|lm) - (lm|K|ml) \quad (2.7)$$

and the total energy E of the system is then

$$\begin{aligned} E &= \sum_l T_l + \sum_{l<m} \epsilon_{lm} \\ &= \sum_l T_l + \frac{1}{2} \sum_l V_l \ . \end{aligned} \quad (2.8)$$

We do not go into the details of the Brueckner theory, since these are adequately described in literature, and the present work does not deal with it. It is enough to point out that the determination of the

energy shift or the energy of the system is very similar to the usual Hartree-Fock method, except that here instead of the simple two-body interaction V_{ij}, one uses the reaction matrix K.

Let us summarise some of the results of the Brueckner formalism which are of interest to us.

(i) The single particle potential V occuring in the above formalism is a non-local potential, and therefore clearly the question arises as to how far it is proper to approximate it by the harmonic oscillator potential. We do not know about this, but most of the calculations on nuclear spectroscopy that have been recently performed following the ideas of Brueckner[17,18,19,22,23] appear to avoid this problem and use harmonic oscillator wavefunctions ϕ_ℓ to evaluate the reaction matrix. Banerjee and Dutta Roy remark that this procedure will not produce any large errors.

(ii) Although the two-body interaction V_{ij} is singular containing infinite repulsive core etc., it turns out that the K-matrix is much weaker, finite and analytically smooth and well-behaved. Thus it is possible to justify the use of first order

perturbation theory for the K-matrix (or its approximations i.e. the effective interactions), whereas for the V-matrix, this would lead to infinities. On the other hand even if the V_{ij} is local, the K-matrix is non-local and density dependent, as well as dependent on the configuration of the shell model states that is being considered. Thus in a strict sense the K-matrix is not a two-body operator, but for a given configuration space, it may be approximately considered as a two-body potential.

(iii) The effective nuclear interactions that have been used in shell model computations should not then be compared with the real nucleon-nucleon interaction V_{ij}, but should be regarded as approximate models of the K-matrix. Thus one should not expect them to have hard-cores or saturating properties etc.

(iv) One of the most important results that emerges is a consequence of the Pauli principle operating in nuclei. It is found that the form of the K-matrix in configuration space differs from V_{ij} only

at short distances $r \lesssim 1\,fm$ (called the healing distance). We shall have occasion to comment on this feature later in this thesis.

(v) In the shell model calculations, it was invariably assumed that for the configuration space one should include only the (energetically) lowest few configurations, and then the Hamiltonian matrix constructed in Born approximation in this space should be diagonalised. This approximation has received justification from Brueckner theory. As may be seen from equation (2.4) the higher two-particle excitations are all included already in the definition of the K-matrix. In practice one defines the operator Q so that in the sum over all excited states, all those states which are approximately degenerate with the ground state are excluded. The "approximately degenerate" has to be defined, but perhaps it is alright to define this to mean all configurations within about 2 MeV of the ground state. This should be adequate for considering the low lying states of nuclei. We shall adopt this definition[17] in our work. It is clear that the form of the K-matrix or the effective interaction will depend upon

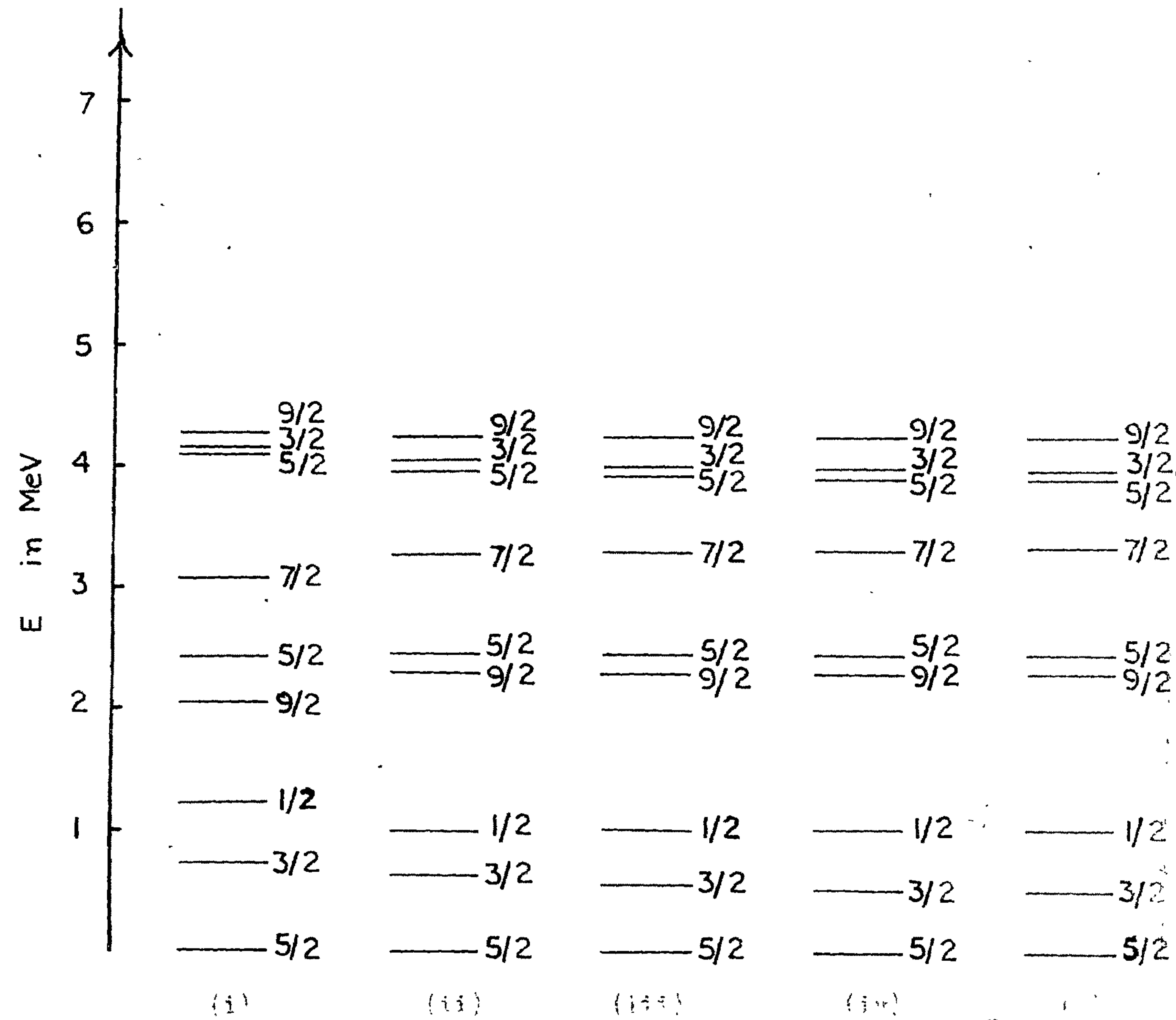
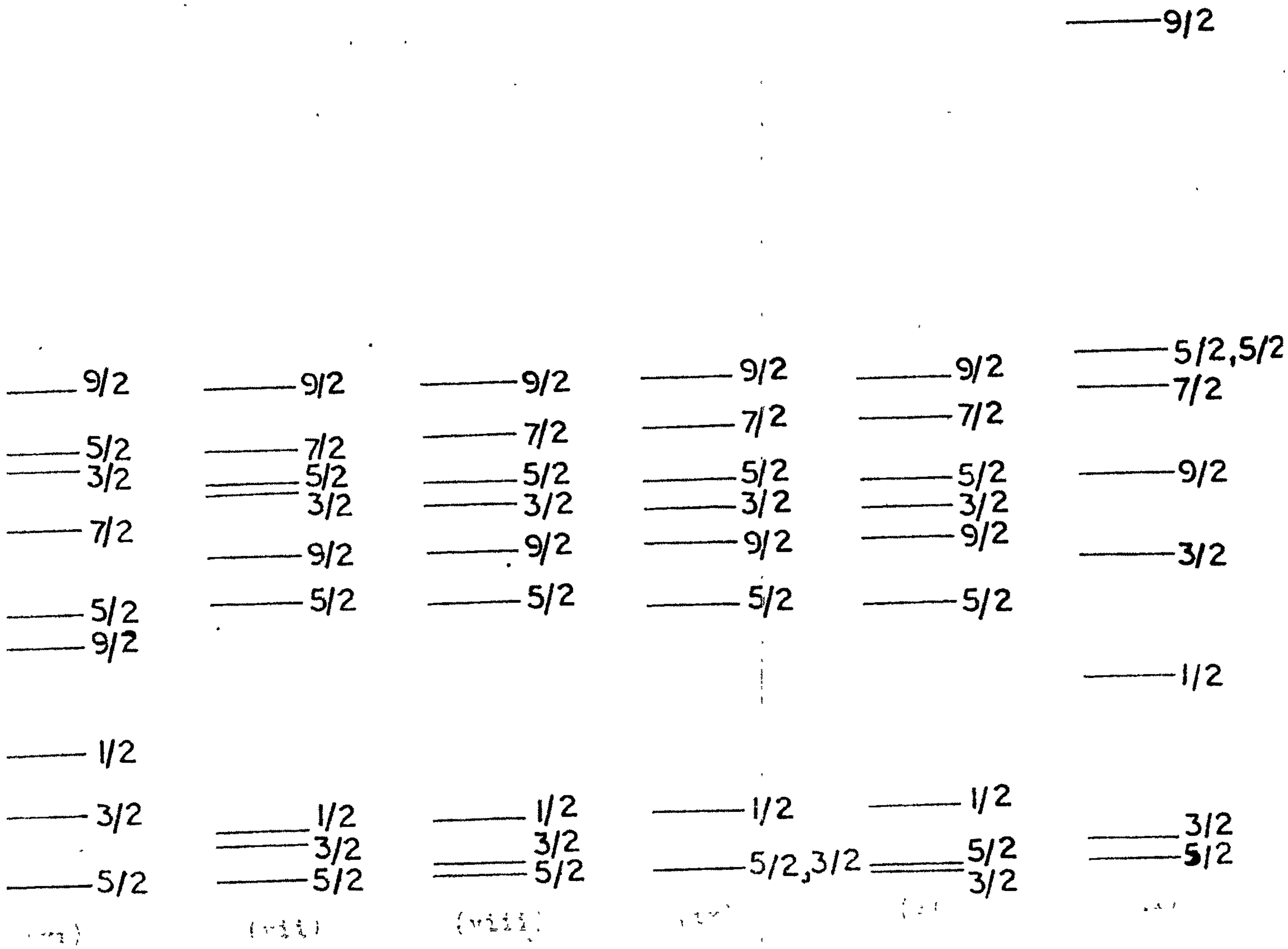


Fig. [illegible] Theoretical energy level scheme for [illegible] ^{19} [illegible] and (v) with parameters of (i) plus [illegible] and V_1 = [illegible].7 MeV λ = 1.[illegible] respectively. [illegible] (iv) and (v) with parameters of (vi) plus [illegible] λ = 1.0; and V_1 = −10.60 MeV, λ = [illegible] respect[illegible]



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the choice of the configuration space in which the Hamiltonian matrix is constructed. Although this was intuitively recognised, it is very well brought out from the Brueckner formalism, and this fact has to be borne in mind while comparing the different effective interactions.

We have summarised the results that are of interest to us, and hope to discuss the results of our calculations of effective interactions in various nuclei in the light of the above concepts.

3. Scope of the thesis

We have seen in the previous section that to evaluate the energy of a nuclear state, one must evaluate the corresponding K-matrix. The practical evaluation of the K-matrix for finite nuclei, is however quite difficult, particularly for potentials which are singular and contain infinite hard cores. As we mentioned above, the actual self-consistency problem is generally not attempted; even so the evaluation of the K-matrix involves a considerable amount of numerical computation. Since the work in this thesis was begun, several calculations[17,18,19] have been published which evaluate the K-matrix for various potentials and the energy levels of some nuclei. Although larger and larger number of such calculations will be performed in the near future, it would perhaps still be

desirable to have a simple model interaction, an approximation to the actual K-matrix which one can use in shell model calculations quickly, simply and effectively, to calculate the nuclear energy levels.

Usually, in the shell model calculations of nuclear spectra, one assumes some interaction as discussed in the previous section and calculates the resulting spectrum for comparison with experiment. In recent years an alternate procedure is also widely used. This is to take the observed spectrum and deduce from it some properties of the effective interaction. This process can be described as follows: For a given nucleus experiments may provide spins and parities and energies of a number of low levels. Other experiments such as stripping, or pick up of a nucleon or electromagnetic transitions might provide some information regarding the wavefunction of these states. If we have thus enough information on the eigenvalues (energies) and the eigenfunctions of different states, it may be possible to invert the Hamiltonian matrix (completely or partially) to obtain explicitely (all or some)the matrix elements of the interaction. We shall discuss it in detail later, but only mention it here that this entire procedure depends upon the choice of a suitable configuration space. Thus from a given nucleus or several nuclei of neighbouring mass values involving the same configurations, it may be possible to extract several matrix elements of the interaction. These matrix elements may then be analysed further

to obtain some properties of the effective interaction and its parameters. With some luck and enough experimental data, one may be thus able to obtain some information on the variation of the K-matrix with mass or configurations of nuclei etc. In chapter II we discuss in detail the methodology adopted by us. We would like to consider that the method of approach and analysis presented here is an important contribution, and a very useful one, whether or not the results obtained in this and subsequent chapters are completely satisfactory. This technique is then applied to simple nuclei such as Li^{6}, O^{18}, Ti^{50} etc. The energy levels are analysed and the results on effective interactions are presented.

In chapter III we present some additional calculations on the nuclei O^{18} and O^{19}. Combining the available information on these two nuclei, it is possible again to obtain more information on the nature of the effective interaction.

An additional investigation carried out during the course of this work is presented in the Appendix. This includes an analysis of effective nuclear interaction in $s_{1/2}$-$d_{3/2}$ subshell.

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