Part I

* Shell Model Studies of Nuclear Spectra *
Part I: SHELL MODEL STUDIES OF NUCLEAR SPECTRA.

CHAPTER I: Introduction

The basic postulate of the shell model is that the nucleons inside a nucleus move independently and the overall interaction between the nucleons can be replaced by an effective potential field $V$ acting on each nucleon independently. Such a spherical shell model potential is found to be valid only for nuclei having a few nucleons (or holes) outside closed shells. In making a shell model calculation of nuclear spectra one has to resort to several simplifying assumptions. It is assumed that the nature of the single-particle potential in nuclei with closed shell plus a few extra nucleons is exactly the same as for a nucleus with closed shell plus one extra nucleon. In other words, the single particle wavefunctions are generally chosen to be those of a simple harmonic oscillator type and the single-particle energies, appropriate to the nucleus under study, are taken from experimental levels for a nucleus with one nucleon outside the closed shell. In addition one has to assume the proper coupling scheme, the configuration space and some effective interaction between the nucleons.

The harmonic oscillator wavefunctions have been found to be very handy in all shell model calculations and give the single particle level schemes quite satisfactorily with the proper strength for spin-orbit coupling. The spin-orbit coupling was originally introduced by Mayer and others to explain the magic numbers. There is now a considerable evidence that it is real. A nucleus with magic neutron or proton (or both) number is called a closed (or doubly closed) shell nucleus. The
strength of the spin-orbit coupling defines the coupling of the shell model nuclei. If this term dominates we get the JJ-coupling in contrast to I2-coupling, A Jj-coupling configuration involves several JJ-coupling configurations, and the interactions between them. Generally Jj-coupling has been used in the shell model calculations except for very light nuclei. The strong faith in this coupling, however, is based on its accurate description of nuclear spectra. The agreement in many cases has been remarkable.

The next important concept in the shell model calculations is that of the configuration space. A configuration space is defined as the set of configurations of extra-core nucleons for which the Hamiltonian matrix is to be constructed. A configuration, however, defines a set of quantum numbers giving the state that are occupied by the individual nucleons. Thus a complete configuration space is given by the product of so-called states of one or more configurations. The question whether configuration mixing of all these states of the individual nucleons forming a new particular nuclear state is important or not is not a matter of belief or arguments. In the case of every nuclear state it is decided by the ratio of non-diagonal matrix elements to the separation of the corresponding perturbing levels. The effect may be negligible for certain levels and more important for others. However, in shell model calculations generally it has been assumed that only
the lowest few configurations with energies 'nearly degenerate' with ground state configuration need be mixed to obtain the low-lying energy levels. This assumption has received its justification from the recent works of Brueckner and others. This theory has provided a theoretical basis to many of the procedures followed in shell model calculations. It is on this basis that the shell model is now thought to be the basic model upon which the entire nuclear structure theory has to be built up. The study of configuration mixing effects, in a way, takes account of the collective effects in a nucleus.

Finally, we discuss the effective interactions without which the shell model calculations of nuclear energy levels can not be carried out. No theoretical derivation for this quantity has yet been given; this rather makes it impossible to know a priori whether the shell model can be used for the calculations of nuclear energies. This leaves us with the only choice of making such calculations for specific nuclei. Various authors have calculated the level spectra for various nuclei and configurations in an attempt to find the effective nuclear interactions in a particular case. Mention may be made of the two different approaches, followed by Talmi and his collaborators and by Pandya and his collaborators. Talmi group determines the effective nuclear interactions from the experimental energies whereas Pandya group assumes a particular type of interaction and predicts the energies to be compared with the experimental data. Talmi rewrites the experimental data in terms of numerical values of the matrix elements of the effective nuclear interactions and obtains the parameters
of his model by least square fit. Evidently such an approach
is very useful in correlating a large amount of experimental
data and then predicting new levels. Such a technique is
obviously independent of any detailed assumption regarding the
explicit nature of the two-body interaction and the independent
particle wave functions. Hence such an analysis cannot by its
very nature, yield any information on the properties of the
phenomenological two-body interaction\(31\). Since the aim of our
present study is to derive the nature of the two-body effective
interaction, we adopt the method used by Pandya and perform the
shell model calculations assuming a particular form \(w\) for the
effective two-body forces. However, the choice of an effective
interaction is generally done with some arbitrariness. Simplicity
and inclusion of several empirically adjustable parameters, e.g.,
range, depth, exchange nature etc. are the main considerations
for such effective forces. Usually central forces with no hard
core or central repulsive regions (monotonic behavior) are
assumed for simplicity in calculations. Then the parameters are
adjusted to reproduce as much as possible the observed features
of the spectra and to predict additional levels or other
properties.

The most general form for the central two-body interaction
can be written as

\[
H_{12} = \left[ A_0 + A_1M + A_2B + A_3MB \right] V (r_{12}) \quad ---(1.1)
\]

where \(M\) and \(B\) are respectively space and spin exchange operators
(Majorana and Bartlett) and \(A_k\)'s are constants. The constants
are so normalized that

\[
A_0 + A_1 + A_2 + A_3 = 1 \quad ---(1.2).
\]
The radial dependence has been chosen to be of Gaussian shape

\[ V_0 \exp \left[ - \frac{(r/r_0)^2}{2} \right] \]  

as a matter of convenience in computations; \( V_0 \) and \( r_0 \) being the strength and range of the potential. Since in the evaluation of the Hamiltonian matrix in a given configuration space, we shall consider states with definite isotopic spin \( T \), so that \( MB = \pm 1 \), expression (1.1) giving the exchange character\(^{36,37} \) can be directly written in the form

\[ H_{12} = \left[ a + b \begin{pmatrix} \sigma_1^+ \cdot \sigma_2^+ \end{pmatrix} \right] V_0 \exp \left( -\frac{r^2}{r_0^2} \right) \]  \( \text{---(1.3)} \)

where

\[ a = A_0 \pm A_3 \quad \text{and} \quad b \begin{pmatrix} \sigma_1^+ \cdot \sigma_2^+ \end{pmatrix} = (A_2 \pm A_1) 0 \]  \( \text{---(1.4)} \).

Putting in terms of triplet \((S = 1)\) and singlet \((S = 0)\) strengths, we get

\[ H_{12} = \left[ V_t \begin{pmatrix} \pi_t \end{pmatrix} + V_s \begin{pmatrix} \pi_s \end{pmatrix} \right] V \left( r_{12} \right) \]  \( \text{---(1.5)} \)

with

\[ \begin{pmatrix} \pi_t \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 3 + \sigma_1^+ \cdot \sigma_2^+ \end{pmatrix}, \quad \begin{pmatrix} \pi_s \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 - \sigma_1^+ \cdot \sigma_2^+ \end{pmatrix} \]  \( \text{---(1.6)} \)

and

\[ V_t = a + b \quad S = 1 \]

\[ V_s = a - 3b \quad S = 0 \]  \( \text{---(1.7)} \).

The parameters \( V_t \) and \( V_s \) in expression (1.5), giving the triplet and singlet strengths of the potential, are to be evaluated from experimental data. These parameters can be connected to the coefficients \( A_{TS} \), defined by Barker\(^{36} \), through the following relations, for \( T = 1 \) states

\[ A_{10} = \frac{1}{V_0} (a - 3b) = V_s/V_0 \]  \( \text{---(1.8)} \)

\[ A_{11} = \frac{1}{V_0} (a + b) = V_t/V_0 \]

However, the effective interactions derived above are different from the interactions between 'free' nucleons. The interaction between free nucleon is highly singular and leads
to strong short range correlations between them. Shell model wave functions contain no such correlation and therefore do not furnish an exact description of nuclear states. Still, under certain conditions, these functions can be used for energy calculations. To do this it is necessary to introduce the effect of the short range correlation into the interaction Hamiltonian. Under favourable conditions this modification results in the replacement of the free nucleon interaction by a 'reaction matrix'. This is then used as an effective interaction for calculations of nuclear spectra. Several such calculations have been made\(^3\). Although this approach is most satisfactory but, in practice, apart from our incomplete knowledge of the free nucleon-nucleon forces, the mathematical difficulties in deriving the reaction matrix, explicitly for finite nuclei are so many that one certainly requires a large computer. In view of this, usual shell model calculations are very useful for learning the effective nuclear interactions in different nuclei. We shall be contented here with such calculations only. It may, however, be mentioned that Pandya\(^4\) has recently constructed a simple analytical model for the effective interactions (using experimental data on oxygen isotopes) instead of the hypothetical and highly simplified forces mentioned above. Taking the available experimental data for the spectra of several nuclei having essentially the same configuration, the Hamiltonian matrices are inverted to obtain matrix elements of the interaction in various two-particle states. The matrix elements (or Talmi integrals) deduced in the above fashion may then be compared directly with the results of calculations of "reaction matrix". A determination of such Talmi Integrals of the effective
interaction by nuclear spectroscopy calculations, rather than the labourous reaction matrix evaluation, in several nuclei may yield considerable information from a phenomenological point of view on the properties of the reaction matrix in nuclei and ultimately also on the nature of the free nucleon-nucleon force. It is hoped that in future many more calculations will be done in this direction so as to get the free nucleon-nucleon interaction, which is a real effective nuclear interaction, by using only the simple shell model calculation techniques. Pandya's study for oxygen isotopes has pointed out that the singlet even forces are rather short ranged and have a repulsive central region (first time shown by simple shell model calculations). Further triplet odd state interaction is pointed out to be complex in nature and should not be approximated in a shell model calculation by a simple monotonic central potential such as a Gaussian or a Yukawa potential.

In conclusion of this chapter, mention may be made of some other properties observed in shell model spectra. In shell model nuclei if jj-coupling scheme were exactly valid, it is expected that the level spectrum derived for a particle-particle configuration would be exactly identical with the level spectrum of the nucleus having the same hole-hole configuration. However, certain exceptions to this description have been noticed in the examples of \( K^{38} \rightarrow \text{Cl}\text{34} \) and \( S^{33} \) (or \( \text{Cl}^{33} \)) \( \rightarrow \) \( K^{39} \) pairs having the configurations \((d_{3/2})^{-1} (d_{3/2})^{-1} \) \( \rightarrow \) \((d_{3/2})^{1} (d_{3/2})^{1}\) and \((d_{3/2})^{1} \rightarrow \) \((d_{3/2})^{-1}\) respectively. The energy levels given by the configuration \((d_{3/2})^{1} (d_{3/2})^{1}\) are found to be a better approximation in \( K^{38} \) rather than in \( \text{Cl}^{34} \). There exists no
theoretical explanation for such a phenomena. The only generally accepted arguments is that jj-coupling scheme has a better validity near the end of the subshell than at the beginning.

The energy levels of a hole-particle configuration can be directly derived from the particle-particle configuration\textsuperscript{41,42} Pandya\textsuperscript{41} has derived a theorem connecting a proton (or neutron) hole and a neutron (or proton) configuration with the proton (or neutron) and a neutron (or proton) configuration. The method is independent of the nature of the two-body interaction. Goldstein and Talmi\textsuperscript{42} have obtained the same results by using the actual numerical values of the coefficients of fractional parentage. The application of these considerations can be taken as an indication whether jj-coupling is a good approximation or not. It may be noted that the relations between the particle-hole configuration and the particle-particle configuration are different for LS-coupling and jj-coupling. Such considerations can also be applied to even-even nuclei, showing a proton (or neutron) hole and a proton (or neutron) configuration, by introducing the proper antisymmetrisation.

Finally, mention may be made of an interesting feature noted in the single particle nuclei. One observes the crossing of levels belonging to neighbouring major shells\textsuperscript{19}. As a typical example of light nuclei, may be taken, the spectrum of $^0\text{O}_\text{17}$ whose ground state is $1d_{5/2}^1$. Experimental data on $^0\text{O}_\text{17}$ shows that $1f_{7/2}$ state occurs lower than $1d_{3/2}$. Various statements have been made about the separations of major oscillator shells from each other and here is an example of how
schematic such statements are. When we approach the closure of 1d-2s shell, the addition of more and more $d_{5/2}$ nucleons would, presumably, interact strongly with $d_{3/2}$ nucleon and lower its position relative to $f_{7/2}$ orbit. Thus we notice that the order of single-particle levels depend critically on the occupied orbits and may differ considerably from any schematic picture. In heavier nuclei, usually one does not observe such crossings and the levels belonging to different major shells are separated by clear gap.

In the next chapter we discuss the method of calculations and the parameters used in our calculations. In Chapter III and IV we consider the specific examples to illustrate some of the concepts discussed here.