CHAPTER - 1

INTRODUCTION

Characterisation of a nuclear system in terms of its symmetry properties and its behaviour in terms of certain statistical quantities is important for the overall understanding of various nuclear phenomena. Here, it is implied that for overall understanding of the system, the vast detailed information is somehow not necessary and only few relevant "statistical quantities" are to be dealt with. There is a clear similarity between this and the statistical mechanics where detailed is glossed over and one deals only with thermodynamical variables which are defined in a statistical sense. It is in this sense that the word 'statistical spectroscopy' /1/ is coined to describe the subject. The spectral distribution methods (SDM) developed by Prof. French and co-workers /2,3,4/ are precisely based on these two underlying principles, namely the symmetry and the statistical spectroscopy. The information derived in statistical spectroscopy falls mainly in three categories:

(i) the level density I(E)dE which gives the total number of states in an energy interval between E and E+dE,

(ii) expectation value of any operator K with respect to hamiltonian eigenvalues and various symmetries, and

(iii) transition strength of various operators R(E,E') between hamiltonian eigenstates at energies E and E'.

Each of these is further subdivided /5/ into (a) locally smoothed forms, and (b) fluctuations around the locally smoothed forms. The SDM concentrate on

the behaviour of locally smoothed forms of observables. Fluctuations, which cannot be handled in the same manner as averaged forms, are studied separately. The study of fluctuations requires introduction of ensembles of hamiltonians /5,6/, whose matrix elements are randomly distributed. In other words, fluctuations may be studied through statistical considerations involved in random matrix theories.

In a quantum mechanical system, occurrence of symmetries implies that the eigenstates of the system can be characterised by additional quantum numbers corresponding to symmetry labels. Also, symmetry considerations are useful in finding conserved quantities which lead to selection rules. Some of the obvious implications of symmetries are degeneracies in mass or energy and relationship between energies and transition probabilities. Transformations which leave the hamiltonian of a quantum mechanical system invariant lead to symmetry groups. These groups usually correspond to space-time symmetries of angular momentum and parity arising out of invariance of H under rotations and reflections in a three-dimensional space, and dynamical symmetries like isospin which describe charge independence of nuclear forces. These symmetries are taken care of through complex nuclear spectroscopy, which makes use of second quantisation and spherical tensors in order to account for Pauli's exclusion principle and rotational invariances implied by a spherically symmetric, charge independent hamiltonian. The model spaces can be decomposed into subspaces defined by JT symmetries, thereby causing the dimensionality of states to reduce considerably. For example, in the 2s-1d shell, the four-particle space $(ds)^4$ has dimensionality of 10626. After (JT) decomposition, the largest subset has dimensionality 69. This feature is not very useful as the dimensionality even after (JT) decompositon is very large for higher particle cases even in s-d shell itself.

The standard approach followed in the conventional spectroscopy for studying nuclear properties is this: one starts by defining a Hilbert space which should in principle be an infinite-dimensional Hilbert space but is taken to be finite in practice. A model space is defined by distributing the particles over N single particle states. A hamiltonian is constructed, which acts on a set of basis states defined in the model space. Eigenvalues and eigenvectors are then obtained by the usual diagonalization of hamiltonian matrices. Once the wave functions corresponding to a given hamiltonian are obtained, various nuclear properties like transition rates, expectation values of operators, level densities, etc. can be obtained. Unfortunately, except for the simplest system, an exact solution of such a many-body problem is impossible due to the computational limitations in dealing with large spaces. For example, in the s-d shell which consists of 24 single-particle states, size of the largest JT matrix for $(ds)^4$ is 69, for $(ds)^8$ is 2268 and for $(ds)^{12}$ is 6706. Dimensionality of the hamiltonian matrices increases very rapidly as the number of active particles in the space increases, which causes the model space to enlarge. In the fp shell consisting of 40 single particle states, the largest JT matrix for $(fp)^4$, $(fp)^8$ and $(fp)^{12}$ has dimensionality of the order of 300, 10^5 and 4×10^6 respectively, which is a massive number.

One way of partially overcoming these difficulties is to choose an appropriate basis state such that the dimension of the hamiltonian matrix is appreciably reduced. This procedure is not entirely satisfactory, since it assumes goodness of symmetries, which may not necessarily hold true.

The SDM have proved to be a powerful alternative to the conventional approach. This method deals with the kind of spectroscopy that is well

adapted to study general aspects of nuclear structure like the distribution of levels, goodness of group symmetries and also to search for simplicities in a complicated system. Besides searching for general simplicities, this method allows us to study the details of low-lying states of a nuclear system. A knowledge obtained from such a study is helpful in suggesting a good approximation method for detailed problems.

In SDM, instead of studying the detailed spectrum of various quantities, one deals with their distributions in energy with respect to configuration, isospin, angular momentum, etc. The distributions are examined in terms of their moments /7/, which are in turn expressed as traces of products of operators. These moments are calculable without knowledge of eigenvalues or eigenfunctions. Moreover, in this approach, the model space may be decomposed into subspaces which are defined by various symmetries like U(N), $U(N_1) \otimes U(N_2) \otimes \ldots\ldots \otimes U(N_i)$ of the system. The action of the central limit theorem (CLT) of statistics in spaces of our interest gives rise to further simplicities - it enables us to express smoothed forms of observables in terms of few low order moments only. Through the virtue of CLT, the density of states $\rho(E)$ in large particle number space turns out to be nearly a gaussian. While using SDM, we take advantage of the fact that the many particle nuclear system is dominated by interactions of two or maximum three - body rank. If the body rank of the interaction is much smaller than the number of interacting particles, so that only few particles can interact simultaneously, then the eigenvalue density of states tends to a gaussian as a result of the CLT /8,9,10/. For all interactions considered by us, H is defined by maximum rank - 2, or two - body interactions. The CLT approximation is therefore valid.

In the following sections, we discuss few specific characteristics of SDM like moments, distributions, trace propagation etc.

A Moments and Distributions

In spectroscopy, we start by defining the eigenvalue problem

$$H\Psi_i = E_i \Psi_i \tag{1}$$

where H is the hamiltonian operator, Ψ_i and E_i denote eigenfunctions and eigenvalues respectively, in a model space. We can expand the functions Ψ_i in terms of the basis states ϕ_α, transforming the eigenvalue problem into a matrix problem :

$$\Psi_i = \sum_\alpha C_{\alpha i}\, \phi_\alpha$$

so that the inverse transformation would be

$$\phi_\alpha = \sum_i C^*_{\alpha i}\, \Psi_i \,. \tag{2}$$

A plot of $|C_{\alpha i}|^2$ vs. eigenvalues E_i defines a distribution which can be studied via its energy moments. The p-th moment is defined as

$$M^p = \sum_i |C_{\alpha i}|^2 E_i^{\,p} = \langle \phi_\alpha | H^p | \phi_\alpha \rangle \,. \tag{3}$$

Instead of considering the distribution of a single state α , let us choose a

set of states $\underset{\sim}{\alpha}$, and define average moments for the set $\underset{\sim}{\alpha}$ as

$$M^p_{\underset{\sim}{\alpha}} = 1/d(\underset{\sim}{\alpha}) \sum_{\alpha \in \underset{\sim}{\alpha}} \langle \emptyset_\alpha | H^p | \emptyset_\alpha \rangle \tag{4}$$

where $d(\underset{\sim}{\alpha})$ denotes the number of states or the dimensionality of the space $\underset{\sim}{\alpha}$. In case of continuous eigenvalues, the summation can be replaced by integration. The moments of distribution are then calculated with respect to a weight factor, so that

$$M^p_{\underset{\sim}{\alpha}} = \frac{\int \rho_{\underset{\sim}{\alpha}}(x)\ x^p\ dx}{\int \rho_{\underset{\sim}{\alpha}}(x)\ dx} , \tag{5}$$

$\rho_{\underset{\sim}{\alpha}}(x)$ is called the density of states defined in $\underset{\sim}{\alpha}$-space and x denotes the energy. The moments defined with respect to the state density are called density moments. For a normalized state density, we have $\int \rho_{\underset{\sim}{\alpha}}(x)\ dx = 1$. The first moment $M^1_{\underset{\sim}{\alpha}}$ defines the centroid energy, or centroid of the density function $\Theta\ (\underset{\sim}{\alpha})$.

Equation (4) expresses the moments $M^p_{\underset{\sim}{\alpha}}$ as a sum over all diagonal matrix elements of powers of H which correspond to the trace of powers of H in the basis-state representation. The evaluation of moments for an arbitrary space would involve a large number of matrix elements of the hamiltonian, and is therefore extremely difficult. If however, the space is selected with symmetry considerations in mind, $\underset{\sim}{\alpha}$ defining the irreducible representation (irrep) of some group, methods which rely upon invariance properties of traces become available for the evaluation of moments. Besides, there also

are other advantages - no restrictions regarding the size N of single particle states and the number of active nucleons need to be imposed. Also, for invariant subspaces, the distributions are close to normal and therefore one needs a small number of moments to characterise them.

The advantage of expressing moments in terms of invariant traces is that they are calculable exactly without any knowledge of either eigenvalues or eigenfunctions of the hamiltonian. From equation (4), the centroid of the density function would simply be averaged sum of all eigenvalues. One can deduce an expression for the density function in equation (5) as a sum over a series of δ-functions.

$$\rho_{\underset{\sim}{\alpha}}(x) = \sum_i \delta(x-E_i) \; / \; d(\underset{\sim}{\alpha}) \tag{6}$$

implying a discrete structure for the eigenvalue density of states; which is in general true since the space is finite dimensional. However, in large spaces, with the number of eigenvalues in a small energy interval being much larger, the density of states is assumed continuous.

In terms of the centroid energy, we can define the more significant central moments /11,12/ as:

$$\mu_{p\underset{\sim}{\alpha}} = [1/d(\underset{\sim}{\alpha})] \sum_{\alpha \in \underset{\sim}{\alpha}} \langle \phi_\alpha | (H-M^1_{\underset{\sim}{\alpha}})^p | \phi_\alpha \rangle \tag{7}$$

Obviously, $\mu_{1\underset{\sim}{\alpha}} = 0$. The second central moment is given by

$$\mu_{2\underset{\sim}{\alpha}} = \sigma^2 \; (\underset{\sim}{\alpha}) = M^2_{\underset{\sim}{\alpha}} - (M^1_{\underset{\sim}{\alpha}})^2$$

$\sigma(\underset{\sim}{\alpha})$ defines the width of the density function, which gives the spread about the centroid energy. The higher moments are related to the shape parameters. The first and the second shape parameters namely the skewness γ_1 and excess γ_2 are given by

$$\gamma_{1\underset{\sim}{\alpha}} = \mu_{3\underset{\sim}{\alpha}} / (\sigma(\underset{\sim}{\alpha}))^3 \quad \text{and} \quad \gamma_{2\underset{\sim}{\alpha}} = \mu_{4\underset{\sim}{\alpha}} / (\sigma(\underset{\sim}{\alpha}))^4 - 3 .$$

The relation between moments and the density function can be obtained through a characteristic function $\phi(t)$ defined by

$$\phi(t) = \int_{-\infty}^{\infty} e^{ixt} \rho(x)dx = \sum_{p=0}^{\infty} (it)^p/p!\ M^p \tag{8}$$

so that the state density is given explicitly in terms of moments as:

$$\rho(x) = \int_{-\infty}^{\infty} e^{-ixt}\ \phi(t)dt = \int_{-\infty}^{\infty} e^{-ixt} \sum_{p=0}^{\infty} (it)^p/p!\ M^p\ dt . \tag{9}$$

It is not possible to calculate $\rho(x)$ exactly, as higher order moments are difficult to evaluate. One can nevertheless approximate $\rho(x)$ in terms of its low-order moments. Once the centroid and width of a distribution are known, it is possible to define a gaussian approximation to the density function:

$$d(\underset{\sim}{\alpha})\,\rho_{\underset{\sim}{\alpha}}(E) = \left[d(\underset{\sim}{\alpha}) / \sqrt{2\pi\sigma^2(\underset{\sim}{\alpha})}\right] \exp\left\{ - (E-G(\underset{\sim}{\alpha}))^2 / 2\sigma^2(\underset{\sim}{\alpha}) \right\} . \tag{10}$$

The higher moments can be incorporated into the density of states by defining the density function as an Edgeworth or a Cornish-Fisher expansion /13/ around a gaussian density. For a normal density $\mu_3 = 0$ and $\mu_4 = 3\sigma^4$, $\mu_5 = 0$, etc., so that γ_1, γ_2 and all higher order shape parameters go to zero.

It is important that distributions be describable via their low-order moments. For subspaces defined by group symmetries, nearly gaussian distributions are expected. In choosing the subspace $\underset{\sim}{\alpha}$ which defines a certain symmetry, no assumptions regarding the goodness of the symmetry are made. The choice of $\underset{\sim}{\alpha}$ helps us in learning about the goodness of group symmetries /14/, proving therefore that distribution methods combined with group theory is a good way of investigating group symmetries.

B Evaluation of spectral moments

The spectral distribution methods seek a direct way of calculating moments without evaluating many-body matrix elements. This can be seen as we obtain an expression for the moments of a k-body operator in an m-particle space. Let us consider a general k-body operator O(k). The average expectation of O(k) in k-particle space is

$$\langle O(k) \rangle^{k} = \langle\langle O(k) \rangle\rangle^{k} \; / \; \binom{N}{k}$$

where $\langle\langle O(k) \rangle\rangle^{k}$ denotes the trace of the operator O(k) in k-particle space and N denotes the total number of single particle states. Similarly in the m-particle space, we have

$$\langle O(k) \rangle^{m} = \langle\langle O(k) \rangle\rangle^{m} \; / \; \binom{N}{m} .$$

It is possible to relate the above two averages through a binomial coefficient

$$\langle O(k) \rangle^{m} = \binom{m}{k} \langle O(k) \rangle^{k} \qquad (11)$$

Such an average over m-particle states is called 'scalar' average. It can be considered to be an average over the irreducible representation $[1^m]$ of U(N). The binomial coefficient $\binom{m}{k}$ which propagates the average of O(k) in the defining k-particle space to the rest of the space is called a 'propagator'. If the operator whose average we wish to calculate does not have a definite particle rank, one could decompose it into operators of definite particle ranks. The propagation concept can be generalized to operators of mixed particle ranks. For any operator O having different particle ranks starting from 0 to a maximum rank ν, $O = \sum_{t=0}^{\nu} O(t)$. The total average of O in m-particle space is

$$\langle O \rangle^m = \sum_{t=0}^{\nu} \binom{\nu-m}{\nu-t} \binom{m}{t} \langle O(t) \rangle^t, \qquad (12)$$

The propagation formula for scalar averaging requires input information $\langle O(k) \rangle^t$ for t = 0 to ν particle rank. While dealing with finer averages (i.e. over states defined by subgroups defined by U(N)), the principle remains exactly the same as in the scalar averaging, though the propagators might be difficult to construct. The moments of operators in m-particle space are then evaluated by expressing them as a linear combination of averages over simpler subspaces involving only few particles.

C Central Limit Theorem and Normality of Distributions

As mentioned earlier, the state density can be well described in terms of its low-order moments, through the application of a strong result in statistics namely the central limit theorem (CLT). This can be shown to hold exactly for noninteracting particles. In a noninteracting particle system, the m-

particle eigenvalue density can be expressed as convolution

$$\rho_m(E) = \int \rho_{m-1}(E')\,\rho_1(E-E')\,dE' . \qquad (12)$$

The characteristic function in m-particle space would be

$$\phi_m(t) = \iint e^{itE}\,\rho_{m-1}(E')\,\rho_1(E-E')\,dE'\,dE , \qquad (13)$$

On repeated convolutions, one gets

$$\phi_m(t) = (\phi_1(t))^m \text{ so that } \ln \phi_m(t) = m \ln (\phi_1(t)) .$$

Expanding both the ln-functions in a series in terms of paramters $K_p(i)$ we have

$$\sum_p (it)^p/p!\; K_p(m) = m \sum_p (it)^p/p!\; K_p(1)$$

$$\text{or} \qquad K_p(m) = m\, K_p(1) .$$

K_p are called cumulants of the distribution. These are directly related to the central moments. The first few cumulants are

$$K_1 = \mu_1 = 0$$
$$K_2 = \mu_2 = \sigma^2$$
$$K_3 = \mu_3$$
$$K_4 = \mu_4 - 3\mu_2^2 ,$$

so that the shape parameters can be directly defined in terms of cumulants

$$\gamma_p = K_{p+2} / \sigma^{p+2}$$

For m-particle space, we have

$$\gamma_{p-2}(m) = m K_p(1) / (m\sigma^2(1))^{p/2} = m^{-p/2+1} K_p(1) / \sigma^p(1). \qquad (13)$$

For $p>2$, $\gamma_{p-2}(m) \longrightarrow 0$ as $m \longrightarrow \infty$.

Hence in the limit of large particle number, all shape parameters rapidly vanish. This is the CLT result for noninteracting particles. Essentially, additivity of cumulants indicates that the distribution tends to normality for large m.

Though no rigorous proof of the application of the CLT to the case of interacting-particles has yet been formulated, there are indications that the CLT result continues to hold for interacting particles too. This implies that since the interaction within the nucleus is predominantly two-body in nature, the CLT is expected to work in large particle number spaces as long as the interaction rank remains much smaller than the number of interacting particles.

Analysis of shell model calculations has shown that the shell model spectrum is essentially a gaussian. Calculations using a two-moment and a four-moment distribution for the energy eigenvalues in many particle spectra have been done by Chang and Zuker /15/. Exact shell model calculations in the ds

shell, with JT matrix dimensionalities ranging upto 1200 using a realistic interaction have been compared with moment-method results, and excellent agreement is obtained. A detailed numerical study regarding the origin of normality of distributions has been carried out by French and Wong /8/ and by Bohigas and Flores /9/, suggesting that the gaussian nature of the spectrum is connected with the two-body nature of effective interaction and the direct product nature of the m-particle states. The normality of distributions is quite rigorously proved (for studies belonging to a fixed exact symmetry) using two-body gaussian orthogonal ensembles (GOE) by Mon /10/. It is expected that the extensions of the central limit theorem give rise to the normality of distributions over states of fixed unitary symmetry.

D Applications of SDM

The density of states $\rho(E)$ plays a very important role in SDM. Its statistical implication can be derived from the fact that the eigenvalue density of states is a laplace transform of the partition function. The discrete eigenvalue spectrum can be recovered from the density function using Ratcliff's /16/ procedure. This is described in detail in the fourth chapter. For an approximately normal density function, the region near the centroid where the density of states is large, will have small level to level fluctuations. Error expected in eigenvalue calculations in that region will not be large. As one moves towards the tail region (where the ground state is expected to lie), the density of states rapidly decreases, and level to level fluctuations increase. Values obtained using Ratcliff's procedure are not expected to yield a good eigenvalue spectrum. It then becomes necessary to either consider higher moments or partition the space into configurations.

Accuracy in the calculations increases tremendously, as can be seen by comparing ground state binding energy with exact shell model results.

Apart from binding energies, ground state occupancy /17,18/ is another important parameter which is easily calculable using SDM. Experimentally, one can deduce the ground state occupancy through stripping and pickup reactions. Since they are directly comparable with experimental results, occupancies can be used to test the validity of different effective interactions /17/. Also, occupancies being the expectation value of one-body operator (the number operator), are useful in the study of single particle behaviour inside the nucleus.

An important application of SDM is to obtain the expectation value of an arbitrary operator K with respect to the hamiltonian eigenstates. The hamiltonian H is perturbed by the operator αK, where α is a small perturbative parameter. The eigenvalues of the hamiltonian get perturbed so that $E \to E_\alpha$. The expectation value of K is then expressed as a parametric derivative of the perturbed eigenvalues E_α:

$$K(E) = \langle E|K|E\rangle = \partial E_\alpha / \partial \alpha \Big|_{\alpha=0} .$$

Recently, Halemane /19/ obtained a variety of inverse energy weighted sum-rules by applying SDM to Rayleigh-Schroedinger pertubation expansion of E_α. The second chapter here deals with few inverse energy weighted sum rules. Correction to the ground state binding energy has been obtained in terms of inverse energy weighted sums when the effective interaction hamiltonian H_{eff} is approximated by various model hamiltonians H_{model}. These model

hamiltonians have been constructed by taking different linear combinations of pairing and quadrupole operators. The difference between H_{eff} and H_{model} is small, and is treated as a perturbation. The first correction term to the eigenvalue expression corresponds to K(E), or the expectation value of K as a function of energy E. The second correction term gives the first inverse energy weighted sum, and so on. The results have been applied to ^{20}Ne, which lies in the s-d shell. The PW effective interaction is taken as H_{eff}. This work has partially been done by Ms. Pramila Shenoy /20/ who calculated scalar corrections and few configuration space corrections to the binding energy. This chapter gives a review of her work, and gives a complete result in the configuration space for five model hamiltonians.

Besides the hamiltonian, there are other interesting operators like the number operator n_s, the quadrupole operator Q.Q., other electromagnetic transition operators, etc. whose expectation values are of considerable interest. The SDM provide smoothened forms for expectation values of such operators in terms of energy. Attempts have been made to figure out dependence of smoothened forms on other quantum numbers like J,T. The complete analytical expression in terms of averages of product of operators involves series of orthogonal polynomials defined for the state density function. A similar expansion can also be written down using bivariate orthogonal polynomials (if possible to define) for a bivariate density function. The exact result would require evaluating all terms in the series which would be tedious for higher orders. However, due to the application of the CLT in many-particle system, this approach becomes meaningful as one would obtain a good approximation by using only low-order terms, which are easily calculable. One gets the CLT limit by retaining only linear terms. The third chapter presents a simple

geometrical way to obtain the CLT result for the expectation value of an operator K as a function of one as well as two variables using univariate and bivariate gaussian densities respectively. For the univariate case, the calculations are straight forward, and one defines shift in the eigenvalues due to changes in centroid and width of the given density function. For the bivariate case, we proceed via conditional density $\eta(x|y)$ of the bivariate gaussian $G(x,y)$ to obtain shift in eigenvalues.

The fourth chapter deals with an extensive study of single particle aspect of various nuclei via single nucleon transfer (SNT) reactions. The SDM provide a useful approach for studying these, as most measurable properties of a nucleus are expectation values of one-body operators in the ground state. For example, the occupancies are the expectation values of the number operator. In the ground state, these alongwith other properties are measured via the single nucleon transfer reactions. In this chapter, we calculate further single particle properties namely the centroids and widths for particle removal and particle addition strengths for various nuclei in the s-d, f-p and upper f-p-g shells. These numbers are important for experimentalists as they provide information for the excitation energy in the final nucleus upto which an experiment must be conducted so as to exhaust the entire strength for a pickup or a stripping reaction. The occupancies, centroids and widths are defined in terms of moments $M^p(E)$ of the strength distribution, which are defined through expectation values of operators of the kind O^+H^pO. The centroid for the pickup strength is calculated using two different methods. One of them is the polynomial expansion in which only terms upto linear in energy are considered. In the other method, we use a recent result obtained by Kota and Kar /4/ in which the density of the strength function for a set

of initial and final states is expressed in terms of a bivariate gaussian, which can be easily integrated to obtain moments. For the centroid of the stripping strength, we make use of an identity /21/; the difference between particle occupancy weighted pickup strength centroid and the hole occupancy weighted stripping strength centroid gives the effective single particle energy. It is interesting to study these, as they can be compared with experimentally obtained figures from particle removal and addition centroids. The widths for pickup and stripping strengths are calculated using moments of the bivariate strength function.

The fifth and the final chapter presents a summary of the work done and includes an approach to future problems related to this field.