

INTRODUCTION

In general, theoretical nuclear physicists are interested mostly in the following three problems : (a) The spectrum of low lying states, (b) The wave functions of low lying states, from which nuclear moments and transition rates can be calculated, (c) The level density and other average properties of more highly excited states. Almost all the theories and models are designed to obtain solutions of these three problems, so that the results give best fit with the experimental data.

Until a few years ago, attempts were made to solve these problems by the method of complex spectroscopy. However, as we shall see later, complex spectroscopy has its own drawbacks. Here we give a brief account of conventional complex spectroscopy and its difficulties, because the results of complex spectroscopy provide a check for the new methods which have been introduced and developed recently by French¹⁾, and which we have used to study various problems in this thesis.

The essential features of complex spectroscopy with spherical orbits are based on the use of second quantization and spherical tensors. By using the former, Pauli's antisymmetrization principle is satisfied, while by representing all quantities by spherical tensors we can take into account all rotational invariances implied by a spherically symmetric, charge-independent Hamiltonian. This means that we can decompose the model vector space into subspaces which

are defined by the exact symmetries, angular momentum, isospin and parity and which are invariant under operation of the hamiltonian. For example, in the ds shell, the 4 particle space has dimensionality 10626, but after decomposition by (J,T) the largest subspace has dimensionality only 69. From this example, we realise how important and powerful this feature is. However, it is not sufficiently powerful for more complicated cases; for example, the largest invariant subspace for $(ds)^{12}$ has dimensionality about 7000!

In principle, for nuclear calculations one should consider an infinite dimensional Hilbert space, but in practice we always use finite dimensional space. In conventional spectroscopy, we first set up a hamiltonian defined by its single particle energies and two body matrix elements in a given model space of m particles distributed over N single particle states. These N single particle states form a set of basis states. Then the hamiltonian matrix is formed by calculating matrix elements between these basis states and the eigenvalues and eigenvectors are obtained by diagonalizing this matrix. The eigenvalues and eigenvectors are associated with nuclear energies and wave functions respectively. After obtaining the wave functions, the calculation of transition rates, occupancies and other nuclear properties is very simple.

However, as the number of active particles increases, the dimensionality of the hamiltonian matrix increases rapidly and so does the complexity of the problem. For example, in the ds shell, with 24 single particle states, the dimensionalities of the largest of a (JT) matrix in $(ds)^4$, $(ds)^6$ and $(ds)^{12}$ are 69, 500 and over 6000 respectively. The number of matrix elements for a 6000 dimensional matrix is 1.8×10^7 . It is easy to see that the setting up and diagonalization of such a large matrix is far beyond the ability of sophisticated computers. Moreover, if we consider excitation of particles so as to include the $f-p$ shell (these excitations are necessary to understand some phenomena such as electric quadrupole transitions), the largest dimensionality of a Si^{28} matrix grows by many orders of magnitude.

Besides this difficulty in computation associated with large dimensional matrices, we come across another problem. Large matrices produce large number of eigenvalues and eigenvectors, and except for particular properties like level densities and properties of certain states near the ground states, most of the resulting output is redundant. Also, without redoing the calculation, it is difficult to say how the results depend on the chosen interaction and which aspects of the results are of importance and which are of no particular interest.

The recently introduced Spectral Distribution Methods¹⁾ provide us with a powerful alternate tool to overcome the difficulties mentioned above. This method deals with a spectroscopy which is well adapted to study some general aspects of nuclear structure and also to search for general simplicities in complicated systems. Besides searching for general simplicities, this method also allows us to study the details of low lying states of a nuclear system. Thus Spectral Distribution Method helps us to study the basic structure without going too much in detail.

Instead of attempting a detailed solution of spectroscopic problems, the spectral distribution method adopts a statistical approach. In this approach too we set up a Hamiltonian matrix in a model space of m particles distributed over N single particle states. After that we study how the basis state (formed by the N single particle states) distributes among the eigenstates of the system. In other words, Spectral Distribution Method allows us to study the distribution of various quantities of interest in energy, configuration, isospin etc. Such distributions when averaged over all the states of the system or over appropriate subsets, can be studied by their energy moments. We shall see later that due to a certain statistical "simplicity" in the spectral distribution we need only a few lower moments to describe the system with reasonable accuracy.

Let us now study what are moments. Spectroscopy deals with the solution of the problem, $H\psi_i = E_i \psi_i$ where H is the hamiltonian operator and ψ_i and E_i denote the eigenfunctions and eigenvalues respectively. The functions ψ_i are expanded in terms of a set of basis states ϕ_α as

$$\psi_i = \sum_{\alpha} b_{\alpha i} \phi_{\alpha}$$

This is the usual matrix problem. Let us consider the inverse problem, where the basis states ϕ_α are expanded in terms of ψ_i 's, as

$$\phi_{\alpha} = \sum_i c_{i\alpha} \psi_i$$

Now a plot of $|c_{i\alpha}|^2$ vs E_i defines a distribution of the basis state, which can be studied via its energy moments, the p^{th} moment being defined as

$$\begin{aligned} M_{\alpha}^p &= \sum_i |c_{i\alpha}|^2 E_i^p \\ &= \langle \phi_{\alpha} | H^p | \phi_{\alpha} \rangle \end{aligned}$$

Now if we define M_{α}^p as the average moment over a set of states α then

$$M_{\alpha}^p = \frac{1}{d(\alpha)} \sum_{\alpha \in \alpha} \langle \phi_{\alpha} | H^p | \phi_{\alpha} \rangle$$

where $d(\alpha)$ denotes the number of states in the set α . The first moment $p = 1$ defines the centroid energy of the distribution $M_{\alpha}^1 = E_c(\alpha)$. In terms of the centroid energy the central moments $\mu_{p,\alpha}$ are defined as

$$\mu_{p,\underline{\alpha}} = \frac{1}{d(\underline{\alpha})} \sum_{\alpha \in \underline{\alpha}} \langle \phi_{\alpha} | (H - M_{\underline{\alpha}}^1)^p | \phi_{\alpha} \rangle$$

The second central moment $\mu_{2,\underline{\alpha}} = \sigma^2(\underline{\alpha})$ is given by

$\sigma^2(\underline{\alpha}) = M_{\underline{\alpha}}^2 - (M_{\underline{\alpha}}^1)^2$ and is called the energy variance and describes the spreading of the states about the centroid energy. It is related to the width of the distribution. The higher central moments define the shape of the distribution.

In the evaluation of the spectral moments, we encounter the first simplifying feature of the spectral distribution methods. From the defining expression of moments, we notice that moments are nothing but, to within a dimensionality factor, the traces of appropriate powers of the hamiltonian. Since the traces can be calculated without evaluating the many-body matrix elements, the problem of calculating the moments simplifies to a great extent. The expression for the average of a k-body operator in m-particle states belonging to the symmetry $\underline{\alpha}$ is given by ¹⁾

$$\langle O(k) \rangle^{m\underline{\alpha}} = \frac{1}{d(m\underline{\alpha})} \sum_{\alpha \in \underline{\alpha}} \langle m\alpha | O(k) | m\alpha \rangle$$

and hence the trace is given by

$$\begin{aligned} \langle\langle O(k) \rangle\rangle^{m\underline{\alpha}} &= d(m\underline{\alpha}) \langle O(k) \rangle^{m\underline{\alpha}} \\ &= \sum_{\alpha \in \underline{\alpha}} \langle m\alpha | O(k) | m\alpha \rangle \end{aligned}$$

Using the anticommutation relations for creation and destruction operators (A_i & B_i respectively) the definition

of a k body operator and the properties of particle - hole transformations, it has been shown that ¹⁾

$$\langle O(k) \rangle^{m\alpha} = \sum_{\beta} \langle m\alpha | \rho(k\beta) | m\alpha \rangle \langle O(k) \rangle^{k\beta}$$

where the k particle states have been divided into sets β and summed over all β . This expression reveals an important feature that the trace of a k -body operator in various k -particle spaces ($k\beta$) can be related to the trace of $O(k)$ in the space $m\alpha$. Thus we have another simplifying factor, since a k -body operator is completely specified by its matrix elements in k -particle states (defining space), we see that the trace in the defining space propagates to other spaces by means of the density operator ' ρ '. In general the propagation formula can be written as

$$\langle O \rangle^m = \sum_{t=0}^{\nu} \rho_t^{\nu}(m) \langle O \rangle^t$$

where $\rho_t^{\nu}(m)$ are the density operators and possess the following properties :-

1. $\rho_t^{\nu}(m)$ is a ν^{th} degree polynomial in m .
2. $\rho_t^{\nu}(m) = \delta_{mt}$, $0 \leq m \leq \nu$

Thus, we see that the calculation of moments becomes very straightforward. We first calculate the required moments in a space of very few particles (usually 2), and then propagate this information to desired space with any number of particles.

Another very important simplifying feature is the recognition of the role played by the Central Limit Theorem (CLT) in many particle spaces. By virtue of this theorem, in the limit of large number of particles, the smoothed eigenvalue distributions for most Hamiltonian operators in the given space become close to Gaussian. Analysis of shell model results has shown that the shell model spectrum is essentially a Gaussian. French and Wong (1970)²⁾, and Bohigas and Flores (1971)³⁾ have carried out detailed numerical studies and suggested that the gaussian nature of the spectrum is related with the two body nature of the effective interaction and the direct product nature of the m -particle states. The normality of distribution is now quite rigorously proved (for states belonging to a fixed exact symmetry) using two body Gaussian orthogonal ensembles. The fact that the distributions are close to normal suggests that there exist closely related asymptotic forms for expectation values and strengths of operators.

This idea was the origin of the polynomial expansion⁴⁾ (usually rapidly convergent) for expectation values and strength of operators. These polynomials P_μ are orthogonal polynomials and associated with the eigenvalue density and can be constructed explicitly in terms of the density moments given by

$$M^P = \int \rho(z) z^P dz = \langle H^P \rangle^m = \frac{1}{d} \langle\langle H^P \rangle\rangle^m$$

When the density is gaussian, the polynomials are related to Hermite polynomials H_μ by

$$P_\mu(E) = (\mu!)^{-\frac{1}{2}} He_\mu[(E - E_c)/\sigma] \text{ where}$$

$$He_\mu(z) = 2^{-\mu/2} H_\mu(z/\sqrt{2})$$

E = Energy

σ = Width

and E_c = Centroid of the distribution.

Orbit occupancies are the expectation values of the number operator n_i in the state. It has been shown by Draayer et.al. (1977)¹⁵⁾ that the expectation value of any operator O at E can be expanded in terms of orthogonal polynomials $P_\mu(E)$ as

$$O(E) = \langle O \rangle + \sum_{\mu=1}^{\infty} \langle O P_\mu(H) \rangle P_\mu(E)$$

In Chapter II we have used this important fact to evaluate the orbit occupancies of ground states of nuclei in the mass range $A = 60-80$. The spectroscopic space used consists of the f-p shell and the g $9/2$ orbit and the single particle energies are 0.0, 0.78, 1.08 and 3.0 MeV for $p_{3/2}$, $f_{5/2}$, $p_{1/2}$ and $g_{9/2}$ orbits respectively. We have used the modified fully renormalised Kuo-Brown interaction. The calculated results have been compared with experimental data.

Given a set of moments, one can represent an eigenvalue distribution in terms of these moments. But there does not exist a unique way to do this. It is important that we have a proper representation of the eigenvalue distribution which satisfies certain theoretical and physical norms. In Chapter III we have studied various methods of representing a density function when its moments upto 4th order are given; the use of Edgeworth expansion and the Gram Charlier expansion has been reviewed. We have introduced the Cornish Fisher expansion to represent the density function and it has been shown to be very useful in studies using spectral distribution methods.

As stated earlier, the moments and eigenvalues of a distribution characterising a given Hamiltonian are important ingredients of spectral distribution methods. In Chapter IV we have developed two methods of calculating eigenvalues without resorting to numerical integration which is tedious and time consuming. In this chapter we have also studied various uses of the Cornish Fisher (CF) expansion, and the CF expansion appears to be quite promising. Various numerical calculations have been done in this regard and the results have been compared with those obtained by exact shell model calculations.

Besides studying eigenvalue distributions with respect to energy, spectral averaging methods can also be used to evaluate the expectation values of various operators as a function of energy. These are obtained by statistically testing the response of the system as measured by its state density, when the Hamiltonian is modified by adding to it an appropriate function of the operator. These expectation values then allow one to obtain various sum rules. Halemane used these methods to obtain a set of inverse energy weighted sum rules. We have adopted a simple and different approach to derive the same. Chapter V deals with this derivation. We have also studied the CLT limit of the rule and its extension to configuration spaces. The results of the analytic study are used to obtain correction to ground state energy when an effective interaction (PW interaction in our study) is approximated by a linear sum of Q.Q and Pairing interactions. Results are given for calculation in scalar and configuration spaces.

Chapter VI gives the conclusion and future prospects.

