CHAPTER VI

SUMMARY AND FUTURE PROSPECTS

In this thesis, we have studied applications of Spectral Distribution Methods.

Using these methods we have calculated the orbit occupancies in the ground states of nuclei in the mass range A = 60-80, and compared the results with experimental data wherever available. We have also studied various ways of representing a density function, both empirical and based on transformations of variable. In particular, the Cornish Fisher expansion has been found to be very promissing, not only as a representation of density function, but also for calculating energy eigenvalues, expectation values and orbit occupancies. We have developed methods to calculate eigenvalues without numerical integration. Using these methods we have calculated eigenvalues for several cases and compared the results with exact shell model data. Besides this we have also derived expressions for statistically averaged inverse energy weighted sum rules and used them to calculate corrections to estimates of ground state energy when an effective interaction is approximated by a linear conbination of well known simple operators. The results are very encouraging.

Besides the applications mentioned above we have also used spectral distribution methods to derive analytical expressions for the averaged third and fourth moments of intensity in the partitioned spaces. Here we present the derivation of these reseults and some future prospects.

1. When the scalar space is decomposed according to some symmetry representations (configurations for example), then the calculation of the third and fourth moments of intensity in the partitioned spaces becomes extremely difficult, more so, because the number of such partitions is quite large. As against this, there are several studies demonstrating the goodness of constant width approximation when the number of partitions is large; where it has been implicitly assumed that on an average, the intensity in each configuration can be represented by a Gaussian with same width. If the scalar skewness and excess parameters are known, with the knowledge of centroid distribution of the intensity in configurations, we can infer about average γ_1 and γ_2 values for each configuration and hence, one can test the validity of the assumption of using gaussian shape for each configuration intensity. One can go a step further and evaluate average γ_1 and γ_2 values without recourse to constant width approximation.

To begin with, let us assume that all the configuration intensities have same shapes and same widths,

$$\rho_{conf}(x) = \frac{1}{\sqrt{2\pi}\ \sigma_{conf}} \exp\left(-\frac{x^2}{2\sigma^2_{conf}}\right) * S(x)$$

where $S(x)$ is the shape function depending upon the shape parameters like γ_1 and γ_2 which are assumed to be same for all configurations; centroid of configuration intensity is assumed to be zero here and σ_{conf} is the constant width. We can represent the distribution of configuration centroids by $\rho_c(E)$, where $\rho_c(E) = \sum_{\vec{m}} \frac{d(\vec{m})}{D}\, \delta(E - E_{\vec{m}})$, $D = \sum_{\vec{m}} d(\vec{m})$

$d(\vec{m})$ is the configuration dimensionality and $E_{\vec{m}}$ is the configuration intensity centroid. Then, it is clear that the total state density can be represented by a convolution.

$\rho(E) = \rho_c \otimes \rho_{conf} = \int \rho_c(x)\ \rho_{conf}(E-x)\ dx$. The p^{th} moment of the total state density is given by

$\mu_p = \int x^p\ \rho(x)\ dx$ and can be shown to be equal to

$\mu_p = \sum_{r=0}^{p} \binom{p}{r} \mu_r\,(\text{cent})\ \mu_{p-r}\,(\text{conf})$ where $\binom{p}{r}$ is a

binomial coefficient and we have shifted the energy scale in such a way that over all centroid is zero. The value of the configuration width σ_{conf} in constant width approximation automatically follows from $\mu_2 = \sigma^2_{total} = \sigma^2_{cent} + \sigma^2_{conf}$

Similarly $\mu_3 = \mu_3\,(\text{cent}) + \mu_3\,(\text{conf})$

$$\therefore \gamma_1 = \mu_3/(\mu_2)^{3/2} = \frac{(\gamma_1 \text{ (cent)} \sigma^3_{\text{cent}} + \gamma_1 \text{ (conf)} \sigma^3_{\text{conf}})}{(\sigma^2_{\text{cent}} + \sigma^2_{\text{conf}})^{3/2}}$$

and fourth moment gives the relation between various γ_2 values;

$$\gamma_2 = \frac{\gamma_2\text{(cent)} \sigma^4_{\text{cent}} + \gamma_2 \text{ (conf)} \sigma^4_{\text{conf}}}{(\sigma^2 \text{ cent} + \sigma^2 \text{ conf})^2}$$

One can immediately estimate average γ_1 and γ_2 values for configuration intensity using the knowledge of (i) skewness and excess foroverall state density and (ii) centroid distribution of configurations.

We can relax constant width approximation by introducing a bivariate eentroid and width distribution for configurations.

$$\rho_M (E, \quad) = \sum_{\vec{m}} \frac{d\ (\vec{m})}{D} \quad \delta (E - E_{\vec{m}}) \ \delta (\sigma - \sigma_{\vec{m}}) ,$$

here we have assumed constant shape parameters for each configuration intensity

$$\rho_{\text{conf}} (x, \sigma) = \frac{1}{\sqrt{2\pi}\ \sigma} e^{-x^2/2\sigma^2} \ S \ (x)$$

The overall state density can again be written down as a linear combination of convolutions.

$$\rho(E) = \int d\sigma \ \rho(E/\sigma) = \iint d\sigma \ \ dx \ \rho_M (E- x,\sigma) \ \rho_{\text{conf}} (x, \sigma)$$

where $\rho(E/\sigma)$ = state density coming from all those configurations which have width σ. It is given by

$$= \int \rho_M(E-x, \sigma) \quad \rho_{conf}(x, \sigma) \quad dx.$$

The moments of the overall state density are given by

$$\mu_p = \iiint dE \, d\sigma \, dx \quad \rho_M(E-x, \sigma) \; (E-x+x)^p \rho_{conf}(x, \sigma)$$

substituting E' for E - x we get

$$\mu_p = \sum_{r=0}^{p} \binom{p}{r} \int d\sigma \int \rho_M (E', \sigma) \; (E')^{p-r} \; dE' * \int x^r \rho_{conf}(x, \sigma) \; dx$$

$$= \sum_{r=0}^{p} \binom{p}{r} \int d\sigma \int dE' \quad \rho_M(E', \sigma)(E')^{p-r} \sigma^r \eta_r$$

Here η_r gives the information about shape of configuration intensity and has the following values $\eta_0 = 1$, $\eta_1 = 0$, $\eta_2 = 1$, $\eta_3 = \gamma_1$, $\eta_4 = \gamma_2 + 3$ and so on. We can immediately recognise the integral over σ and E as the moments of a bivariate density function $\rho_M (E, \sigma)$, hence

$$\mu_p = \sum_{r=0}^{p} \binom{p}{r} \; M_{p-r,\, r} \; \eta_r.$$

$$M_{p,q} = \iint d\sigma \; dE \quad E^p \quad \sigma^q \; \rho_M (E, \sigma)$$

From these expressions, it is clear that knowing the bivariate moments of centroid and width distribution along with the scalar moments, we can find out the average γ_1, γ_2 values for configuration intensity distribution.

Numerical calculations have been done in the s-d shell to determine the average values of γ_1 and γ_2 in the configuration spaces, and they are found to be quite small. It is relevant to mention here that if the spread in these values is large, the calculation of average values is pointless, because they cannot be used, in principle, as the constant shape parameters. For calculating the spread in γ_1, γ_2 values, one would need to calculate scalar moments upto the 8^{th} order.

2. In general, the effective interaction Hamiltonian matrix elements are derived in two ways: (i) From the bare G-matrix by renormalisation and (ii) this renormalised interaction is used for detailed shell - model calculation to determine the eigenvalue spectrum, this spectrum is compared with the experimentally obtained spectrum and with the help of least square fitting method the effective interaction Hamiltonian matrix elements are modified. Here we propose that a method for modification of effective interaction matrix elements based on empirically fitting observed ground state occupancies(which considers the experimentally observed trends) can be given. As an illustration, the sudden change of proton occupancy structure for germanium isotopes when the neutron number in the space crosses 12 can be simulated by properly adjusting the induced proton single particle energies, (Chang et.al. 1977) for p

orbits and $f_{5/2}$ orbit such that these cross over when the number of neutrons becomes 12. There are several advantages in the proposed scheme (i) calculations involved are simple, (ii) only few parameters like induced single particle energies (which depend on sums of two body matrix elements) need be varied and (iii) modification relates to the wave function of the ground state rather than the eigenvalues.

Besides these, we should be able to solve the following problems.

3. The Cornish Fisher expansion around a nôn gaussian random variable, which will allow a direct evaluation of expectation values of various operators of interest.

4. We have seen how to calculate the orbit occupancies by applying Cornish Fisher expansion to a ratio of densities representing positive definite operators (number operator in this case). We can study how to do such calculations for any operator in general (negative or positive).

5. We know that the eigenvalues of a random matrix yield a semi-circular distribution. We also know that when a constant matrix is added to a random matrix, there is a shift in the ground state on the energy scale. An analytical expression can be derived for this shift by representing the density function by

Cornish Fisher expansion using the moments of a random matrix.

6. We have approximated an effective interaction in terms of the quadrupole and the pairing operators and then applied the perturbation theory to inverse energy weighted sum rules to calculate corrections to estimates of ground state energy given by the empirical interactions. It has been seen that the empirical interactions so generated in various spaces do have large correlation coefficients with the effective interactions, and in that sense we can say that a large part of the effective interaction on the average does come from these two operators. However, these empirical interactions connot, to a good accuracy, reproduce the low lying energy levels generated by the effective interaction. We thereforefeel that addition of other operators such as L.S., $Y^4 \cdot Y^4$ etc. may not only improve the correlation but the predictions of low lying levels as well.