CHAPTER IV

MOMENTS AND EIGENVALUES

In the theories of nuclear structure, the eigenvalues of operators of interest are very important quantities. Of particular interest are the energy eigenvalues of a given hamiltonian operator in a given model space. Knowing the energy eigenvalues, one can calculate level density, transition probability, spin cut-off factors, orbit occupancies etc. Conventionally the eigenvalues are obtained by solving the eigenvalue equation $H\psi = E\psi$, where H is the hamiltonian and ψ is the eigenvector corresponding to the eigen energy E. This is a matrix problem, first of all constructing it from 1 + 2 - body hamiltonian and then solving it becomes tedious and time consuming as the matrix dimensionalities (which depend on the number of active nucleons) increase.

Spectral distribution methods provide an easier and more elegant way to solve the problem approximately. As mentioned in the previous chapter, spectral distribution methods deal with moments of operators of interest, and the density of energy levels (in case of a given hamiltonian) can be represented in terms of a few low order moments of the hamiltonian. In order to obtain fluctuation free spectrum of diserete energy eigenvalues; the density function has to

be numerically integrated using the Ratcliffe's procedure[39]. The averaged eigenvalue of the i^{th} state is given by

$$\int_{-\infty}^{E_i} \rho(E)\, dE = (i - \tfrac{1}{2})/D.$$

where $\rho(E)$ is the density function, E_i are the eigenvalues $i = 1,2 \ldots\ldots, D$, D is the dimensionality of the spectroscopic space used. The process of numerical integration, however, has two disadvantages (i) the process is tedious, more so if the dimensionality of the spectroscopic space is large and (ii) the truncated series expansions which are used to represent the density function are not necessarily positive definite functions for all values of the variable E. In section A we develop two methods of calculating eigenvalues without resorting to numerical integration. In section B we present various uses of Cornish Fisher (CF) expansion. The results and discussion follow in the last section.

A NEW METHODS FOR CALCULATING EIGENVALUES

If the density function is taken as a gaussian, one can straight away utilize the inversion formula quoted by Abramowitz and Stegun[35], and obtain correspondingly the discrete spectrum. The i^{th} eigenvalue $\hat{X}_i$ for $\rho_o(x)$ in terms of standardized variable, in a space of D eigenstates is

given by ($i \leq D/2$)

$$X_i = -\left(t - \frac{C_0 + C_1 t + C_2 t^2}{1 + d_1 t + d_2 t^2 + d_3 t^3}\right)$$

$$t = \sqrt{\ln \frac{1}{p^2}} \qquad ; \quad p = (i - \tfrac{1}{2})/D$$

C_o, C_1, C_2, d_1, d_2 and d_3 are numerical constants given by

C_o = 2.515517

C_1 = 0.802853

C_2 = 0.010328

d_1 = 1.432788

d_2 = 0.189269

d_3 = 0.001308

Since the gaussian is symmetric about its centroid, the eigenvalues corresponding to $i > D/2$ are given as

$$\hat{X}_i = -\hat{X}_{(D-i)} \qquad \text{for } i > D/2$$

These expressions have been developed by Hastings. For any other form of density function one has to perform numerical integration to obtain the discrete spectrum. As mentioned earlier, numerical integration has obvious short comings. To avoid numerical integration, we adopt a completely different approach to the problem.

In general, it is found that the fluctuation free spectrum when used to recalculate the moments of the density function, shows slight discrepancy with respect to the original moments which were used to write the continuous density function $\rho(x)$. This is clearly due to the discretization of the continuous density function. Our aim now is to obtain the discrete spectrum in such a way that even after discretization of the density function, recalculation of moments gives the exact original moments of the continuous density function. As far as the first two moments, that is, centroid and width are concerned, these discrepancies can be corrected by shifting and stretching or contracting the energy scale, that is, the corrected eigenvalue E_i' of the i^{th} eigenstate can be written as $E_i' = a + bE_i$

where E_i is the discretized eigenvalue obtained by Ratcliffe's procedure, 'a' is the shifting parameter which fixes the centroid and 'b' is the stretching parameter which fixes the width of the distribution. Thus,'a' and 'b' can be obtained by demanding that the centroid and width of the discretized spectrum be the same as the centroid and width respectively of the original continuous density function $\rho(x)$. The parameters 'a' and 'b' can be calculated as follows .

Let M_1 and M_2 be the first and second moments of a continuous density function $\rho(x)$ and let E_i be the corresponding discretized eigenvalues, $i = 1,2,.....,D$, and D is the dimensionality of the spectroscopic space. After discretization, let the new moments be M_1' and M_2'. Due to the reason mentioned above $M_1 \neq M_1'$ and $M_2 \neq M_2'$. Using the equation $E_i' = a + bE_i$, where E_i' are the corrected eigenvalues and using the condition that the moments remain the same we have

$$\frac{1}{D} \sum_{i=1}^{D} E_i' = M_1 = \frac{1}{D} \sum_{i=1}^{D} a + b E_i = a + b M_1'$$

$$\frac{1}{D} \sum_{i=1}^{D} E_i'^2 = M_2 = \frac{1}{D} \sum_{i=1}^{D} (a+bE_i)^2 = a^2+b^2M_2'+2abM_1'$$

Now, for simplicity and without loss of generality, we assume $M_1 = 0 = M_1'$. So, we obtain $a = 0$ and

$$b = \sqrt{\frac{M_2}{M_2'}} = \frac{\sigma_{continuous}}{\sigma_{discrete}}$$

(since $M_1 = M_1' = 0, \sqrt{M_2/M_2'} = \frac{\sigma}{\sigma'}$)

It is found that the stretching parameter 'b' depends on the dimensionality D of the spectroscopic space considered. Figure 7 shows the relationship between 'b' and D. From the figure it is obvious that as $D \to \infty$, $b \simeq 1$. In other words, this means that as the dimensionality increases, the discrepancy with respect to moments upto second order on

FIGURE 7

The relationship between the stretching parameter 'b' and the dimensionality D of the spectroscopic space used. The dimensionality is represented on a log scale. Here $\sigma_{continuous} = 1$, therefore $b = 1/\sigma_{discrete}$.

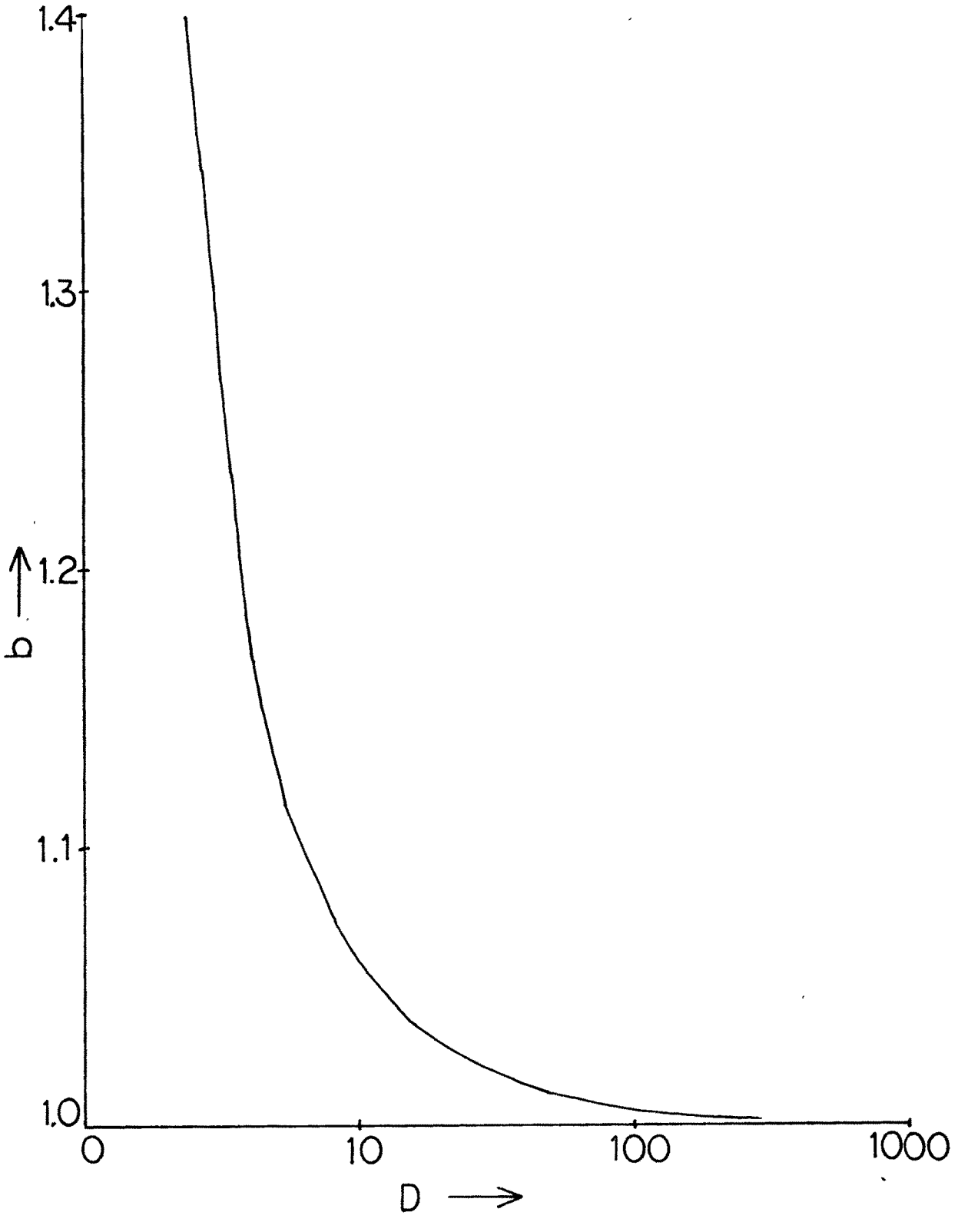

FIGURE 7

discretization decreases. A function which fits properly with the curve drawn in figure may be quite useful to incorporate the stretching correction.

Thus knowing the first two moments of the original continuous density function and the corresponding moments after discretization, one can calculate the constants 'a' and 'b' which in turn enable one to calculate eigenvalues E_i' so that the moments remain the same. This however suggests that in order to obtain proper fit with first three moments one may extend the procedure by writing

$$E_i' = a + bE_i + cE_i^2$$

where the discrete eigenvalues E_i are obtained from Hasting's expressions corresponding to a gaussian level density. Let us begin with known moments M_1, M_2 and M_3 of a density function with dimensionality D. For simplicity we assume $M_1 = 0$. Let the recalculated moments (calculated by using the discrete eigenvalues E_i) be M_1', M_2' and M_3' respectively. Here also, we can arrange to have $M_1' = \frac{1}{D}\sum_{i=1}^{D} E_i = 0$. As a consequence all the odd moments of the discretized spectrum automatically vanish, since Ratcliffe's procedure is symmetric with respect to the two ends of a gaussian. The corrected eigenvalues $E_i' = a + bE_i + cE_i^2$ must now reproduce the original moments M_1, M_2 and M_3, that is,

$$M_p = \frac{1}{D}\sum_{i=1}^{D} (E_i')^p = \frac{1}{D}\sum_{i=1}^{D} (a+bE_i+cE_i^2)^p \quad \text{for } p=1,2,3.$$

Using the fact that all the odd moments M'_{2n+1} vanish due to symmetric nature of a gaussian and that $M_1 = 0$, we get three algebraic equations for the three unknowns a, b and c.

$$a+cM_2' = 0 \qquad (1)$$

$$a^2+ (b^2+2ac)M_2'+c^2M_4' = M_2 \qquad (2)$$

$$a^3+ 3(a^2c + ab^2)M_2'+ 3(ac^2+b^2c)M_4'+c^3M_6' = M_3 \qquad (3)$$

Substituting the value of $a=-cM_2'$ in (2), we get

$$b^2 = M_2/M_2' - c^2 (M_4'/M_2' - M_2')$$

using the values of b^2 and a in (3), we obtain a cubic equation in 'c' i.e.

$$c^3 + 3c \left(\frac{M_2 M_4'/M_2' - M_2 M_2'}{DR}\right) - \frac{M_3}{DR} = 0$$

where $DR= (M_6' + 3M_2'M_4' - M_2'^3 - 3M_4'^2/M_2')$

This equation is numerically solved to obtain its smallest root. Using this value of 'c' we calculate 'b' and 'a' from their explicit expressions. Now corresponding to each E_i, E_i' can be calculated and the moments can be recalculated. When the dimensionality of the spectroscopic space used is large, that is, in the limit $D \to \infty$, the recalculated moments

would have the values $M_2' = M_2$, $M_6' = 15M_2^3$, $M_4' = 3M_2^2$ etc., identical to the moments of a gaussian. We also see that in the limit $M_3 \to 0$, the discrete spectrum reduces to a spectrum corresponding to a gaussian level density. Similarly, extension to exact fit with known values of first four moments can also be worked out using the correction polynomial $E_i' = a + bE_i + cE_i^2 + dE_i^3$.

The main assumption that is the basis of this fitting procedure is that the discrete spectrum corresponding to a given density function can be calculated from a discrete spectrum corresponding to a zero centered gaussian (obtained using Hasting's expressions) and then by the proper adjustment of the energy scale. The higher the order of moments to be fitted, the larger is the order of the fitting polynomial. Results of calculations with taking 3 moments into consideration are given ahead.

Instead of using such a fitting procedure, one may adopt another approach, which approximately takes into account the skewness γ_1 and excess γ_2 of the density function $\rho(x)$. Let the density function be represented as a truncated series in terms of γ_1 and γ_2 as follows

$$\rho(\hat{x}) = \frac{1}{\sqrt{2\pi}} e^{-\hat{x}^2/2} \left(1 + \frac{\gamma_1}{6} (\hat{x}^3 - 3\hat{x}) + \frac{\gamma_2}{24} \right.$$

$$\left. * (\hat{x}^4 - 6\hat{x}^2 + 3) + \ldots\ldots \right) \quad \ldots \qquad (4)$$

and as explained in the previous chapter, $\hat{x}$ is a standardized variable. Now Ratcliffe's procedure [39] gives an average eigenvalue X_i, corresponding to the i^{th} eigenstate of the density function $\rho(x)$. It is given by.

$$p = (i-\tfrac{1}{2})/D = \int_{-\infty}^{\hat{X}_i} \rho(\hat{x})\, d\hat{x}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\hat{X}_i} e^{-\hat{x}^2/2} \left(1 + \frac{\gamma_1}{6}(\hat{x}^3 - 3\hat{x}) + \frac{\gamma_2}{24} * (\hat{x}^4 - 6\hat{x}^2 + 3) + \ldots.\right) d\hat{x} \qquad .. (5)$$

From this expression it is clear that the eigenvalue $E_i = \hat{X}_i * \sigma + M_1$ is a function of γ_1 and γ_2 (and other higher order moments if they are included in the representation of $\rho(x)$; M_1 is the 1^{st} moment and σ the width of the given density function). We know that the truncated series representing $\rho(x)$ converges asymptotically to a gaussian. Hence provided that the γ_1 and γ_2 are small, that is, $|\gamma_1|, |\gamma_2| \leq 0.3$, the eigenvalue $\hat{X}_i(\gamma_1, \gamma_2)$ (since $\hat{X}_i$ depends on γ_1 and γ_2) can be expressed as a Taylor series expansion around $\hat{X}_i(G)$, where $\hat{X}_i(G)$ is the corresponding i^{th} eigenvalue of zero centered unit width gaussian (obtained by using Hasting's expressions).

Therefore

$$\hat{X}_i(\gamma_1,\gamma_2) = \hat{X}_i(G) + \frac{\gamma_1 \partial \hat{X}_i}{\partial \gamma_1}\Bigg|_{\substack{\gamma_1=0\\ \gamma_2=0}} + \frac{\gamma_2\, \partial \hat{X}_i}{\partial \gamma_2}\Bigg|_{\substack{\gamma_1=0\\ \gamma_2=0}} +$$

$$\frac{\gamma_1^2}{2}\ \frac{\partial^2 \hat{X}_i}{\partial \gamma_1^2}\Bigg|_{\substack{\gamma_1=0\\ \gamma_2=0}} \qquad .. \quad (6)$$

where we have used terms upto second order only, as we have considered moments only upto γ_2. If higher order moments are also taken into account, then the above expression should also include corresponding higher order terms. The coefficients $\frac{\partial \hat{X}_i}{\partial \gamma_1}$, $\frac{\partial \hat{X}_i}{\partial \gamma_2}$ and $\frac{\partial^2 \hat{X}_i}{\partial \gamma_1^2}$ can be obtained by the parametric differentiation of (5). We have

$$\frac{\partial p}{\partial \gamma_1} = 0 = \frac{\partial \hat{X}_i}{\partial \gamma_1} * \varphi(\hat{x}) + \int_{-\infty}^{\hat{X}_i} \frac{\partial}{\partial \gamma_1}\ \varphi(\hat{x})\, d\hat{x}$$

$$= \frac{\partial \hat{X}_i}{\partial \gamma_1} * e^{-\hat{x}^2/2} \left(1 + \frac{\gamma_1}{6}(\hat{x}^3 - 3\hat{x}) + \frac{\gamma_2}{24}(\hat{x}^4 - 6\hat{x}^2 + 3) + ..\right)$$

$$+ \int_{-\infty}^{\hat{X}_i} e^{-\hat{x}^2/2} * (1/6\ (\hat{x}^3 - 3\hat{x}))\, d\hat{x}$$

$$\therefore \frac{\partial \hat{X}_i}{\partial \gamma_1} = \frac{-\int_{-\infty}^{\hat{X}_i} e^{-\hat{x}^2/2} * (1/6(\hat{x}^3 - 3\hat{x})) \, d\hat{x}}{e^{-\hat{x}^2/2} * (1 + \frac{\gamma_1}{6}(\hat{x}^3 - 3\hat{x}) + \frac{\gamma_2}{24}(\hat{x}^4 - 6\hat{x}^2 + 3) + \ldots)}$$

Since $\gamma_1 \to 0, \gamma_2 \to 0$ in the asymptotic limit and $\hat{X}_i \to \hat{X}_i(G)$, on integrating the numerator and taking limit $\gamma_1, \gamma_2 \to 0$ on both sides, we have

$$\left.\frac{\partial \hat{X}_i}{\partial \gamma_1}\right|_{\gamma_1, \gamma_2 = 0} = 1/6 \, (\hat{X}_i^2 \, (G) - 1)$$

Following the same procedure we get

$$\left.\frac{\partial \hat{X}_i}{\partial \gamma_2}\right|_{\gamma_1, \gamma_2 = 0} = 1/24 \, (\hat{X}_i^3 \, (G) - 3 \, \hat{X}_i \, (G))$$

$$\left.\frac{\partial^2 \hat{X}_i}{\partial \gamma_1^2}\right|_{\gamma_1, \gamma_2 = 0} = -1/36 \, (\hat{X}_i^5 (G) + 2\hat{X}_i^3 (G) - 9\hat{X}_i (G))$$

Now, since the Gram Charlier expansion, Edge-worth expansion and Cornish Fisher expansion all asymptotically converge to a gaussian, all of them have the same partial derivatives with respect to γ_1 and γ_2 (and higher order moments if they are considered). Using these partial derivatives in (6) we can calculate the corresponding eigenvalues $\hat{X}_i(\gamma_1, \gamma_2)$ and

consecutively the actual energy eigenvalues can be calculated by using $E_i = \hat{X}_i\ (\gamma_1,\gamma_2) * \sigma + M_1$. It is important to note that this procedure can be used only if γ_1 , γ_2 are small. Results of calculations using this method are given in the last section.

Numerical calculations have been performed using the energy eigenvalues obtained from the shell model calculations using the Kuo[40] interaction and ^{17}O single particle energies in the $(2s\text{-}1d)^{m=5,\ T=\frac{1}{2}}$ space. We have also used the 307 eigenvalues obtained by a similar calculation in the $(2s\text{-}1d)^{m=6,\ J=2,\ T=0}$ space. From these eigenvalues, we calculated the moments of the hamiltonian matrices upto the fourth order. They are given by

$$M_1 = 1/D \sum_{i=1}^{D} E_i = \text{Centroid of distribution}$$

$$M_p = 1/D \sum_{i=1}^{D} E_i^{\,p} \quad ; \quad p=2,\ 3,4$$

where E_i are the eigenvalues and D is the dimensionality of the spectroscopic space. The corresponding width σ, skewness γ_1 and excess γ_2 are given by

$$\sigma = \sqrt{\mu_2} = \sqrt{M_2 - M_1^{\,2}}$$

$$\gamma_1 = \mu_3/\sigma^3 = 1/\sigma^3 *(M_3 - 3M_1M_2 + 2M_1{}^3)$$

$$\gamma_2 = \mu_4/\sigma^4 \ -3 = 1/\sigma^4 *(M_4-4M_1M_3+6M_2M_1{}^2-3M_1{}^4)-3$$

Using these moments as the given moments, we recalculated the eigenvalues, using the moment fitting procedure described earlier, which requires the discrete spectrum obtained with the help of Hasting's expressions, corresponding to a unit width, zero centered gaussian.

Next we evaluated the eigenvalues using successive approximations in the Taylor series expansion by taking into account (i) only first correction term (ii) first and second corrections and (iii) first, second and third correction terms respectively. This amounts to making γ_1, γ_1 and γ_2, and γ_1, γ_2 and γ_1^2 corrections respectively to $\hat{X}_i(G)$, in the i^{th} eigenvalue of a unit gaussian.

Each time after evaluation of eigenvalues, we recalculated the first four moments and scaled the new spectrum with respect to the width of the original spectrum. This partly takes into account the distortion introduced when discretizing the continuous level density forms in spectral distribution methods. Also the level-to-level comparison between the original spectrum and the numerically obtained, can be done easily.

A comparative study of the given and the calculated eigenvalues can be done in two ways (i) in terms of fluctuations of the calculated results from the corresponding original values and (ii) by calculating the root mean squard deviation (RMSD) in terms of the mean spacing and by performing a running average over the entire spectrum.

The fluctuation Δ_i of the i^{th} calculated eigenvalue and the original i^{th} eigenvalue is given as, $\Delta_i = E_i' - E_i$ where E_i' = calculated i^{th} eigenvalue and E_i = giyen i^{th} eigenvalue. Using these fluctuations, the root mean squard deviations of the calculated eigenvalues from the original eigenvalues are given as

$$RMSD = (1/D \sum_{i=1}^{D} \Delta_i^2)^{\frac{1}{2}}$$

On the other hand, running average is performed by using these fluctuations and local spacing taken with 5 levels as follows

$$d(E_i) = 1/5 \left(\frac{E_{i+3} + E_{i+2}}{2} - \frac{E_{i-2} + E_{i-3}}{2} \right)$$

where $d(E_i)$ is the mean local spacing. $\delta_i^2 = \left(\frac{\Delta_i}{d(E_i)} \right)^2$ gives square of the fluctuation in terms of the mean local spacing and the corresponding root mean squared deviation is given by

$$RMSD = \left(1/(D-6) \sum_{i=4}^{D-3} \delta_i^2 \right)^{\frac{1}{2}}$$

The factor of D-6 comes because the running average is done by taking 5 levels for calculating local mean spacing, starting with the 4^{th} level and continuing upto D-3 levels. In this way the entire spectrum can be spanned. Results are presented in tabular and graphical forms in a section ahead.

B CORNISH FISHER EXPANSION - APPLICATIONS

Besides giving a good fit to the exact density, the CF expansion has several other uses (as mentioned in chapter 3), which are discussed below.

1. In section A of this chapter, we have studied two methods of calculating eigenvalues of a given Hamiltonian. The first of the two methods fits moments exactly where as the second takes them into account approximately. The CF expansion has a large region of applicability in the γ_1, γ_2 plane (described in chapter 3 Fig. 4). So, instead of using Taylor series expansion for calculating eigenvalues, we can use the CF expansion directly, which takes a full account of γ_1 , γ_2 values of the given density function, provided that γ_1, γ_2 lie in the region shown in the figure 4. For this purpose, we used equation (8) of chapter 3, that is

$\hat{x} = y + (\gamma_1/6)(y^2-1) + (\gamma_2/24)(y^3-3y) - (\gamma_1^2/36)(2y^3-5y)$ where

y corresponds to a gaussian random variable. The first step was to generate the smooth spectrum for a gaussian using Hasting's expressions. Then knowing the centroid and width of the given density function, we scaled the spectrum so obtained with respect to the width of the given density function. We also shifted the energy scale so that the smooth spectrum had the same centroid as that of the given density function. Putting it in a different way we used the formula $Z_i = \hat{X}_i\ (G) * \sigma + x_c$ where $\hat{X}_i\ (G)$ is the i^{th} eigenvalue of a unit gaussian, x_c and σ are the centroid and width of the given density function. Now using (8) we incorporated γ_1, γ_2 values and obtained the eigenvalues corresponding to the given density function. The results of calculation of eigenvalues using this method are discussed in the next section.

2. We can obtain series expansions for expectation values of operators of interest using the parametric derivative approach[37] and CF expansion.

Let H be the hamiltonian operator of a system of D states and let E_i be the corresponding eigenvalues i = 1,2, ..., D.

Let K be another (perturbative) operator, not necessarily positive definite. We are interested in smoothed form for the

expectation values $K(E_i)$ of the operator K in terms of the eigenvalues E_i of H.

For simplicity of calculation, and without any loss of generality, we assume that both H and K are represented by zero centered, unit width densities, that is to say

$$\langle H \rangle = \langle K \rangle = 0 , \quad \sigma_H = \sigma_K = 1$$

Even if the above conditions do not hold, we can always shift and stretch or contract the appropriate scales to make the centroid zero and width unity (as explained in the previous section). At the end of calculations, we can apply the inverse transformations to obtain the original centroid and width.

Let $H(\alpha) = H + \alpha K$ where α is a small parameter. This addition amounts to a small perturbation of the hamiltonian. Due to this perturbation, the eigenvalues E_i shift along the energy scale, the shift depending on the parameter α. Let us represent the shifted eigenvalues by $E_{i,\alpha}$. The expectation values of the operator K can now be calculated by the well known equation[37]

$$K(E_i) = \left. \frac{\partial E_{i,\alpha}}{\partial \alpha} \right|_{\alpha=0} \qquad .. (7)$$

Now, the eigenvalues E_i can be written in terms of the moments of H using the Cornish Fisher expansion (Equation 7

of chapter 3) as follows.

$$E_i = \hat{x}_i - (\gamma_1/6)(\hat{x}_i^2 - 1) - (\gamma_2/24)(\hat{x}_i^3 - 3\hat{x}_i) + (\gamma_1^2/36)(4\hat{x}_i^3 - 7\hat{x}_i)$$

where $\hat{x}$ is a standardized variable and γ_1 and γ_2 are shape parameters related to the 3rd and 4th moments of H namely μ_3 and μ_4 as $\gamma_1 = \mu_3$ and $\gamma_2 + 3 = \mu_4$, because $\sigma_H = 1$. In a similar way, the new shifted eigenvalues $E_{i,\alpha}$ can also be expreseed using moments of H (α) and the CF expansion. However due to the perturbation, the moments of H change. Hence to write down the shifted eigenvalues $E_{i,\alpha}$, we need the moments of $H + \alpha K$.

Let us start from the centroid. It is given as

$\mathcal{E}_\alpha = \langle H + \alpha K \rangle = \langle H \rangle + \alpha \langle K \rangle = 0$ which means that the centroid remains unaffected by the shift under the chosen condition i.e. $\langle H \rangle = \langle K \rangle = 0$.

Similarly, the width σ_α can be calculated

$$\sigma_\alpha^2 = \langle (H + \alpha K)^2 \rangle = \langle H^2 \rangle + 2\alpha \langle HK \rangle + \alpha^2 \langle K^2 \rangle$$

$$\therefore \quad \sigma_\alpha = (1 + 2\alpha \langle HK \rangle + \alpha^2)^{\frac{1}{2}} \quad \because \langle H^2 \rangle = \langle K^2 \rangle = 1.$$

We can immediately see that in case limit $\alpha \to 0$, $\sigma_\alpha \to 1$.

The 3rd moment $\mu_{3,\alpha}$ comes out as $\mu_{3,\alpha} = \langle (H + \alpha K)^3 \rangle$

$= \langle H^3 \rangle + 3\alpha \langle H^2 K \rangle + 3\alpha^2 \langle HK^2 \rangle + \alpha^3 \langle K^3 \rangle$ and $\mu_{4,\alpha}$, the 4th moment as

$$\mu_{4,\alpha} = \langle (H+\alpha K)^4 \rangle = \langle H^4 \rangle + 4\alpha \langle H^3 K \rangle + 6\alpha^2 \langle H^2 K^2 \rangle + 4\alpha^3 \langle H K^3 \rangle + \alpha^4 \langle K^4 \rangle$$

The shape parameters of H (α), that is, $\gamma_{1,\alpha}$, $\gamma_{2,\alpha}$ are now given as $\gamma_{1,\alpha} = \mu_{3,\alpha} / \sigma_\alpha^3$; $\gamma_{2,\alpha} = (\mu_{4,\alpha} / \sigma^4) - 3$

Knowing these moments, we are now in a position to write $E_{i,\alpha}$ as a CF expansion in terms of these moments. We notice that the perturbation $H \rightarrow H(\alpha)$ does not affect the centroid. However, the width has changed from 1 to σ_α. Hence the shifted eigenvalues have to be properly scaled by multiplying with σ_α. Hence we can write,

$$E_{i,\alpha} = \sigma_\alpha * \left(\hat{x}_i - \frac{\gamma_{1,\alpha}}{6} (\hat{x}_i^2 - 1) - \frac{\gamma_{2,\alpha}}{24} (\hat{x}_i^3 - 3\hat{x}_i) + \frac{\gamma_{1,\alpha}^2}{36} (4\hat{x}_i^3 - 7\hat{x}_i) \right) \ldots . \qquad (8)$$

Now using (7) we can obtain the expectation values $K(E_i)$ of the operator K. However, for this purpose, we need partial derivatives of σ_α, $\gamma_{1,\alpha}$ and $\gamma_{2,\alpha}$ with respect to α. They are given as follows.

$$\frac{\partial \sigma_\alpha}{\partial \alpha} = (\langle HK \rangle + \alpha) * (1 + 2\alpha \langle HK \rangle + \alpha^2)^{-\frac{1}{2}}$$

$$\frac{\partial \gamma_{1,\alpha}}{\partial \alpha} = \frac{1}{\sigma_\alpha^6} \left(\sigma_\alpha^3 \left(3\langle H^2K\rangle + 6\alpha\langle HK^2\rangle + 3\alpha^2\langle K^3\rangle\right)\right.$$

$$- \left(\langle H^3\rangle + 3\alpha\langle H^2K\rangle + 3\alpha^2\langle HK^2\rangle + \alpha^3\langle K^3\rangle\right)$$

$$\left.* 3\sigma_\alpha^2 * 1/2 \left(1+2\alpha\langle HK\rangle + \alpha^2\right)^{-\frac{1}{2}} * \left(2\langle HK\rangle + 2\alpha\right)\right)$$

$$\frac{\partial \gamma_{2,\alpha}}{\partial \alpha} = \frac{1}{\sigma_\alpha^8} \left(\sigma_\alpha^4 \left(4\langle H^3K\rangle + 12\alpha\langle H^2K^2\rangle + 12\alpha^2\langle HK^3\rangle + 4\alpha^3\langle K^4\rangle\right)\right.$$

$$- \left(\langle H^4\rangle + 4\alpha\langle H^3K\rangle + 6\alpha^2\langle H^2K^2\rangle + 4\alpha^3\langle HK^3\rangle + \alpha^4\langle K^4\rangle\right)$$

$$\left.* 4\sigma_\alpha^3 * 1/2 \left(1+2\alpha\langle HK\rangle + \alpha^2\right)^{-\frac{1}{2}} * \left(2\langle HK\rangle + 2\alpha\right)\right)$$

Now partially differentiating (8) with respect to α, substituting the above values and taking limit $\alpha \to 0$, we have

$$\left.\frac{\partial E_{i,\alpha}}{\partial \alpha}\right|_{\alpha=0} = \hat{x}_i \langle HK\rangle - 1/6 \left(\hat{x}_i^2 - 1\right)\left(3\langle H^2K\rangle - 2\langle HK\rangle\langle H^3\rangle\right)$$

$$- 1/24 \left(\hat{x}_i^3 - 3\hat{x}_i\right)\left(4\langle H^3K\rangle - 4\langle HK\rangle\langle H^4\rangle + \left(\langle H^4\rangle - 3\right) * \langle HK\rangle\right)$$

$$+ 1/36 \left(4\hat{x}_i^3 - 7\hat{x}_i\right)\left(6\langle H^2K\rangle\langle H^3\rangle - 6\langle HK\rangle\langle H^3\rangle\right.$$

$$\left. + \langle H^3\rangle^2\langle HK\rangle\right) \quad .. \quad (9)$$

This is a new polynomial expansion for expectation values and can be used to obtain the expectation values. The validity of

this expansion can be checked in the CLT limit, which is shown below. Now in the CLT limit, the shape parameters γ_1 and γ_2 are zero and hence $\langle H^3 \rangle = 0$ and $\langle H^4 \rangle = 3$. Therefore (9) reduces to

$$\left.\frac{\partial E_{i,\alpha}}{\partial \alpha}\right|_{\alpha=0} \overset{CLT}{=} K(E_i) = \hat{x}_i \langle HK \rangle - 1/2\ (\hat{x}_i^{\,2} - 1) \langle H^2K \rangle - 1/6\ (\hat{x}_i^{\,3} - 3\,\hat{x}_i)\ (\langle H^3K \rangle - 3\langle HK \rangle)$$

which is the well-known polynomial expansion for the expectation value[37] of an operator, $K(E) = \sum_i P_i(E) \langle K\ P_i\ (H) \rangle$ where the P_i's are Hermite Polynomials.

We have done this calculation in two steps, that is, by expanding the eigenvalues of both the operators H and $H+\alpha K$ by using CF expansion around a gaussian random variable. This is because, as yet, we have not used the CF expansion around a non-gaussian random variable[36] to represent a density function. If this is known, then we can straight away write the eigenvalues $E_{i,\alpha}$ and proceed to calculate the corresponding expectation values, which is definitely a shorter procedure.

3. Cornish Fisher expansion can be used to derive smooth forms for the spherical orbit occupancies over the entire spectrum corresponding to a given density function $\rho(E)$ in a

given space of m particles.

Consider a density function $\rho_k(E)$, which is the density function $\rho(E)$ weighted by the expectation value of an operator K. Strictly speaking, $\rho_k(E)$ represents a density function only if K is a positive definite operator. This is so because a good representation of a density function should be positive definite. Then we may define[37)]

$$K(E) = \rho_k(E) / \rho(E) \qquad .. \quad (10)$$

The moments of $\rho(E)$ and $\rho_k(E)$ are given as

$$M_p = 1/D \sum_i E_i^p = 1/D \int_{-\infty}^{+\infty} \rho(E)\, E^p \, dE = \langle H^p \rangle^m \quad \text{and}$$

$$W_{p,0} = 1/D \sum_i \langle \psi_i | K | \psi_i \rangle E_i^p = 1/D \int_{-\infty}^{+\infty} \rho_k(E)\, E^p dE$$

$$= \langle H^p K \rangle^m$$

where D is the dimensionality of the space used. As an example, let us consider K = n (E), where n (E) is the number operator and E represents the energy. Since the number operator is a positive definite operator, using (10) we can straightaway obtain an expression for average exepctation value of the number operator, that is, average spherical orbit occupancy at a given energy E. Thus we have

$$n(E) = \rho_n(E)/\rho(E) \qquad \ldots (11)$$

An expression for n(E), equivalent to the above result, can also be derived from the definition of strength function $S_1(E)$, which is $S_1(E) = D\,\rho(E) \langle E \mid K^+K \mid E \rangle / \ll K^+K \gg$

$$= \frac{D\,\rho(E)\; n(E)}{\ll K^+K \gg}$$

$$\therefore \quad \frac{S_1(E)}{\rho(E)} * \langle n \rangle = n(E) \qquad \ldots (12)$$

where $(1/D) \ll K^+K \gg = 1/D \sum_i n_i = \langle n \rangle$ is the average occupancy of a given i^{th} spherical orbit. The moments of $S_1(E)$ are given by $W_{p,\theta} = \langle K^+K H^p \rangle^m / \langle K^+K \rangle^m$

Thus knowing the moments of $\rho(E)$ and $\rho_n(E)$ or $S_1(E)$, we can express the density (strength) function in terms of these moments using CF expansion. Then using either of the expressions (11) and (12) we can derive expression for smooth forms of orbit occupancies. The CF representation for a density function is

$$\rho(\hat{x}) = \frac{1}{\sqrt{2\pi}} \left| \left(1 - \frac{\gamma_1}{6}\,\hat{x} + \frac{\gamma_1^2}{36}\left(12\hat{x}^2 - 7\right) - \frac{\gamma_2}{8}\left(\hat{x}^2 - 1\right)\right)\right| *$$

$$\exp\left(-1/2\left(\hat{x} - \frac{\gamma_1}{6}\left(\hat{x}^2 - 1\right) - \frac{\gamma_2}{24}\left(\hat{x}^3 - 3\hat{x}\right) + \frac{\gamma_1^2}{36}\left(4\hat{x}^3 - 7\hat{x}\right)\right)^2\right)$$

.. (13)

where γ_1, γ_2 are the skewness and excess of the density (strength) function and $\hat{x}$ is a standardized variable.

At this juncture, we would like to add that in principle, all the moments of a given density can be calculated. In practice, however, the calculation of moments higher than the second moment is extremely difficult and time consuming. Since higher moments are not available, we have used exact results obtained by shell model calculations to calculate the first four moments to be used for our calculations.

We have used the exact results obtained by performing shell model calculations for all J$_z$ values in $(2s - 1d)^{m=5}$, $T=\frac{1}{2}$ space. The interaction used was Kuo[40] interaction with ^{17}O single particle energies. Out of all the cases available, for occupancy calculation we have used the J= 1/2 case with 109 energy eigenvalues and the corresponding occupancies for the $d_{5/2}$ and $d_{3/2}$ orbits over the entire spectrum in the space considered.. Using the eigenvalues E_i and the corresponding occupancies n_i for an orbit, we calculated moments of S_1 (E) and

$\rho(E)$ (We have used (12)) as follows

$$W_{p,0} = 1/D \sum_{i=1}^{D} n_i E_i^p \Big/ 1/D \sum_{i=1}^{D} n_i$$

$$M_p = 1/D \sum_{i=1}^{D} E_i^p$$

From these moments, we calculated the centroid, width, skewness and excess and using (13) we obtained CF expansions for S_1 (E) and $\rho(E)$ respectively. Finally we used equation (12) to evaluate the average orbit occupancies. However, since these occupancies were calculated by using CF expansion around a standardized variable, we scaled the occupancies with respect to the widths of the strength function S_1 (E) and density function $\rho(E)$. The results of these calculations are graphically presented and compared with exact shell model results and the results obtained by assuming a gaussian form for both S_1 (E) and $\rho(E)$.

For the calculation of eigenvalues using CF expansion, we have used the exact results of shell model calculations in the $(2s - 1d)^{m=5,\ T=\frac{1}{2}}$ and $(2s - 1d)^{m=6,\ J=2,\ T=0}$ spaces, using Kuo [40] interaction and ^{17}O single particle energies.

C RESULTS AND DISCUSSIONS

The results of the moment calculations are tabulated in Table III for eigenvalue spectra of different dimensionalities. The initial moments σ, γ_1 , γ_2 and the moments after making approximations by incorporating γ_1, γ_1 and γ_2 and γ_1, γ_2 and γ_1^2 (Taylor series) and those calculated by the CF expansion are given. We see that the widths do not change. This is because we had scaled the calculated eigenvalues with respect to the width of the given eigenvalue distribution for each case. The values of skewness for each case obtained by different approximations appear to be more or less equal, but about 5 - 8% less than the corresponding initial values. This can be attributed to the fact that we have calculated eigenvalues by taking into account only a few lower order moments and the corresponding truncated series expansions. As far as the excess (γ_2) values are concerned, from the results, it is evident that the approximation which takes into account only γ_1 gives a larger value of excess compared to the initial values; where as the rest of the approximations give values of γ_2 which are quite smaller than the initial values.

Table IV shows the root mean squared deviations obtained by the two methods a) RMSD in terms of mean spacing b) RMSD

TABLE - 3

Moments of distributions with different dimensionalities, recalculated using various approximations. The first, second and third rows in the first column for each case correspond to the initial width σ, skewness γ_1 and excess γ_2 respectively. The second, third, fourth and fifth columns correspond to moments calculated by using γ_1, γ_1 and γ_2, γ_1, γ_2 and γ_1^2 and CF expansion respectively.

T A B L E III

DIMENSIONALITY	INITIAL MOMENTS	MOMENTS AFTER FITTING			
	σ γ_1 γ_2	γ_1 ONLY	γ_1 AND γ_2	γ_1, γ_2 & γ_1^2	C.F. EXPANSION
	9.4644	9.4644	9.4644	9.4644	9.4644
109	0.1131	0.1036	0.1030	0.1021	0.1033
	-0.0293	-0.1438	-0.1634	-0.1918	-0.1749
	7.8449	7.8449	7.8449	7.8449	7.8449
167	0.0225	0.0211	0.0200	0.0199	0.0200
	-0.2808	-0.1130	-0.3071	-0.3082	-0.309
	9.1739	9.1739	9.1739	9.1739	9.1739
188	0.0369	0.0349	0.0339	0.0338	0.034
	-0.1399	-0.1024	-0.2046	-0.2082	-0.2066
	8.3545	8.3545	8.3545	8.3545	8.3545
209	0.0333	0.0316	0.0301	0.0301	0.0302
	-0.2325	-0.0946	-0.2636	-0.2664	-0.2656
	8.9177	8.9177	8.9177	8.9177	8.9177
223	0.0444	0.0423	0.0407	0.0407	0.0408
	-0.1748	-0.0890	-0.2193	-0.2246	-0.2219
	10.2387	10.2387	10.2387	10.2387	10.2387
307	0.0531	0.0511	0.0491	0.049	0.049
	-0.1815	-0.0680	-0.2094	-0.2176	-0.2127

TABLE - 4

Root mean squared deviations of the recalculated eigenvalues (of distributions of different dimensionalities) from the given eigenvalues. The various columns give results obtained by using different approximate methods and the CF expansion.

TABLE IV

DIMENSIONALITY	ROOT MEAN SQUARED DEVIATION AFTER FITTING				
	3 MOMENTS EXACTLY	γ_1 ONLY	γ_1 AND γ_2	γ_1, γ_2 AND γ_1^2	C.F. EXPANSION
109	0.3253	0.3254	0.3332	0.3511	0.3385
	0.6616	0.6560	0.6583	0.6678	0.6611
167	0.2584	0.2556	0.1884	0.1884	0.1886
	0.9578	0.9614	0.7555	0.7561	0.7567
188	0.2180	0.2181	0.2240	0.2255	0.2247
	0.8147	0.8215	0.8009	0.8032	0.8027
209	0.2375	0.2375	0.1914	0.1918	0.1917
	1.1615	1.1687	1.0082	1.010	1.010
223	0.2393	0.2370	0.2157	0.2163	0.2162
	0.7952	0.8001	0.6850	0.6900	0.6883
307	0.2363	0.2364	0.1829	0.1812	0.1834
	0.8664	0.8759	0.9815	0.9990	0.9937

in terms of local spacing (also called a running average); for each case using the same approximations as mentioned above. Here again, it is clearly seen that there is not much difference between the RMSD values obtained by first method. For some cases, however, the γ_1, γ_2 and γ_1^2 and CF. approximations give smaller values of RMSD. As far as running averages are concerned, the successive approximations show approximately a decreasing trend, the exception being the case of 307 eigenvalues.

Figure 8 (a,b) and Figure 9 (a,b) show the plot of the fluctuations Δ_i vs the number of the eigenstates for cases with dimensionality 109 and 167 and for two approximations, that is the γ_1 and γ_2 correction and the CF expansion respectively.

It is interesting to note that though both the plots (a) and (b) in both figures follow a similar trend, their scales are quite different. In both cases, the fluctuations obtained by using the CF expansion appear to be considerably smaller than those obtained by other approximations.

On the other hand, the tables show that the RMSD's obtained by both the methods are of the same order. The plots however are very illuminating about the difference between the two approximations. This can be because while calculating

FIGURE 8

Fluctuation Δ_i vs the eigenvalue numbers for 109 eigenvalues, obtained using

(a) γ_1 and γ_2 correction and

(b) CF expansion

Note that the fluctuations have reduced considerably in (b). Also note the difference in scales in (a) and (b).

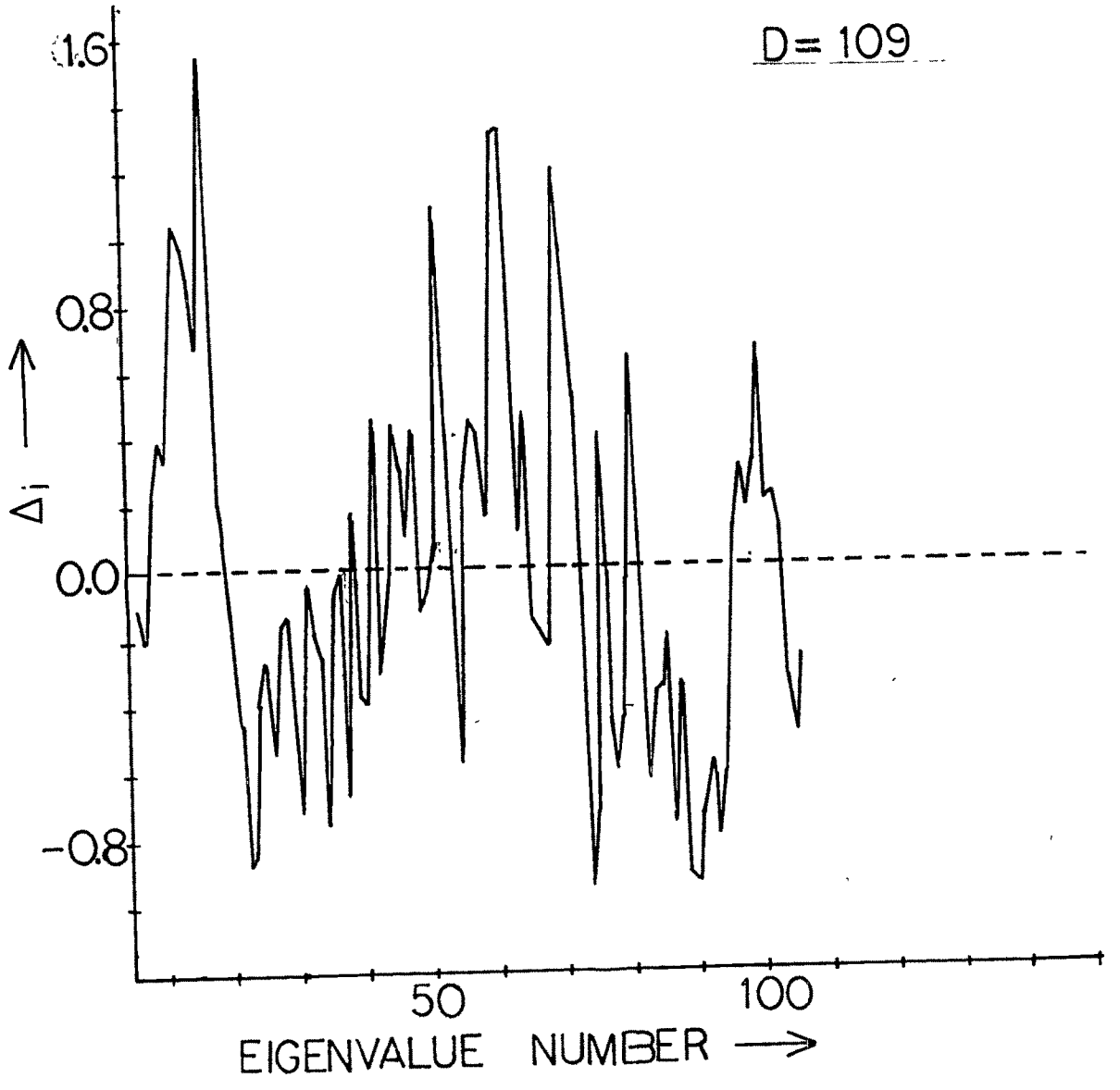

FIGURE 8 (a)

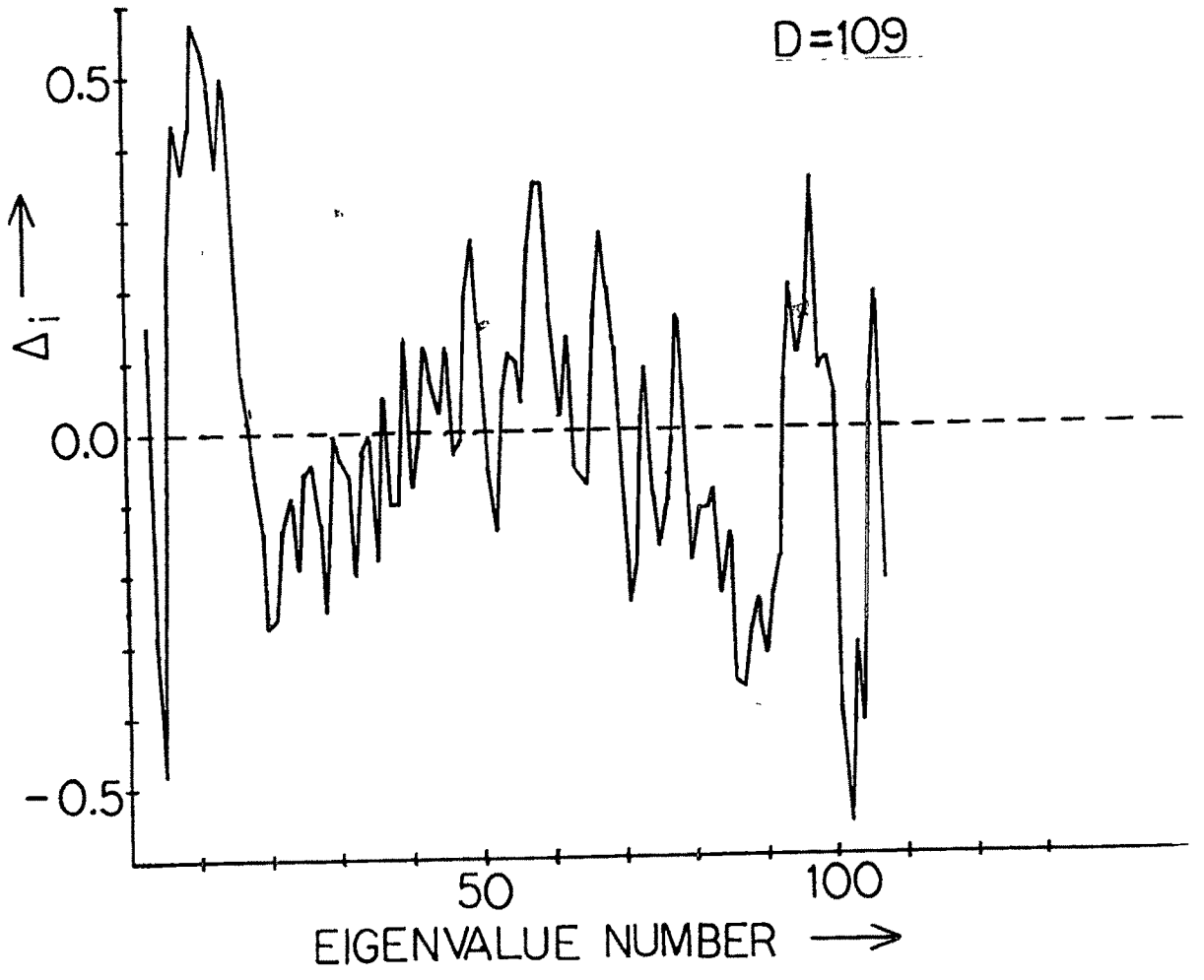

FIGURE 8(b)

FIGURE 9

Fluctuation Δ_i vs the eigenvalue number for 167 eigenvalues, obtained using

(a) γ_1 and γ_2 correction and

(b) CF expansion

Note that the fluctuations have reduced considerably in (b). Also note the difference in scales in (a) and (b).

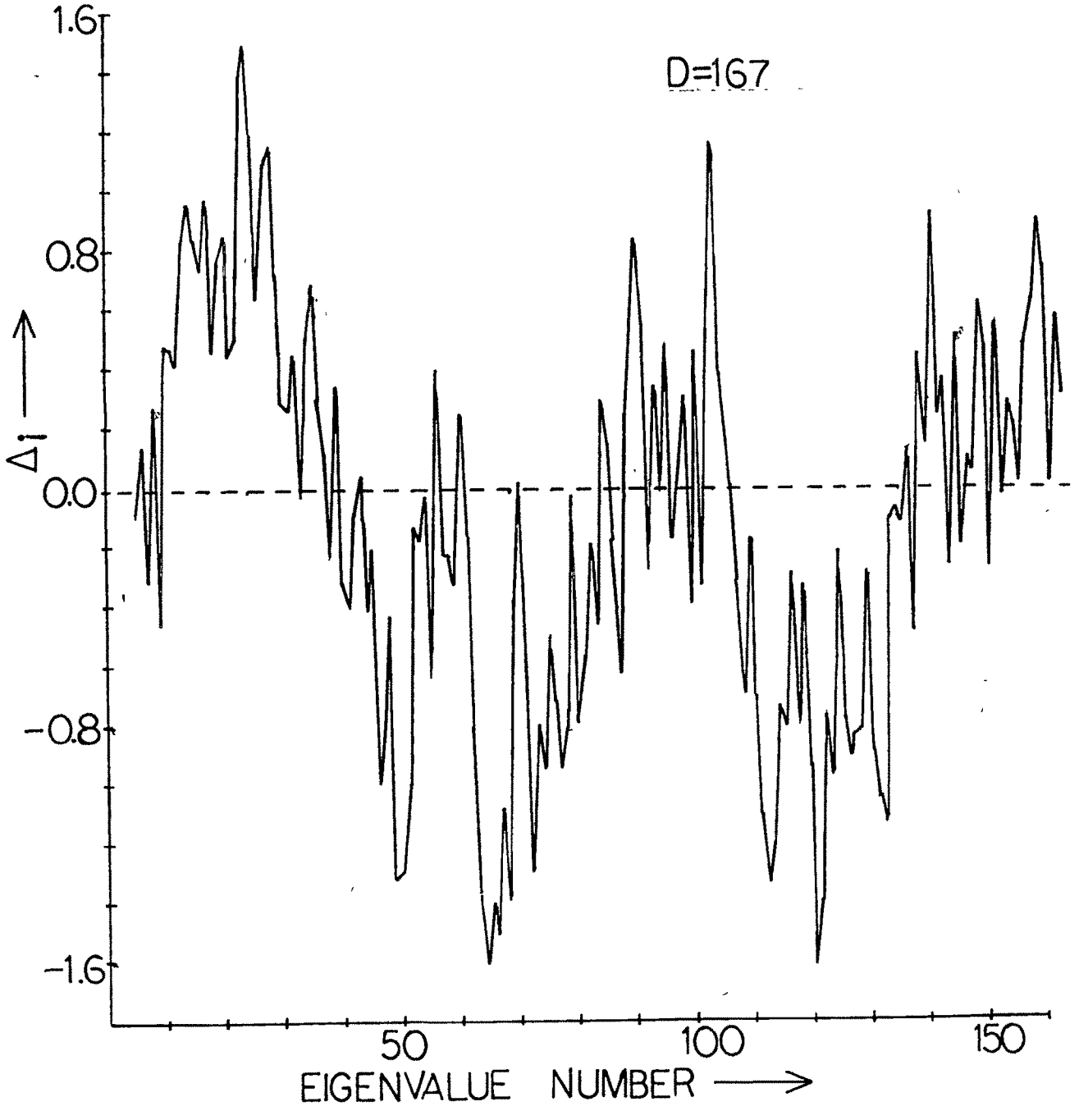

FIGURE 9(a)

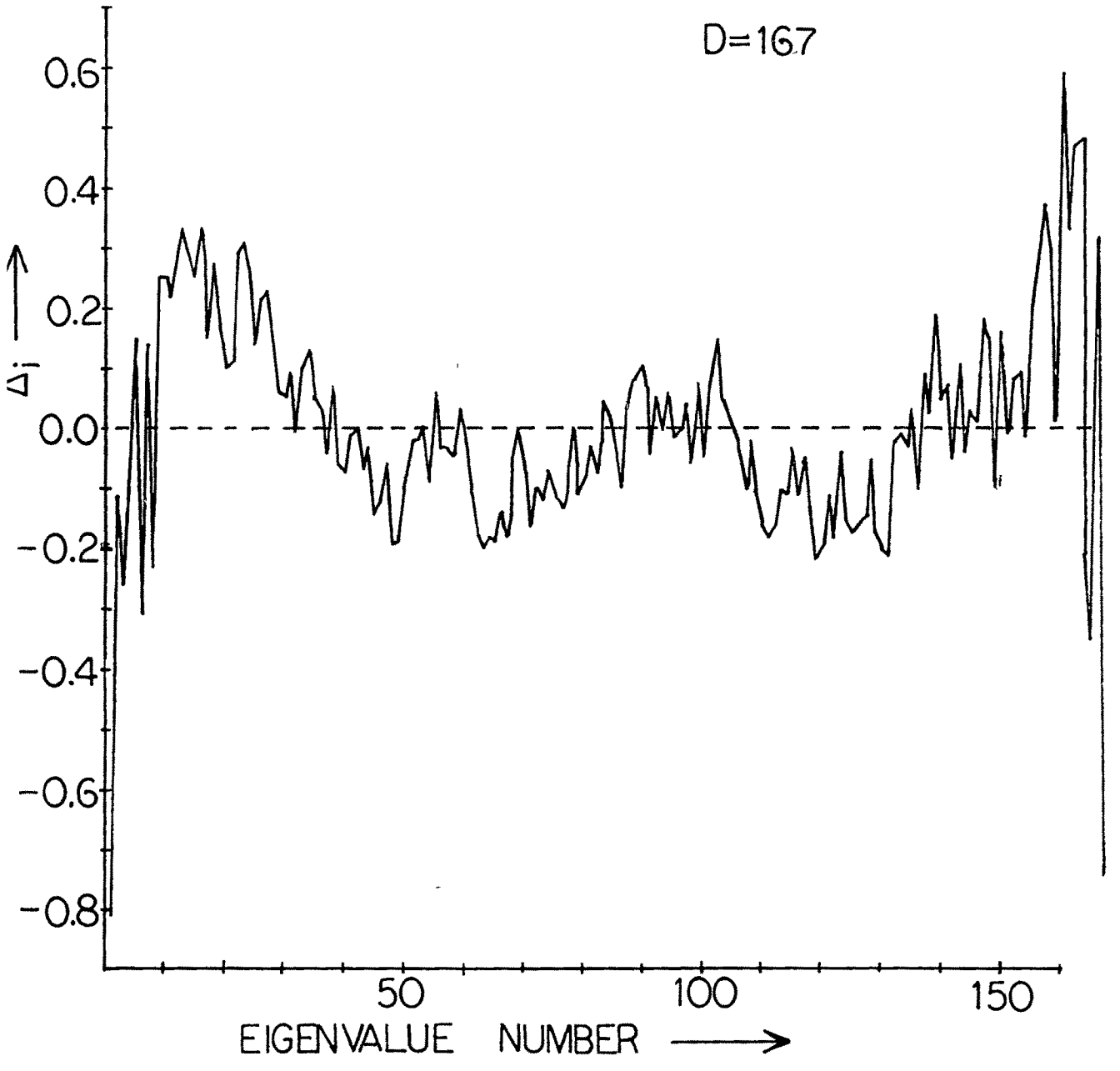
D=167
0.6
0.4
0.2
0.0
-0.2
-0.4
-0.6
-0.8
Δ_i
50
100
150
EIGENVALUE NUMBER

FIGURE 9(b)

FIGURE 10

The orbit occupancies n_i obtained by CF expansion against the energy E_i of the i^{th} state, indicated by _____. For comparison, the exact shell model results are given by the zig-zag solid curve. The - - - - curve shows the results obtained by representing the density function by a gaussian. The results are for the $d_{5/2}$ and $d_{3/2}$ orbits, in the $(2s\text{-}1d)^{m=5,\ T=\frac{1}{2}}$ space with dimensionality D=109.

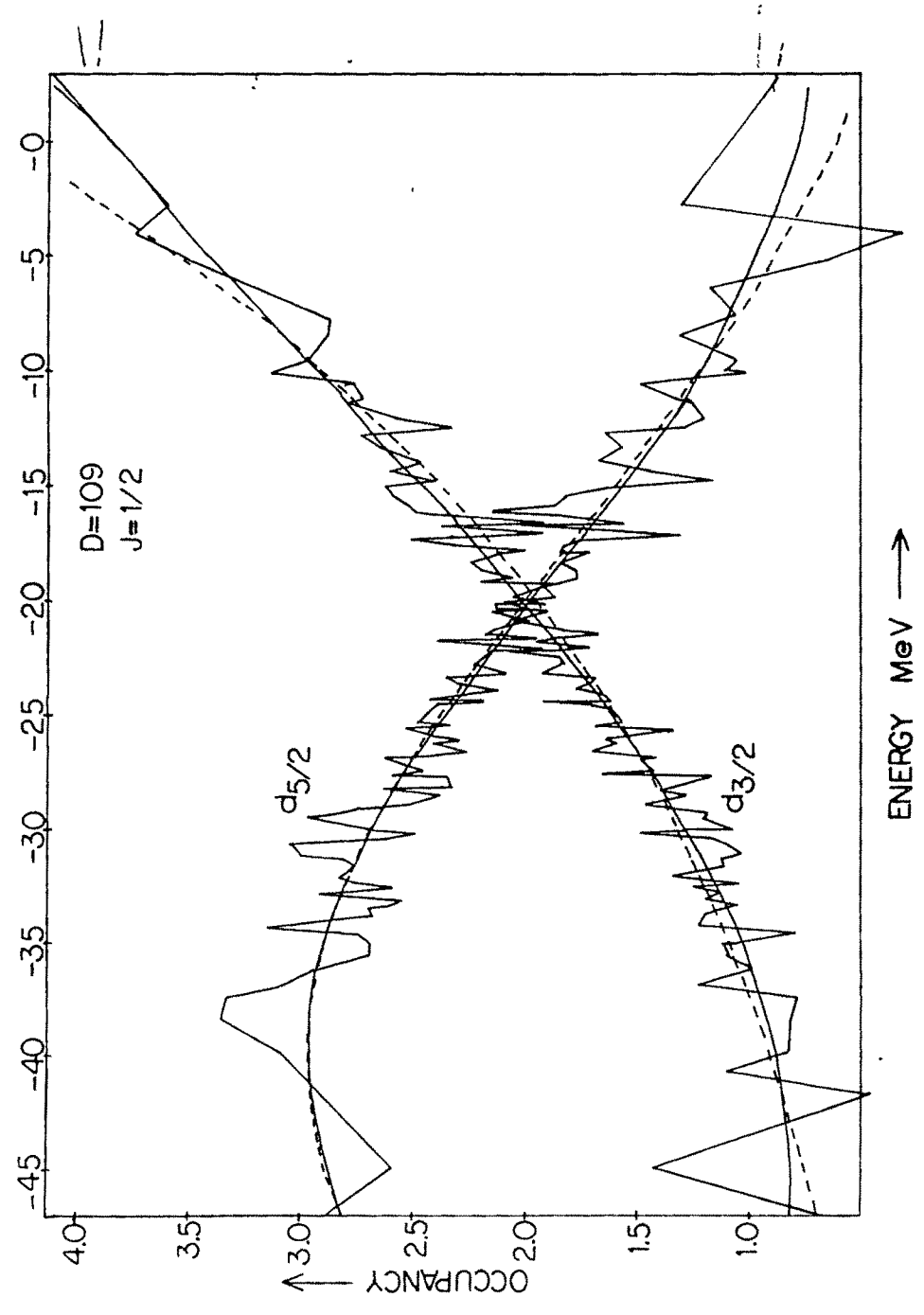
D=109
J=1/2
$d_{5/2}$
$d_{3/2}$
ENERGY MeV
OCCUPANCY
-0
-5
-10
-15
-20
-25
-30
-35
-40
-45
4.0
3.5
3.0
2.5
2.0
1.5
1.0

FIGURE 10

the RMSD's, all the fluctuations are averaged out. The fluctuations obtained by other approximations are even larger than those shown here.

Thus, we see that besides giving a good fit to the density function, the CF expansion gives a very simple and elegant method to calculate eigenvalues also. The results of occupancy calculations are shown graphically in Figure (10) where the orbit occupancies n_i obtained by CF expansion are plotted against the energy E_i corresponding to i^{th} state. The relevant parameters are shown in the figure. For comparison we have also given the exact shell model results and also the curves obtained by representing the density (strength) function by a gaussian. We see that the smooth curves for orbit occupancies obtained by using CF expansion follow the trend of the exact results quite well. Here we have used only one case with dimensionality 109 to verify the validity of CF expansion for calculating occupancies. If higher moments of the density (strength) function are available, then this method can be effectively used for predictive purposes as well.