CHAPTER III

VARIABLE TRANSFORMATION AND REPRESENTATION OF DENSITY FUNCTION

In the spectral distribution methods introduced by French [21] to study many-particle nuclear systems, the density of shell model states $\rho(E)$ in a finite dimensional [22] space as a function of energy is an important quantity. A mathematical function which represents the density of states is known as a density function. Experimentally measured state density is an exponentially increasing function on energy[23], while the density function as defined above is bounded on both sides and corresponds to a partial density of states which depends upon the system Hamiltonian and the spectroscopic space used. Therefore it follows that moments of the density function exist and it can be represented in terms of its moments [24]. In principle one would require all the moments of the density function for such a representation. However the spectral distribution methods attempt to construct smooth forms for the density function, in terms of its few low order moments; usually the first four moments which are (or simply related to) (i) the centroid ($E_c = M_1$), (ii) the width ($\sigma = \sqrt{\mu_2}$) (iii) the skewness ($\gamma_1 = \mu_3/\sigma^3$) and (iv) the excess ($\gamma_2 = (\mu_4/\sigma^4) - 3$) where μ_i, i = 2,3, 4

are the central moments.

These moments can be obtained directly from the defining matrix elements of the Hamiltonian in the space of few particles (usually upto 2 particles), without the construction and the diagonalization of large many-particle Hamiltonian matrices.

However, with the information of few low-order moments alone, without general knowledge of its form, one can never attempt to represent the density function, as there can exist a number of different densities with the same set of lower moments but with differences in higher moments. For example, given a set of first two moments one can choose from a gaussian, a poisson a rectangular and many other distributions. It is known that due to the action of Central Limit Theorem (CLT) in spectroscopic spaces of interest, $\rho(E)$ acquires a gaussian shape. A gaussian probability density function $\rho_G(x)$ is fully described by its first two moments i.e. centroid x_c and width σ. Several analytic studies for ensemble averaged density function with embedded gaussian orthogonal ensemble (EGOE) of k-body interactions[25], monte carlo calculations[26], and shell model calculations with "realistic" interactions[27] have established the closeness of density function to a gaussion. Hence it would be

good to get a representation (for density function) which is closely related to a gaussian and flexible enough to incorporate a few corrections to take care of departures from normality. Cohsider the followihg illustrative data; the KLS - R two body interaction[28] with single particle energies from ^{17}O spectrum gives following γ_1, γ_2 values[29]: 0.095 and - 0.11 for 8 particles, 0.085 and -0.17 for 12 particles and 0.055 and - 0.20 for 16 particles in the spectroscopic space of s-d shell. These γ_1 , γ_2 values have been obtained by taking into account all the states with m particles (scalar space). Small values of γ_1 and γ_2 assure us that the actual density function is quite close to a gaussian, with small departures from normality. Therefore due to the asymptotic nature of CLT convergence, in real applications, $\rho(E)$ should be constructed taking into account the departures from normality. In other words, the density function can be written down as a gaussian with few corrections, or in terms of some function which would go smoothly into a gaussian in the limit of γ_1, γ_2 being zero.

Due to the large dimensionalities of spectroscopic spaces considered, the spectroscopically and experimentally interesting region in the scalar space is often more than 3-widths away from the centroid. It is in this region that the departures

from normality (indicated by non-zero though small values of γ_1 and γ_2) turn out to be increasingly significant. This problem is solved by partitioning the spectroscopic space into subspaces according to some symmetry groups and by extending the CLT action to the partitioned subspaces[30]. One can also calculate still higher moments of the density function in scalar space. But this approach is avoided because (i) it becomes difficult to calculate moments higher than 4^{th} moment and (ii) it has been shown that higher moments deal essentially with level-to-level fluctuations rather than the average properties of the density function. Calculations using partitioning of space has two advantages (i) improved accuracy due to detailed additional information and (ii) better understanding of the system structure. Partitioning into configurations $\tilde{m} = (m_1, m_2, ..)$ defined by distributions of m particles into various shell model spherical orbits, is one of the often considered subdivisions of the scalar space. Thus, now $\rho(E)$ decomposes into partial densities $\rho_{\tilde{m}}(E)$, defined in the configuration space; $d(m)\,\rho(E) = \sum_{\tilde{m}} d(\tilde{m})\,\rho_{\tilde{m}}(E)$

where $d(m)$ and $d(\tilde{m})$ are the dimensionalities in the scalar and configuration spaces respectively. In Figure 1 the

configuration shape parameters γ_1 $(\tilde{m})$, γ_2 $(\tilde{m})$ for $\rho_{\tilde{m}}$ (E) corresponding to 35 configurations of 8 particles in (2s-1d) shell are plotted against the configuration centroid energies E_c $(\tilde{m})$. We see that even though the departures from normality for some configurations are quite large (indicated by large values of γ_1 $(\tilde{m})$ and γ_2 $(\tilde{m})$), the low lying configurations (within 10 MeV from the lowest configuration centroid) which dominate the ground state region have quite small values of γ_1 and γ_2, that is, $|\gamma_1|$, $|\gamma_2| \lesssim 0.5$. With such small values of γ_1 and γ_2, it is possible for us to seek a representation for $\rho(E)$ (or $\rho_{\tilde{m}}$ (E)) which is theoretically satisfying and which yields a gaussian in the asymptotic limit. We now study various methods of representing $\rho(E)$ given the first four moments $(E_c, \sigma, \gamma_1, \gamma_2)$, and compare each one with exact shell model results.

A good representation of a density function should (i) correspond to smooth forms of actual density (ii) have an asymptotic nature (iii) be positive definite for all values of the defining variable (iv) give a good fit between theory and experiments.

There are in general, three different methods[31] of representing the density function $\rho(E)$ when the first four

moments E_c , σ, γ_1 and γ_2 are given : (i) a series representation in terms of derivatives of a known asymptotic density function, the well known Gram Charlier and Edgeworth expansions belong to this class; (ii) transformation of the variable such that the transformed variable has the asymptotic density; here there are two choices: one can opt for a functional form for the transformation as that of the Johnson system or choose a series representation for the variable such as the Cornish Fisher expansion (iii) choosing an approximating function from a class of functions such as the Pearson's system of distributions, which satisfy certain differential equation. Since in most of the physically interesting cases the density function turns out to be close to a gaussian, the first method of representing $\varsigma(E)$ has so far been the natural choice of practitioners of spectral distribution methods[32]. Here we lay emphasis on the second method. However, for completeness, we study all the three methods and compare them with the exact shell model results From here onwards, we use the standardized variable $\hat{x} = (x-x_c)/\sigma$, so that the transformed density $\eta(\hat{x})$ has zero centroid and unit width.

Though both Gram Charlier (GC) expansion and Edgeworth (EW) expansion belong to the series representation class, the basic principles involved in their derivation are quite

different. The Gram Charlier expansion for a density $\eta(\hat{x})$ is written in terms of orthogonal polynomials $P_\mu(\hat{x})$ defined by an asymptotic density $\eta_0(\hat{x})$. It can be expressed as

$$\eta(\hat{x}) = \eta_0(\hat{x}) \left(1 + \sum_{\mu \geq 3} a_\mu P_\mu(\hat{x}) \right) \quad .. \quad (1)$$

where $\int_{-\infty}^{\infty} \eta_0(\hat{x}) P_\mu(\hat{x}) P_{\quad}(\hat{x}) d\hat{x} = N_\mu \delta_{\mu\nu}$

Here, N_μ is related to the normalization of the polynomials and a_μ are the polynomial moments expressible in terms of the shape parameters of the density $\eta(\hat{x})$ and are expressed as

$$a_\mu = \frac{1}{N_\mu} \int_{-\infty}^{\infty} \eta(\hat{x}) \; P_\mu(\hat{x}) \; d\hat{x}$$

Now on using the gaussian density $\eta_G(\hat{x}) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-\hat{x}^2}{2}\right)$

for $\eta_0(\hat{x})$, the orthogonal polynomials $P_\mu(x)$ turn out to be Hermite polynomials. To take into consideration the skewness γ_1 and excess γ_2 of $\eta(\hat{x})$, we truncate the series (1) after the fourth term. Thus the truncated GC series with γ_1 , γ_2 corrections is

$$\eta_{GC}(\hat{x}) = \eta_G(\hat{x})\left(1+\left(\frac{\gamma_1}{6}(\hat{x}^3-3\hat{x})\right)+\left(\frac{\gamma_2}{24}(\hat{x}^4-6\hat{x}^2+3)\right)\right) \quad .. \quad (2)$$

The Edgeworth expansion (EW), on the other hand, follows from the fact that given a function $\eta_0(\hat{x})$ with cumulants[+] (on next page) ϵ_1, ϵ_2 ...., it is possible to obtain a function

$\eta(\hat{x})$ with cumulants $\epsilon_1 + k_1$, $\epsilon_2 + k_2$ etc. using the following equation.

$$\eta(\hat{x}) = \exp\left(\sum_{r \geqslant 3} \frac{k_r}{r!} \frac{\partial^r}{\partial \hat{x}^r} \right) \eta_0(\hat{x}) \qquad .. \quad (3)$$

Once again, taking $\eta_G(\hat{x})$ for $\eta_0(\hat{x})$, the expansion (3) can be written in a compact form, presumably familiar to others, as

$$\eta(\hat{x}) = \eta_G(\hat{x}) \left(\sum_{P=0}^{\infty} \left(\sum_{[P]} \left(\prod_{i=1}^{\ell} \frac{1}{s_i!} \left(\frac{k_{p_i+2}}{(p_i+2)!} \right)^{s_i} \right) * \right. \right.$$

$$\left. \left. \mathrm{He}_{P+2S}(\hat{x}) \right) \right) \qquad .. \quad (4)$$

where $\mathrm{He}_\nu(\hat{x})$ are Hermite polynomials and $[P]$ is a partition of integer P written as

$$[p_1^{s_1}, p_2^{s_2}, \ldots\ldots, p^{s}] \quad \text{with } \sum_i s_i = S \text{ and } \sum_i s_i p_i = P$$

With the proposition that the cumulants k_ν ($\nu \geqslant 3$) for a system with large number of particles behave as $b^{-(\nu-2)/2}$,

† Cumulants are coefficients of t^r/r in the expansion of $\log \int e^{tx} g(x)\, dx$ where $g(x)$ is the density function. They are simply related to the central moments, for example $k_3 = \mu_3$ and $k_4 = \mu_4 - 3\sigma^4$

b being a system parameter (here particle number m), all the terms belonging to a given value of P in (4) behave as $m^{-(P-2)/2}$ asymptotically. Therefore, collecting terms upto order 1/m gives the truncated EW series which takes into account γ_1 , γ_2 corrections.

$$\eta_{EW}(\hat{x}) = \eta_G(\hat{x}) \left(1 + \frac{\gamma_1}{6} (\hat{x}^3 - 3\hat{x}) + \frac{\gamma_2}{24} (\hat{x}^4 - 6\,\hat{x}^2 + 3) + \frac{\gamma_1^2}{72} (\hat{x}^6 - 15\,\hat{x}^4 + 45\,\hat{x}^2 - 15) \right) \quad .. \quad (5)$$

It is important to note that the truncated espansions (2) and (5) are not valid in general for all $\hat{x}$, that is, the expansions are not positive definite for all values of $\hat{x}$, with fixed values of γ_1, γ_2. Figure 4 shows the domain [33] of γ_1 and γ_2 values for which (2) and (5) are always valid.

Instead of expanding $\eta(\hat{x})$ around $\eta_G(\hat{x})$, alternatively, one can look for a transformation $y = f(\hat{x})$ such that y has a known asymptotic density $\eta_0(\hat{x})$ and gets transformed into $\eta(\hat{x})$ which has the given moments. One can visualise it like this. Suppose in a given space we have the function $\eta(\hat{x})$. The space is now distorted in such a way that the $\eta(\hat{x})$ of the undistorted space looks like $\eta_0(\hat{x})$. Our problem is of course the inverse of this, that is, the space containing $\eta_0(\hat{x})$ is distorted in such a way that $\eta_0(\hat{x})$ looks like $\eta(\hat{x})$. Thus $\eta(\hat{x})$

can be written as

$$\eta(\hat{x}) = \eta_0 (f(\hat{x})) * \frac{\partial f(\hat{x})}{\partial x} \quad .. (6)$$

The absolute value in the above expression is necessary as both $\eta(\hat{x})$ and $\eta_0(\hat{x})$ should represent positive definite densities. The only condition for this approach to be valid for all $\hat{x}$ is that $\hat{x} = f^{-1}(y)$ is a single valued function of y, that is, the value of $\partial f(x)/\partial x$ always has the same sign.

Johnson [31] has shown that given γ_1, γ_2 of $\eta(\hat{x})$, one can always use one of the transformations from a set of three transformations, applicable in region S_B, in region S_U, and on the lognormal line separating the two regions in the γ_1, γ_2 plane (see figure 11) such that the transformed variable has a gaussian density. The lognormal line in the γ_1, γ_2 plane satisfies the parametric equations

$$\gamma_1^2 = (\omega - 1)(\omega + 2)^2 \quad \text{and} \quad \gamma_2 = \omega^4 + 2\omega^3 + 3\omega^2 - 6.$$

In the region S_B lying below the lognormal line, the representation of $\eta(\hat{x})$ is bounded on both sides, in the S_U region it is unbounded on both sides and for the γ_1, γ_2 values on the lognormal line, it is bounded only on one side [31]. The transformations and the corresponding representations of density function given by Johnson are discussed in Appendix 1.

Instead of using Johnson's transformations which have merely empirical backing, more pleasing procedure would be to write the transformation $y = f(\hat{x})$ as an asymptotic series as Cornish and Fisher did, using polymonials in $\hat{x}$; $y = \sum_{\mu} a_{\mu} g_{\mu}(\hat{x})$. The polynomials $g_{\mu}(\hat{x})$ and the expansion coefficients a_{μ} are derived using the EW expansion given above [31]. With the cumulants k behaving as $m^{-(\nu-2)/2}$, taking y to be a gaussian random variable and collecting the terms which behave asymptotically as the same power of m, the Cornish Fisher (CF) expansion for y to order 1/m, taking into a account γ_1, γ_2 is given by [31]

$$y = \hat{x} - \frac{\gamma_1}{6}(\hat{x}^2-1) + \left(-\frac{\gamma_2}{24}(\hat{x}^3-3\hat{x})\right) + \frac{\gamma_1^2}{36} * (4\hat{x}^3 - 7\hat{x}) \quad .. (7)$$

The inverse transformation to the same order is

$$\hat{x} = y + \frac{\gamma_1}{6}(y^2-1) + \frac{\gamma_2}{24}(y^3-3y) - \frac{\gamma_1^2}{36}(2y^3-5y) \quad ... (8)$$

Using equations (6) and (7), the CF representation of $\eta(\hat{x})$ is

$$\eta_{CF}(\hat{x}) = \frac{1}{\sqrt{2\pi}}\left(1 - \frac{\gamma_1}{3}\hat{x} + \frac{\gamma_1^2}{36}(12\hat{x}^2-7) - \frac{\gamma_2}{8}(\hat{x}^2-1)\right) *$$

$$\exp\left(-1/2\left(\hat{x} - \frac{\gamma_1}{6}(\hat{x}^2-1) - \frac{\gamma_2}{24}(\hat{x}^3-3\hat{x}) + \frac{\gamma_1^2}{36}(4\hat{x}^3-7\hat{x})\right)^2\right) \quad .. (9)$$

Here we would like to make a remark that CF expansion can also be made around a non gaussian random variable. We see that the density function generated by the CF expansion is positive definite, inspite of its truncation. The domain of validity in γ_1 , γ_2 plane for this representation is determined by the condition of monotonicity of $y = f(\hat{x})$. For any distribution, γ_1, γ_2 values must lie below the ------- line (Figure 4). Cross hatched area in the main figure and the area between the two solid lines in the inset figure are for the Cornish Fisher expansion. In the inset figure, the area under -.-.-.-.-. curve and the - - - - curve are for the Gram Charlier and the Edgeworth expansions respectively. We see that the CF expansion is valid in a considerably larger domain of γ_1 , γ_2 as compared to the GC and EW expansions.

The Pearson system of curves comes out as a solution of differential equation

$$\frac{\partial \eta(\hat{x})}{\partial \hat{x}} = \frac{(\hat{x}-a)\ \eta(\hat{x})}{b_0 + b_1 \hat{x} + b_2 \hat{x}^2} \qquad .. \quad (10)$$

The parameters a, b_0, b_1 and b_2 can be expressed in terms of the centroid, width, γ_1 and γ_2 of $\eta(\hat{x})$. The gaussian function is generated as a special case with $b_0 = -1$, $b_1 = b_2 = 0$. The precise functional forms of $\eta(\hat{x})$ to be used in various domains

FIGURE 4

Domain of validity in γ_1, γ_2 plane. For any distribution γ_1, γ_2 values must lie below the ------ line in the main figure. Cross hatched area in the main figure and the area between the two solid lines in the inset figure are for the Cornish Fisher expansion. In the inset figure, the area under -.-.-.-. curve and the - - - - curve are for the Gram Charlier and Edgeworth expansions respectively. Note the difference of scales in the main and the inset figure.

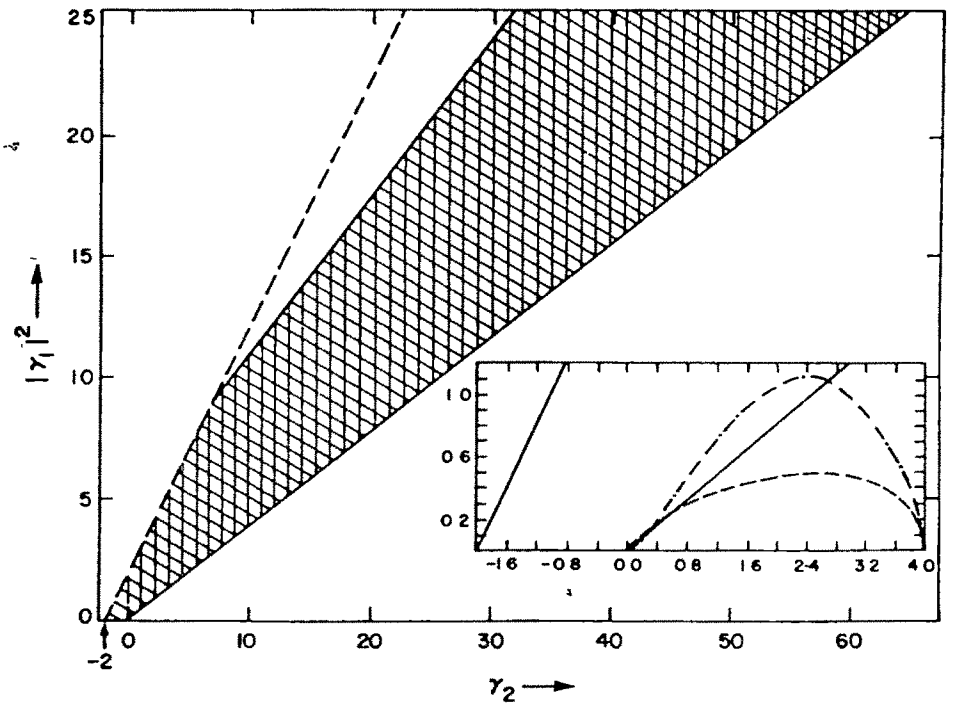
25
20
15
10
5
0
$|\gamma_1|^2$
0
10
20
30
40
50
60
-2
γ_2
1.0
0.6
0.2
-1.6
-0.8
0.0
0.8
1.6
2.4
3.2
4.0

FIGURE 4

of the γ_1, γ_2 plane have also been discussed in Appendix 1.

Using exact shell model calculations performed in $(2s\text{-}1d)^4$ space with Rpsenfeld [34] interaction and ^{17}O single particle energies, the configuration partial densities $\rho_{\tilde{m}}(E)$ were constructed. The exact results for the two configurations are compared with the five representations mentioned above along with the gaussian curve in figure 5 (a,b) and 6 (a,b). The relevant parameters for the configuration have been given along with the figures. We have chosen here to represent two extreme cases of large γ_1 and γ_2 so that the departures of different representations from the exact results can be seen adequately. We see that the Gram-Charlier and Edgeworth representations give unphysical values in the tail regions for the chosen examples. The inadequacy of the Gram Charlier representation is clearly seen from the figures, as was pointed out by others [32]. The Cornish Fisher expansion, as is evident from the figures is as good, if not better than the Edgeworth expansion. It is interesting to note that the Johnson and Pearson systems fit well with the exact results. One can also see that as $\gamma_1, \gamma_2 \to 0$, curves in both these systems approach a gaussian, but then the dependence of their higher cumulants on m (the number of particles) is

FIGURE 5 (a, b)

Comparison of various representations with the shell model results.

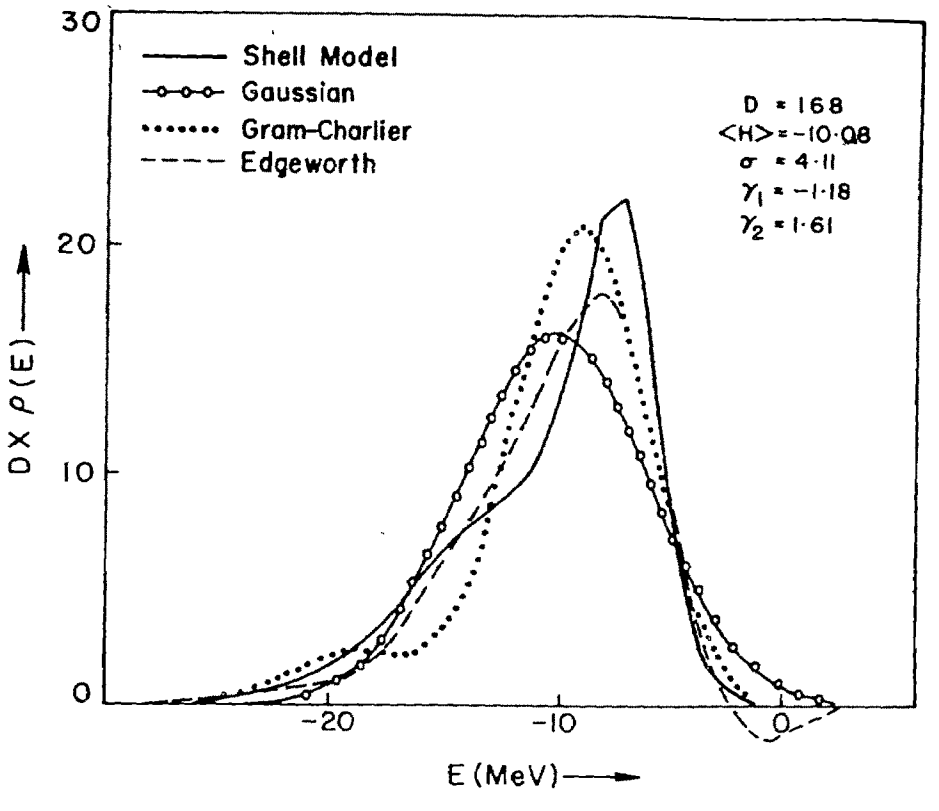
30
20
10
0
Shell Model
Gaussian
Gram-Charlier
Edgeworth
D = 168
<H>=-10·08
σ = 4·11
γ1 = -1·18
γ2 = 1·61
D X ρ(E)
-20
-10
0
E (MeV)

FIGURE 5(a)

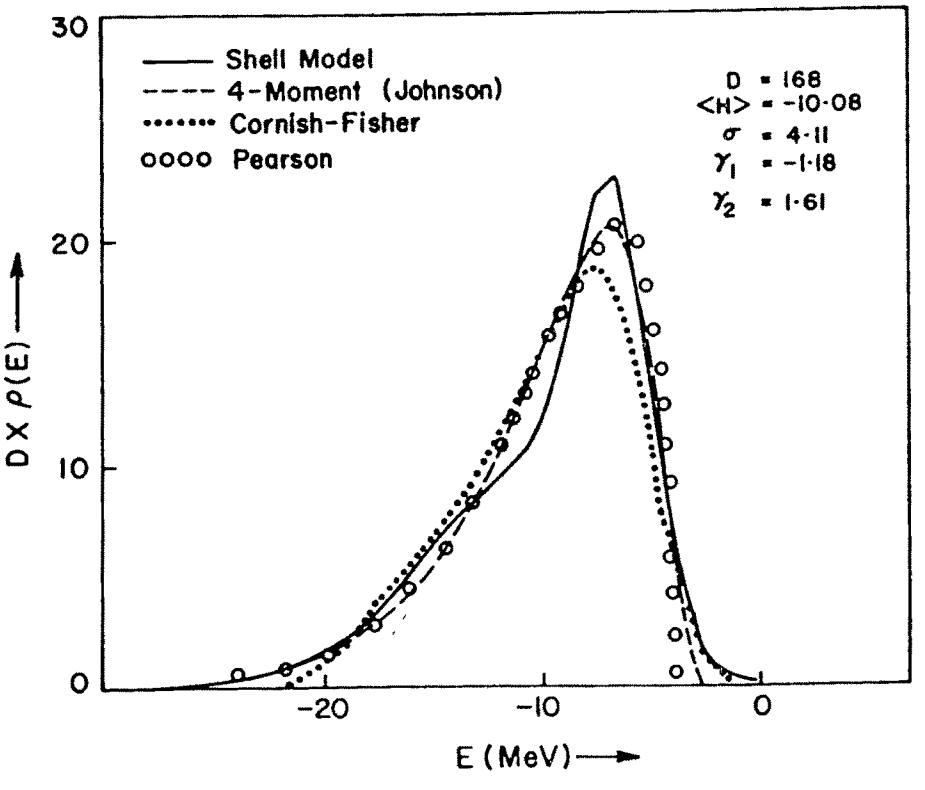
30
20
10
0
D X ρ(E)
Shell Model
4-Moment (Johnson)
Cornish-Fisher
Pearson
D = 168
<H> = -10·08
σ = 4·11
γ1 = -1·18
γ2 = 1·61
-20
-10
0
E (MeV)

FIGURE 5(b)

FIGURE 6 (a, b)

Comparison of various representations with the shell model results.

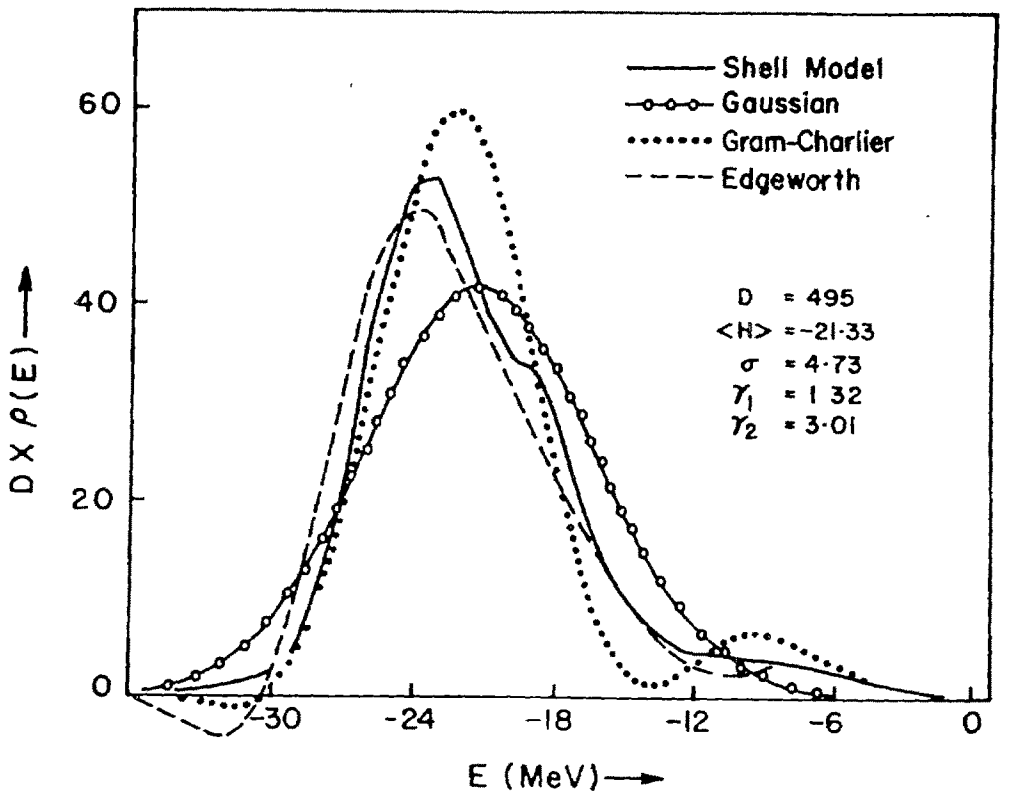
Shell Model
Gaussian
Gram-Charlier
Edgeworth
D = 495
<H> = -21·33
σ = 4·73
γ1 = 1 32
γ2 = 3·01
D X ρ(E)
E (MeV)
60
40
20
0
-30
-24
-18
-12
-6
0

FIGURE 6(a)

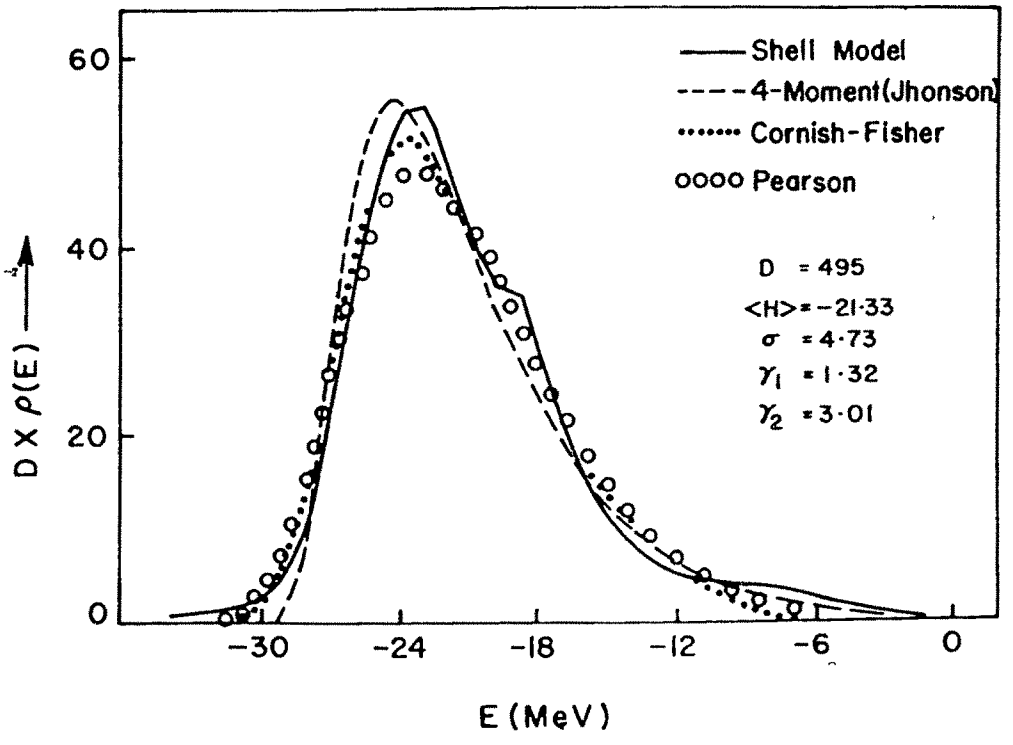
Shell Model
4-Moment(Jhonson)
Cornish-Fisher
Pearson
D = 495
<H>=-21·33
σ = 4·73
γ1 = 1·32
γ2 = 3·01
D X ρ(E)
E (MeV)
60
40
20
0
-30
-24
-18
-12
-6
0

FIGURE 6(b)

unexplored for these systems. In that sense we do not know about their asymptotic convergence properties and hence their study is essential before advocating their use.

Besides giving a good fit to the exact density, the CF expansion has several other uses. Given the centroid and width, for gaussian approximation, using Hasting's expressions[35] one can read off the smooth spectrum. Now using CF expansion (8), it is easy to incorporate γ_1 , γ_2 corrections. Similar calculations for other representations involve numerical integration. The fact that CF expansion can also be done in terms of non gaussian random variables[36], allows us to obtain series expansions for expectation values of operators using parametric derivative approach [37]. Similarly, one can also do statistical perturbation theory [38] using CF expansion. CF expansion gives a very good account of the spherical orbit occupancies as compared to the other available expansions. We study some of the above mentioned uses of CF expansion in detail in the next chapter.

Thus, in conclusion we see that the Cornish Fisher expansion gives a good fit to the exact density and it is theoretically and physically satisfying because of its (i) asymptotic convergence properties (ii) positive definiteness

and (iii) large domain of validity, and hence can be termed as the most appropriate representation for the density function.