CHAPTER - 3

GEOMETRICAL DERIVATION OF CLT RESULT

The spectral distribution methods (SDM), used for the study of nuclear properties, deal with distribution of physical observables rather than the observables themselves. In the case of energy distributions, the discrete eigenvalue spectrum can be recovered through the Ratcliff procedure. The accuracy of such a calculation depends upon the extent to which the approximation is made. One can construct energy eigenvalue distribution fairly well using low-order moments of the hamiltonian. The operation of the central limit theorem (CLT) in model spaces of interest makes this approach meaningful. Besides the hamiltonian, there are other interesting operators namely the number operator n, the quadrupole and other electromagnetic transition operators, operators related to particle transition or a product of these operators, whose expectation values with respect to hamiltonian eigenfunctions are of considerable interest. The spectral distribution methods provide smoothened forms for expectation values of such operators as a function of energy /22/.

Though the smoothened forms for various operators depend largely upon energy, one cannot rule out their dependence on other quantum numbers like angular momentum J, its z-component J_z, isospin T and so on. A beginning has been made to bring out such dependences using bivariate and multivariate distributions defined in terms of these quantum numbers and E /27/. For example, if one seeks a J_z dependence, it is possible to obtain a bivariate level density $\eta(E,M)$, where M is the eigenvalue of J_z. This density can be explicitly constructed in terms of its bivariate cumulants K_{rs}. If the higher order cumulants are small in magnitude, the corresponding bivariate density can be expanded as a series around a bivariate normal $S_G(E,M)$; the expansion involving only few low order cumulants. Measurable properties like binding energies, yrast lines, level densities, spin cutoff factors etc. follow directly from $\eta(E,M)$. There are, however, other measurable properties like the spherical orbit occupancies, static moments, electromagnetic sum-rule quantities, etc. which cannot be derived directly from $\eta(E,M)$ but are expressible as expectation values with respect to E and M. The complete analytical expression in terms of averages of products of operators for the expectation value as a function of two variables turns out to be a series expansion using bivariate orthogonal polynomials defined by the bivariate density function /28/. Under the action of CLT, only terms upto linear in variables contribute in the expansion, other terms becoming negligible.

In this chapter, a simple, geometrical way is presented to obtain the CLT result for the expectation value of an arbitrary operator K in terms of one and two variables. For obtaining the result in the bivariate case, use has been made of the conditional density $\eta(x|y)$ of the bivariate density $S_G(x,y)$; x and y are the eigenvalues of operators X and Y respectively.

A Univariate Case

Let K be an operator in an m-particle space with X as the hamiltonian having eigenvalues x. As a consequence of the CLT, the energy-eigenvalue density function in the first approximation is given by gaussian with centroid ϵ and width σ:

$$\eta(x) = (2\pi\sigma^2)^{-1/2} \exp\{-(x-\epsilon)^2/2\sigma^2\} \tag{1}$$

When a small multiple of an operator K is added to X, so that $X \rightarrow X + \alpha K$; then to the first order in α, the eigenvalue $x \rightarrow x(\alpha) = x + \alpha\langle x|K|x\rangle = x + \alpha K(x)$; where K(x) is the expectation value of K in the m-particle space. Thus, we have $(\partial x_{(\alpha)}/\partial\alpha)|_{\alpha=0} = K(x)$. Again due to the strong CLT action, the new eigenvalue density function $\eta_\alpha(x)$ would be a gaussian but with the centroid and width depending on the parameter α. Because of the change in the hamiltonian, we have

$$\langle X\rangle \rightarrow \langle X\rangle + \alpha\langle K\rangle = \epsilon + \alpha\langle K\rangle\ ,$$
$$\sigma^2 \rightarrow \sigma^2 + 2\alpha\langle(X-\epsilon)K\rangle + \alpha^2 \text{ term}$$
$$\sigma \rightarrow \sigma(1 + \langle(X-\epsilon)K\rangle\alpha/\sigma^2) + \text{higher order terms in } \alpha\,.$$

The centroid of the density function shifts by $\alpha\langle K\rangle$ and the overall scale is changed due to the variation of σ by a factor of $\alpha\langle(X-\epsilon)K\rangle/\sigma^2$. Now it is easy to see how a particular eigenvalue x gets shifted due to these changes. Figure 3.1 indicates these shifts: (i) First of all, shift of centroid introduces a constant shift in all eigenvalues $x \rightarrow x + \alpha\langle K\rangle$. (ii) Secondly, the scale change introduces a shift proportional to the distance from the centroid which is equivalent to stretching or contracting; $x \rightarrow (x-\epsilon)\langle(X-\epsilon)K\rangle\alpha/\sigma^2$. Both these combined produce shift

$$x \rightarrow x + \alpha\{\langle K\rangle + \langle(X-\epsilon)K\rangle * (x-\epsilon)/\sigma^2\}$$

giving rise to the CLT result for expectation value of K as a function of energy;

$$K(x) = \langle K\rangle + \langle(X-\epsilon)K\rangle(x-\epsilon)/\sigma^2\,. \tag{2}$$

The arguments given here will be valid for any density which does not change its shape on introduction of K and then the CLT result is exact. However, if the shape changes, the CLT result corresponds only to the leading terms in the series expansion.

B Bivariate case

Let us extend these arguments to the bivariate gaussian density $\eta(x,y)$, a function of x and y (the eigenvalues of operators X and Y respectively). Such a density is characterised by five parameters namely, two centroids ($\langle X \rangle$ and $\langle Y \rangle$), two widths (σ_x and σ_y) and a correlation coefficient between X and Y denoted by ρ and given as

$$\rho = \frac{\langle (X-\langle X \rangle)(Y-\langle Y \rangle) \rangle}{\sigma_x \sigma_y} = \iint \frac{(x-\langle X \rangle)(y-\langle Y \rangle)}{\sigma_x \sigma_y} \eta(x,y)\, dx\, dy. \tag{3}$$

For simplicity, we assume that centroids are zero and the variables x and y (and corresponding operators) are normalised in such a way that $\sigma_x = \sigma_y = 1$. The density function $\eta(x,y)$ then is given by

$$\eta(x,y) = \frac{1}{2\pi(1-\rho^2)^{1/2}} \exp\left\{-\frac{x^2-2\rho xy+y^2}{2(1-\rho^2)}\right\}. \tag{4}$$

The number of states in the interval x to x+dx and y to y+dy is given by $D^* \eta(x,y)\,dx\,dy$, where D is the total number of states (dimensionality) in the model space. It must be kept in mind that such an interpretation is possible only if operators X and Y commute.

Consider now the conditional density function $\eta(x|y)$ when y is fixed,

$$\eta(x|y) = \eta(x,y)/\eta(y)$$

which is a gaussian. It can be immediately shown that the expectation value of x for $\eta(x|y)$ [centroid of $\eta(x|y)$] is ϱy. In statistical language this is called the regression line (Fig.3.2a)

$$\int_{-\infty}^{\infty} x\ \eta(x|y)\ dx = \varrho y . \tag{5}$$

Let us add a small operator αK to X. Due to the strong action of CLT, we can assume that this does not result in any change of shape, that is, the density function still remains a bivariate gaussian. Such an addition however is going to affect in three ways: (i) change of centroid along the x-axis, (ii) change of scale parameter along the x-axis and (iii) change of the correlation coefficient which results in rotating the regression line. Consider a particular eigenstate with eigenvalue (x_0,y), which can be obtained through Ratcliff procedure using the conditional density $\eta(x|y)$. We would now like to find out how x_0 shifts as a function of α. The value of $dx_0/d\alpha|_{\alpha=0}$ then is the expectation value of K at (x_0,y) in the CLT limit.

The addition of αK shifts the overall centroid of the bivariate density along x-axis by $\alpha\langle K\rangle$, (see Fig.3.2b)

$$x_0 \rightarrow x_0 + \alpha\langle K\rangle \quad \text{or } dx_0 = \alpha\langle K\rangle . \tag{6}$$

Secondly, the width of X also changes

$$\sigma_X^2 \rightarrow \sigma_{(X+\alpha K)}^2 = \sigma_{X,\alpha}^2 = \sigma_X^2 + 2\alpha\langle KX\rangle + \alpha^2\sigma_K^2$$

or $$\sigma_X \rightarrow \sigma_X(1 + 2\alpha\langle KX\rangle + \alpha^2\sigma_K^2)^{\frac{1}{2}} \cdot \tag{7}$$

Since $\sigma_X = 1$, we have an overall change of scale factor given by

$$1 \rightarrow 1 + \alpha\langle KX\rangle + \alpha^2\sigma_K^2/2 + \text{higher order terms in } \alpha.$$

In the limit $\alpha \rightarrow 0$, for $dx_0/d\alpha\,\big|_{\alpha=0}$, we shall see that α^2 and higher order terms vanish. Such a scale change shifts x_o by $\alpha\langle KX\rangle x_o$, as the stretching is proportional to the distance from the centroid on x-axis (see Fig.3.2c. Combining these two effects, we have,

$$dx_o = \alpha\langle K\rangle + \alpha\langle KX\rangle x_o \ . \tag{8}$$

The change of orientation of regression line $\partial\varrho$ due to the addition of αK has two effects; (i) change of centroid of the conditional density and (ii) change of scale factor (stretching) due to change of width of the conditional density $\eta(x|y)$.

$$\varrho \rightarrow \varrho_\alpha = \varrho + \partial\varrho = \frac{\langle XY\rangle + \alpha\langle KY\rangle}{(1 + 2\alpha\langle KX\rangle + \alpha^2\sigma_K^2)^{1/2}} \tag{9}$$

(Note: We have already assumed that both X and Y are unit width operators).

$$\therefore \quad \varrho_\alpha = \varrho + \alpha \langle K(Y-\varrho X)\rangle \quad + \text{higher order terms in } \alpha \,. \tag{10}$$

Hence dx_0 due to centroid change is

$$dx_0 = \partial\varrho * y = \alpha\langle K(Y-\varrho X)\rangle y \,. \tag{11}$$

Width of the conditional density $\eta(x|y)$, which originally was $\sqrt{1-\varrho^2}$ is now changed to $\sqrt{1-(\varrho+\partial\varrho)^2}$:

$$\sqrt{1-\varrho^2} \rightarrow \sqrt{(1-(\varrho+\partial\varrho)^2)}$$
$$= \sqrt{(1-\varrho^2)}\left\{1 - \frac{\alpha\varrho}{1-\varrho^2}\langle K(Y-\varrho X)\rangle\right\} \text{ to the first order in } \alpha. \tag{12}$$

The corresponding change in the scale factor therefore is $\{1-[\alpha\langle K(Y-\varrho X)\rangle/(1-\varrho^2)]\}$. Keeping in mind that this is the change in the scale factor for conditional density and hence the stretching is going to be proportional to the distance from the centroid of conditional density, we have (Fig. 3.2d).

$$dx_0 = -\frac{\alpha\varrho\langle K(Y-\varrho X)\rangle}{(1-\varrho^2)} * (x_0-\varrho y) \,. \tag{13}$$

The shift dx_0 due to all these effects now can be written down to the first order in α,

$$dx_0 = \alpha\langle K\rangle + \alpha\langle KX\rangle x_0 + \frac{\alpha(y-\varrho x_0)}{1-\varrho^2}\langle K(Y-\varrho X)\rangle; \tag{14}$$

Figure captions:

Figure 3.1a-b: Changes in eigenvalue x_0 of operator X when X is perturbed by a small operator αK with respect to a univariate distribution of operator X. (a) change in eigenvalue due to centroid shift and (b) change in eigenvalue due to scale change.

Figure 3.2 a-d: Changes in eigenvalue x_0 of operator X when X is perturbed by αK with respect to a joint bivariate distribution of operators X and Y. (a) conditional density $\eta(x|y)$ with unperturbed centroid at $x = \varrho y$, (b) shift in x_0 due to change of centroid of the conditional density, (c)shift in x_0 due to change of scale of the conditional density and (d) shift in x_0 due to change in orientation of the regression line.

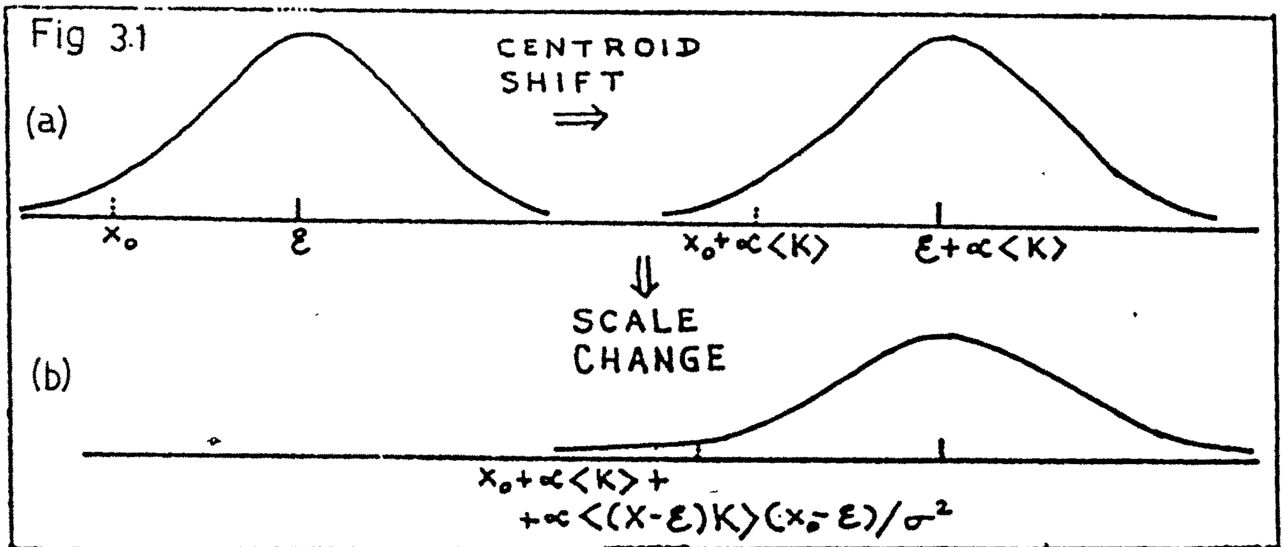
(a)
CENTROID SHIFT
x_o
ε
$x_o + \alpha\langle K \rangle$
$\varepsilon + \alpha\langle K \rangle$
SCALE CHANGE
(b)
$x_o + \alpha\langle K \rangle +$
$+ \alpha\langle (X-\varepsilon)K \rangle (x_o - \varepsilon)/\sigma^2$

Fig 3.1

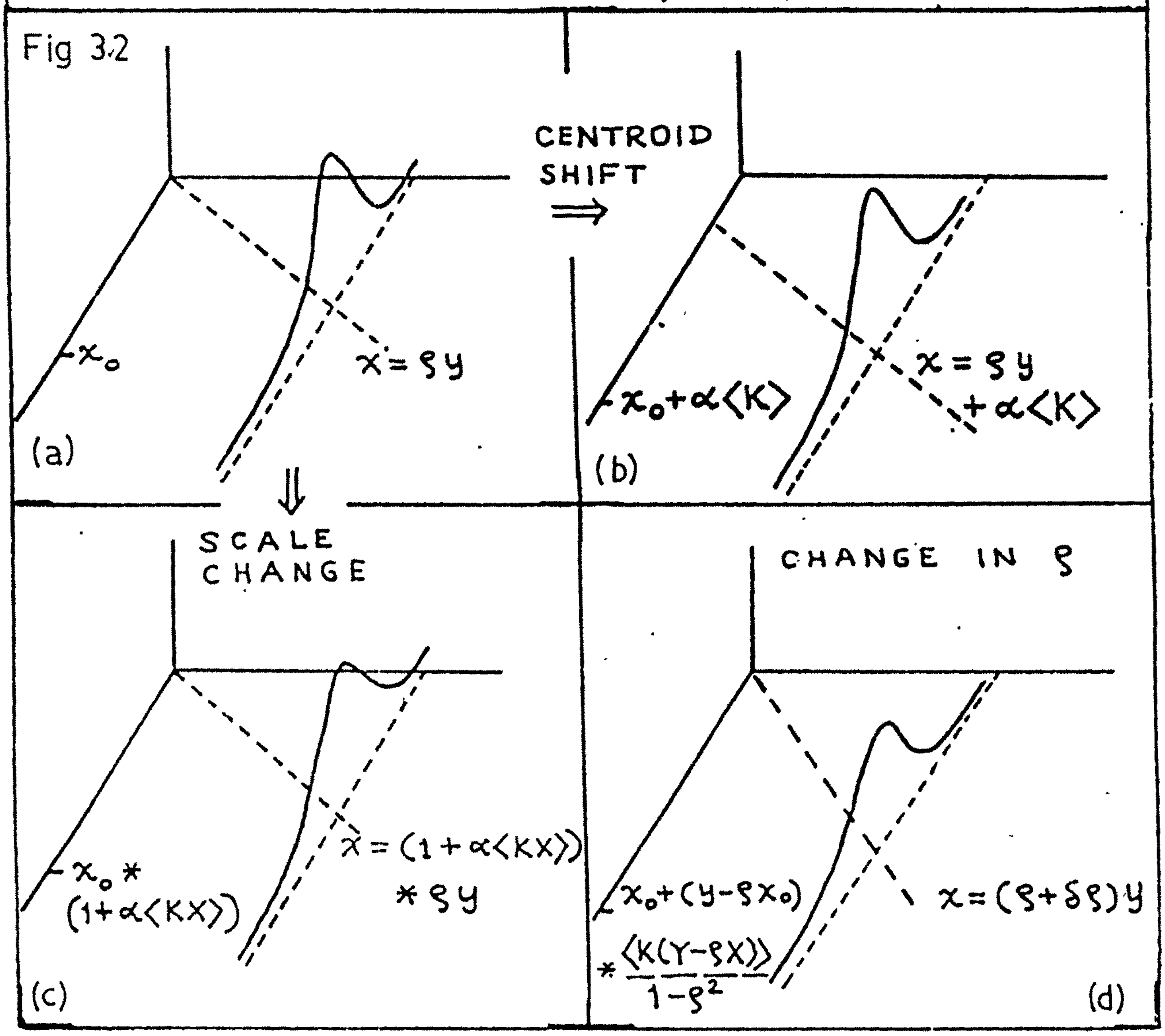
x_o
$x = \varrho y$
(a)
CENTROID SHIFT
$x_o + \alpha\langle K \rangle$
$x = \varrho y + \alpha\langle K \rangle$
(b)
SCALE CHANGE
$x_o * (1+\alpha\langle KX \rangle)$
$x = (1+\alpha\langle KX \rangle) * \varrho y$
(c)
CHANGE IN ϱ
$x_o + (y - \varrho x_o) * \frac{\langle K(Y-\varrho X) \rangle}{1-\varrho^2}$
$x = (\varrho + \delta\varrho) y$
(d)

Fig 3.2

$$K(x,y) = \left.\frac{dx_0}{d\alpha}\right|_{\alpha=0} = \langle K \rangle + \langle KX \rangle\, x + \frac{(y-\rho x)}{1-\rho^2} \langle K\,(Y-\rho X)\rangle . \tag{15}$$

This is the CLT result for expectation value of K as a function of two variables (x,y) when the density is assumed to be a bivariate gaussian.

If, instead of the operator X, the operator Y is perturbed so that $Y \rightarrow Y + \alpha K$, similar result for expectation value K(x,y) can be obtained in terms of shift of eigenvalues of Y. In that case however, it is not possible to define the conditional density $\eta(x|y)$, since for defining $\eta(x|y)$, the bivariate density $\eta(x,y)$ is normalised with respect to the marginal density $\eta(y)$, it is necessary that $\eta(y)$ remain fixed. Shift in eigenvalues of Y would change the centroid and width of the y-distribution, so that $\eta(y) \rightarrow \eta(y_\alpha)$, whereas $\eta(x)$ remains fixed. One can therefore follow a similar procedure as described above, but through the conditional density $\eta(y|x)$.