CHAPTER V

STATISTICALLY AVERAGED INVERSE ENERGY WEIGHTED SUM-RULES

Sum-rules in spectral distribution methods are encounted in two different ways. First, if an excitation operator O acts on an eigenstate with energy E of a hamiltonian H, then the expectation value of $O^{+} O$ as a function of energy E, corresponds to the non energy weighted sum and gives us the expression for the total strength of the excitation operator O, acting on the eigenstate E. The linear - energy - weighted sum given by the expectation value of $O^{+}HO$ as a function of E, relates to the centroid of the strength distribution. Similarly, the quadratically - energy - weighted sum (expectation value of $O^{+} H^{2}O$ as a function of E) has the information about the spread of the strength with respect to energy. Single nucleon transfer provides as example for such sum rules. Secondly, the sums arise when a hamiltonian H is perturbed by a small operator αK, where α is merely a multiplicative parameter. In this case the expectation value of K^{2} as a function of energy E is related to the width of an eigenfunction of H at E, when expressed in terms of eigenfunctions of K. Perturbation of H by any operator provides an example of the second kind. So far not much attention has been paid to the inverse - energy - weighted sums. This is partly due to the notion that one has to deal with Green's function and complete solutions of the problems, for obtaining inverse - energy - weighted sums. However, recently Halemane[38) applied the spectral distribution methods to the Rayleigh-Schrodinger perturbation theory and obtained expressions for varieties of inverse energy weighted sums. Our purpose is to rederive his expressions using a different procedure. In the first section we discuss the new and simple procedure to obtain inverse - energy - weighted sums. The second section deals with the central limit theorem (CLT) limit for the rule. Its extension to configuration spaces is discussed in the third section. We apply these rules in the fourth section to correct the ground state energy estimates when an effective interaction is approximated by linear sum of well known operators.

A. THEORY

The eigenvalue density of a Hamiltonian H in a finite dimensional space is always discrete. However, the spectral distribution methods which generally deal with only few lower order moments, assume a continuous density of states, $\rho(E)$. It has been demonstrated that when the higher order moments are not taken into account, it amounts to ignoring the level to level fluctuations. Ratcliffe's procedure provides us a method to generate a smoothend (fluctuation free) spectrum from the continuous density function which in turn is expressible in terms of few lower moments (traces of powers of Hamiltonian matrix). For example, the n^{th} level starting from the ground - state is given by

$$n - 1/2 = d \int_{-\infty}^{E_n} \rho(x)\, dx = d * F(E_n)$$

where E_n is the eigenvalue (smoothened) of n^{th} level, d is the dimensionality of the space and F is the distribution function. If a small operator αK is added to H, this perturbation will shift the eigenvalues. The new set of eigenvalues can be obtained by the same procedure with the state density function $\rho_\alpha(x)$, which is characterised by few lower order moments of $H + \alpha K$. We denote n^{th} eigenvalue of H by $E_{n,0}$ and corresponding eigenvalue of $H + \alpha K$ by $E_{n,\alpha}$. The value of the distribution function is same for both these eigenvalues; we denote it by p.

$$\int_{-\infty}^{E_{n,0}} \rho_{\alpha=0}(x)\, dx = F_{\alpha=0}(E_{n,0}) = p = F_\alpha(E_{n,\alpha})$$

$$= \int_{-\infty}^{E_{n,\alpha}} \rho_\alpha(x)\, dx \quad .. (1)$$

It should be noted here that, the statistical methods involved here naturally invoke the principle of rigidity (non-crossing of levels). For small values of α, the shifted eigenvalue $E_{n,\alpha}$

can be written down as a series in powers of α, the coefficients of m^{th} power of α denoted by $S_m(E_{n,0})$, where $E_{n,0}$ is the unperturbed energy.

$$E_{n,\alpha} = E_{n,0} + \alpha S_1(E_{n,0}) + \alpha^2 S_2(E_{n,0}) + \quad .. \qquad .. (2)$$

The coefficients $S_m(E_{n,0})$ are explicitly given by the Rayleigh-Schrodinger perturbation expansion :

$$E_{n,\alpha} = E_{n,0} + \alpha\langle E_{n,0} | K | E_{n,0}\rangle + \alpha^2 \sum_{m\neq n} \frac{|\langle E_{n,0} | K | E_{m,0}\rangle|^2}{E_{m,0} - E_{n,0}} \qquad .. (3)$$

Thus S_1 corresponds to the expectation value of K and S_2 is the inverse energy weighted sum of the strength of the operator K. Spectral distribution methods provide the smoothened expressions for these coefficients; to obtain these we turn to equation (1). Differentiating equation 1 with respect to α, we get (since we are interested in smooth forms, we drop the state index n from now on).

$$\frac{\partial p}{\partial \alpha} = 0 = \frac{\partial E_\alpha}{\partial \alpha} \rho_\alpha(E_\alpha) + \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx$$

$$\therefore \quad \frac{\partial E_\alpha}{\partial \alpha} = - \frac{1}{\rho_\alpha(E_\alpha)} \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx \qquad .. (4)$$

In the limit $\alpha \to 0$, we have

$$\left.\frac{\partial E_\alpha}{\partial \alpha}\right|_{\alpha=0} = - \frac{1}{\rho(E_0)} \int_{-\infty}^{E_0} \left.\frac{\partial \rho_\alpha(x)}{\partial \alpha}\right|_{\alpha=0} dx .$$

Now the integration limits do not depend on α, hence interchanging integration over x and differentiation with respect to α, we obtain,

$$\left.\frac{\partial E_\alpha}{\partial \alpha}\right|_{\alpha=0} = - \frac{1}{\rho(E_0)} \left[\frac{\partial}{\partial \alpha} \int_{-\infty}^{E_0} \rho_\alpha(x) \; dx\right]_{\alpha=0} .$$

$$= - \frac{1}{\rho(E_0)} \left[\frac{\partial}{\partial \alpha} F_\alpha \; (E_0)\right]_{\alpha=0} . \qquad .. \; (5)$$

Comparing this with equation 2 we obtain,

$$K\,(E) = S_1\,(E) = - \frac{1}{\rho(E_0)} \left[\frac{\partial}{\partial \alpha} F_\alpha \; (E_0)\right]_{\alpha=0}$$

where K (E) is the expectation value of K at E. This result was originally given by Chang and French[37]. Differentiating equation (4) again with respect to α gives

$$\frac{\partial^2 E_\alpha}{\partial \alpha^2} = - \frac{1}{\rho_\alpha(E_\alpha)} \int_{-}^{E_\alpha} \frac{\partial^2}{\partial \alpha^2} \rho_\alpha(x)\, dx + \frac{1}{\rho_\alpha^2(E_\alpha)} \left.\frac{\partial \rho_\alpha(x)}{\partial \alpha}\right|_{x=E_\alpha} *$$

$$\int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx + \frac{1}{\rho_\alpha^2(E_\alpha)} \frac{\partial \rho_\alpha(E_\alpha)}{\partial \alpha} \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} \; dx \qquad .. \; (6)$$

One has to be careful about keeping all the terms which depend on α. For example $\frac{\partial \rho_\alpha (E_\alpha)}{\partial \alpha}$ can be written as

$$\frac{\partial \rho_\alpha(E_\alpha)}{\partial \alpha} = \frac{\partial}{\partial \alpha} \left\{ \rho_\alpha(E_0) + \left.\frac{\partial \rho_\alpha(x_0)}{\partial x}\right|_{x=E_0} (E_\alpha - E_0) + \frac{(E_\alpha - E_0)^2}{2} \left.\frac{\partial^2 \rho_\alpha(x)}{\partial x^2}\right|_{x=E_0} + .. \right\} \quad .. (7)$$

Substituting equation 7 in equation 6 and then taking the limit as $\alpha \to 0$, we obtain

$$S_2(E) = 1/2 \left.\frac{\partial^2 E_\alpha}{\partial \alpha^2}\right|_{\alpha=0} = - \frac{1}{2 * \rho(E_0)} \left[\left(\frac{\partial^2}{\partial \alpha^2} F_\alpha (E_0)\right)_{\alpha=0} - \frac{\partial}{\partial E_0} \left\{ \frac{1}{\rho(E_0)} \left(\left.\frac{\partial F_\alpha (E_0)}{\partial \alpha}\right|_{\alpha=0} \right)^2 \right\} \right] \quad .. (8)$$

As mentioned earlier, this result was given by Halemane. We have rederived it beginning with the Ratcliffe's procedure[39]. Since the purpose here is to provide an alternative method of deriving the results originally given by Halemane, we merely state that the expressions for S_m (E_0) for higher values of m can be similarly obtained.

B. THE CLT RESULT

The role played by the central limit theorem in spectral distribution methods has been well established and discussed at various places. As a consequence of CLT, we can write the eigenvalue density function as a Gaussian, defined by its centroid $\mathcal{E}$ and width σ. The CLT also allows us to assume that when the hamiltonian H is perturbed by a small operator αK, the new eigenvalue density still remains a Gaussian but with different centroid $\mathcal{E}(\alpha)$ and different width $\sigma(\alpha)$. The change in centroid merely shifts the eigenvalue spectrum while the width change corresponds to the scale change.

$$\mathcal{E} = \langle H \rangle \quad , \mathcal{E}(\alpha) = \langle H \rangle + \alpha \langle K \rangle$$
$$\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2$$
$$\sigma^2(\alpha) = \langle (H + \alpha K)^2 \rangle - (\langle H + \alpha K \rangle)^2$$
$$= \sigma^2 + 2\alpha \zeta \sigma \sigma_K + \alpha^2 \sigma^2_K$$

where ζ is the correlation coefficient between H and K and σ^2_K is the width of eigenvalue density function corresponding to the operator K. The scale change parameter λ is defined by

$$\lambda = \left(\frac{\sigma(\alpha)}{\sigma} - 1\right) = \left(1 + 2\alpha \zeta \sigma_K/\sigma + \alpha^2 \sigma^2_K/\sigma^2\right)^{\frac{1}{2}} - 1 \quad .. (9)$$

Thus if we take into account these two changes, from the eigenvalue E_0 corresponding to unperturbed hamiltonian H we can obtain the eigenvalue E_α as

$$E_\alpha = E_0 + \alpha \langle K \rangle + (E_0 - \mathcal{E})\lambda \quad .. \quad (10)$$

Merely expanding the parameter λ as a series in gives

$$E_\alpha = E_0 + \alpha\langle K \rangle + \alpha(E_0 - \mathcal{E})\zeta\ \sigma_K/\sigma + (E_0 - \mathcal{E})\ \frac{\alpha^2}{2}\left(\frac{\sigma_K^2}{\sigma^2} - \frac{\zeta^2\sigma_K^2}{\sigma^2}\right)$$

$$= E_0 + \alpha\langle K \rangle + \alpha\zeta\sigma_K/\sigma\,(E_0 - \mathcal{E}) + \frac{\alpha^2}{2}\ (E_0 - \mathcal{E})\ (1 - \zeta^2)\ \sigma_K^2/\sigma^2$$

Thus it immediately follows that in the CLT limit we have

$$S_1\ (E_0) = \langle K \rangle + \zeta\,\sigma_K/\sigma\ (E_0 - \mathcal{E})$$

$$S_2\ (E_0) = (1-\zeta^2)\ (E_0 - \mathcal{E})\,\sigma_K^2/2\sigma^2 \quad .. \quad (11)$$

The same expressions can be obtained using equations (5) and (8) if the distribution functions F and F_α are taken to be Gaussian.

C. EXTENSION TO CONFIGURATIONS

The arguements based on the centroid shift and scale change for calculating S_1 (E) and S_2 (E) are easily applicable in the scalar space. If we partition the space according to some symmetry group, we cannot use these simple arguments. Let us, for example, decompose the space into configurations. The over all state density ρ(E) (assumed to be gaussian and hence completely described by its centroid $\mathcal{E}_0$ and width σ_0) is then the sum of all intensities of configurations into which the space has now been subdivided. Thus,

$$\rho(E) = \sum_c \rho^c (E) \frac{dc}{D} = \sum_c I^c(E)$$

with dc being the configuration dimensionality and $D = \sum_c dc$ is the total dimensionality. Each term in the above summation corresponds to the intensity of the configuration c in the eigenvalue distribution at energy E. Further, we assume that each partial state density is a gaussian (higher order configuration moments are usually not easy to calculate because of two reasons : (i) number of configurations involved are prohibitively many (ii) with increasing order of moments, computer time increases at a much faster rate, and hence if one pleads complete ignorance of higher order moments, it turns out that natural choice is a Gaussian) and can be written down as

$$\rho^c (E) = \frac{1}{\sqrt{2\pi}\ \sigma_0 (c)} \exp \left(- 1/2 \left(\frac{E - \mathcal{E}_0 (c)}{\sigma_0 (c)} \right)^2 \right)$$

where $\mathcal{E}_0(c)$ and $\sigma_0 (c)$ are configuration centroid and width respectively. The corresponding distribution function is

$$F (E) = \sum \frac{dc}{D} \int_{-\infty}^{E} \rho^c (x)\, dx = \sum_c \int_{-\infty}^{E} I^c (x)\, dx$$

Now, when the Hamiltonian operator H is perturbed, the new state density $\rho_\alpha(E)$ corresponding to the perturbed hamiltonian operator $H + \alpha K$ is given by $\rho_\alpha(E) = \sum_c I^c_\alpha (E)$

$$= \sum_c \frac{dc/D}{\sqrt{2\pi}\ \sigma_\alpha(c)} \exp \left(- 1/2 \left(\frac{E - \mathcal{E}_\alpha (c)}{\sigma_\alpha (c)} \right)^2 \right) \quad \text{.. (12)}$$

The corresponding distribution function is

$$F_{\alpha}(E) = \sum_{c} \int_{-\infty}^{E} I_{\alpha}^{c}(x)\ dx$$

$$F_{\alpha}(E) = \sum_{c} dc/D \int_{-\infty}^{E} \rho_{\alpha}^{c}(x)\ dx \qquad .. (13)$$

The calculation of $\mathcal{E}_{\alpha}(c)$ and $\sigma_{\alpha}(c)$ is straight forward. By definition we have, $\mathcal{E}_{\alpha}(c) = \langle H\rangle^{c} + \alpha\langle K\rangle^{c}$

$$= \mathcal{E}_{0}(c) + \langle K\rangle^{c}\alpha \qquad .. (14)$$

$$\sigma_{\alpha}^{2}(c) = \langle(H + \alpha K)^{2}\rangle^{c} - (\langle H + \alpha K\rangle^{c})^{2}$$

$$= \sigma_{0}^{2}(c) + 2\,\zeta_{c}\,\sigma_{K}(c)\,\sigma_{0}(c)\,\alpha + \alpha^{2}\sigma_{K}^{2}(c) \qquad .. (15)$$

where $\sigma_0(c)$ corresponds to the configuration width of the unperturbed Hamiltonian H, $\sigma_K(c)$ is the configuration width corresponding to the operator K and ζ_c is the correlation coefficient between the operators H and K in the configuration.

Partially differentiating both sides of (13) with respect to α and interchanging the integration over x and differentiation with respect to α (since integration limits do not depend on α)

we have

$$\frac{\partial F_\alpha(E)}{\partial \alpha} = \sum_c \int_{-\infty}^{E} \frac{\partial}{\partial \alpha} I^c_\alpha(x)\,dx \qquad \text{.. (16)}$$

We are now in a position to define $S_1(E)$ and $S_2(E)$ in configuration spaces.

$$S_1(E) = -\frac{1}{\sum_c I^c(E)} * \left.\frac{\partial F_\alpha(E)}{\partial \alpha}\right|_{\alpha=0}$$

$$S_2(E) = -\frac{1}{2\sum_c I^c(E)} * \left[\left.\frac{\partial^2}{\partial \alpha^2} F_\alpha(E)\right|_{\alpha=0} - \frac{\partial}{\partial E}\left\{\frac{1}{\sum_c I^c(E)}\left(\left.\frac{\partial}{\partial \alpha}F_\alpha(E)\right|_{\alpha=0}\right)^2\right\}\right] \qquad \text{.. (17)}$$

Using equation (12) - (17), we can derive explicit expressions for $S_1(E)$ and $S_2(E)$ in configuration space. For ease of calculation we consider a single term in the expression (12) and perform the summation at the end of the calculation. Partially differentiating I^c_α with respect to α, we have

$$\frac{\partial I^c_\alpha}{\partial \alpha} = \frac{\partial I^c_\alpha}{\partial \sigma^2_\alpha(c)}\,\frac{\partial \sigma^2_\alpha(c)}{\partial \alpha} + \frac{\partial I^c_\alpha}{\partial \mathcal{E}_\alpha(c)}\,\frac{\partial \mathcal{E}_\alpha(c)}{\partial \alpha} \qquad \text{.. (18)}$$

where $\frac{\partial \mathcal{E}_\alpha(c)}{\partial \alpha}$ and $\frac{\partial \sigma^2_\alpha(c)}{\partial \alpha}$ are obtained from (14), (15) by partially differentiating both sides of the equations with respect to α. These partial differential coefficients turn out to be

$$\frac{\partial \xi_\alpha(c)}{\partial \alpha} = \langle K \rangle^c$$

$$\frac{\partial \sigma_\alpha^2(c)}{\partial \alpha} = 2\ \sigma_0^2\ (c)\ \left(\zeta_c \frac{K\ (c)}{\sigma_0\ (c)} + \frac{\sigma_K^2\ (c)}{\sigma_0^2\ (c)} \alpha \right)$$

Similarly the terms $\frac{\partial I_\alpha^c}{\partial \sigma_\alpha^2\ (c)}$ and $\frac{\partial I_\alpha^c}{\partial \xi_\alpha(c)}$ can also be obtained by partial differentiation of I_α^c with respect to σ_α^2 (c) and $\xi_\alpha(c)$ respectively. Substituting the various terms in (18) we have

$$\frac{\partial I_\alpha^c}{\partial \alpha} = \frac{1}{\sqrt{2\pi}\ \sigma_\alpha\ (c)} \exp\left(- \frac{(x - \xi_\alpha(c))^2}{2\sigma_\alpha^2(c)} \right) \Bigg[\langle K \rangle^c \left(\frac{x - \xi_\alpha(c)}{\sigma_\alpha^2\ (c)} \right) + \frac{\sigma_0^2\ (c)}{\sigma^2\ (c)} \left(\zeta_c \frac{\sigma_K\ (c)}{\sigma_0(c)} + \alpha \frac{\sigma_K^2\ (c)}{\sigma_0^2(c)} \right) \left\{ \left(\frac{x - \xi_\alpha(c)}{\sigma_\alpha\ (c)} \right)^2 - 1 \right\} \Bigg] \quad ..\ (19)$$

Taking limit as $\alpha \to 0$ on both sides, we get

$$\left.\frac{\partial I_\alpha^c}{\partial \alpha}\right|_{\alpha=0} = \frac{1}{\sqrt{2\pi}\ \sigma_0\ (c)} \exp\left(- \frac{(x - \xi_0\ (c))^2}{2\ \sigma_0^2\ (c)} \right) *$$

$$\left[\langle K \rangle^c \left(\frac{x - \xi_0\ (c)}{\sigma_0^2\ (c)} \right) + \left\{ \left(\frac{x - \xi_0(c)}{\sigma_0(c)} \right)^2 - 1 \right\} \zeta_c \frac{\sigma_K\ (c)}{\sigma_0\ (c)} \right]$$

Integrating both sides with respect to a standardized variable

$\hat{x} = \dfrac{x - \mathcal{E}_0\ (c)}{\sigma_0\ (c)}$ in the limits $-\infty$ and E, we have,

$$\int_{-\infty}^{E} \frac{\partial I_{\alpha}^{c}\ (x)\ dx}{\partial \alpha}\Bigg|_{\alpha=0} = \frac{1}{\sqrt{2\pi}\ \ \sigma_0\ (c)} \int_{-\infty}^{E} \exp\ (-\frac{\hat{x}^2}{2})\ *$$

$$\left[\langle K\rangle^{c}\ \hat{x} + (\hat{x}^2-1)\ \zeta_c\ \sigma_K(c)\right]\ d\hat{x}$$

where $d\hat{x} = dx/\ _0(c)$ or

$$\int_{-\infty}^{E} \frac{\partial I_{\alpha}^{c}\ (x)\ dx}{\partial \alpha}\Bigg|_{\alpha=0} = -\frac{1}{\sqrt{2\pi}\ \sigma_0(c)}\ \exp\left\{-\ (\frac{E - \mathcal{E}_0\ (c)}{2\ \sigma_0\ (c)})^2\right\}\ *$$

$$\left[\langle K\rangle^{c} + \zeta_c\ \sigma_K\ (c) * (\frac{E - \mathcal{E}_0\ (c)}{\sigma_0\ (c)})\right] = \frac{\partial F_{\alpha}\ (E)}{\partial \alpha}\Bigg|_{\alpha=0} \qquad ..\ (20)$$

Now $\dfrac{\partial F_{\alpha}\ (E)}{\partial \alpha}\Big|_{\alpha=0}$ can be obtained by summing the above expression over all the configurations. Substituting $\dfrac{\partial F_{\alpha}\ (E)}{\partial \alpha}\Big|_{\alpha=0}$ in (17) we have

$$S_1(E) = \frac{\sum_c I^c(E) * \left\{\langle K\rangle^{c} + \zeta_c\ \sigma_K(c) * (\frac{E - \mathcal{E}_0\ (c)}{\sigma_0\ (c)})\right\}}{\sum_c I^c(E)} \qquad ..\ (21)$$

For calculating $S_2(E)$ in the configuration space, we use the second one of the equations (17)

$$S_2(E) = -\frac{1}{2\sum_c I^c(E)}\left[\frac{\partial^2 F_\alpha(E)}{\partial\alpha^2}\bigg|_{\alpha=0} -\right.$$

$$\left.\frac{\partial}{\partial E}\frac{1}{\sum_c I^c(E)}\left(\frac{\partial}{\partial\alpha}F_\alpha(E)\bigg|_{\alpha=0}\right)^2\right] \quad .. \quad (22)$$

The first term contains $\frac{\partial^2 F_\alpha(E)}{\partial\alpha^2}\bigg|_{\alpha=0}$. To calculate this term we need to calculate $\frac{\partial^2}{\partial\alpha^2} I^c_\alpha(x)\bigg|_{\alpha=0}$. We have, using (19)

$$\frac{\partial}{\partial\alpha}\left(\frac{\partial I^c_\alpha(x)}{\partial\alpha}\right) = \frac{\partial}{\partial\alpha}T_1(T_2 + T_3) + T_1\left(\frac{\partial T_2}{\partial\alpha} + \frac{\partial T_3}{\partial\alpha}\right)$$

where $T_1 = I^c_\alpha(x) = \frac{dc/D}{\sqrt{2\pi}\,\sigma_\alpha(c)}\exp\left(-\frac{(x-\mathcal{E}_\alpha(c))^2}{2\sigma^2_\alpha(c)}\right)$

$$T_2 = \langle K\rangle^c\left(\frac{x-\mathcal{E}_\alpha(c)}{\sigma^2_\alpha(c)}\right)$$

$$T_3 = \sigma_0^2(c)\left(\sum_c\frac{\sigma_K(c)}{\sigma_0(c)} + \alpha\frac{\sigma_K^2(c)}{\sigma_0^2(c)}\right)\left(\frac{x-\mathcal{E}_\alpha(c)}{\sigma^4_\alpha(c)} - \frac{1}{\sigma^2_\alpha(c)}\right)$$

where, as before, we have used only one term in the summation

$\sum_c I^c(x)$. Now

$$\frac{\partial T_1}{\partial \alpha} = \frac{\partial}{\partial \alpha} I^c_\alpha(x) = T_1 (T_2 + T_3)$$

$$\frac{\partial T_2}{\partial \alpha} = -\frac{\langle K\rangle^c}{\sigma_\alpha^2(c)}\left[\langle K\rangle^c + \frac{x - \xi_\alpha(c)}{\sigma_\alpha^2(c)} * \left(2\zeta_c \frac{\sigma_K(c)}{\sigma_0(c)} + \alpha \frac{\sigma_K^2(c)}{\sigma_0^2(c)}\right)\sigma_0^2(c)\right]$$

$$\frac{\partial T_3}{\partial \alpha} = \sigma_K^2(c)\left(\frac{(x - \xi_\alpha(c))^2}{\sigma_\alpha^4(c)} - \frac{1}{\sigma_\alpha^2(c)}\right) + \sigma_0^2(c)\left(\zeta_c \frac{\sigma_K(c)}{\sigma_0(c)} + \alpha \frac{\sigma_K^2(c)}{\sigma_0^2(c)}\right) *$$

$$\left[\frac{-2\langle K\rangle^c (x - \xi_\alpha(c))}{\sigma_\alpha^4(c)} + 2\sigma_0^2(c)\left(\zeta_c \frac{\sigma_K(c)}{\sigma_0(c)} + \alpha \frac{\sigma_K^2(c)}{\sigma_0^2(c)}\right) * \left(\frac{1}{\sigma_\alpha^4(c)} - \frac{2(x - \xi_\alpha(c))^2}{\sigma_\alpha^6(c)}\right)\right]$$

. Taking limit as $\alpha \to 0$, the above expressions reduce to

$$\left.\frac{\partial T_2}{\partial \alpha}\right|_{\alpha=0} = -\frac{\langle K\rangle^c}{\sigma_0^2(c)}\left[\langle K\rangle^c + 2(x - \xi_0(c))\zeta_c \frac{\sigma_K(c)}{\sigma_0(c)}\right]$$

$$\left.\frac{\partial T_3}{\partial \alpha}\right|_{\alpha=0} = \sigma_K^2(c)\left\{\frac{(x - \mathcal{E}_0(c))^2}{\sigma_0^4(c)} - \frac{1}{\sigma_0^2(c)}\right\} + \sigma_0(c)\,\zeta_c\,\sigma_K(c) *$$

$$\left\{\frac{-2\langle K\rangle^c\,(x - \mathcal{E}_0(c))}{\sigma_0^4(c)} + 2\,\sigma_0(c)\,\zeta_c\,\sigma_K(c) *\right.$$

$$\left.\left(\frac{1}{\sigma_0^4(c)} - \frac{2\,(x - \mathcal{E}_0(c))^2}{\sigma_0^6(c)}\right)\right\}$$

$$\therefore \left.\frac{\partial^2}{\partial \alpha^2} I_\alpha^c(x)\right|_{\alpha=0} = \left[T_1\,(T_2+T_3)(T_2+T_3) + T_1\left(\frac{\partial T_2}{\partial \alpha} + \frac{\partial T_3}{\partial \alpha}\right)\right]_{\alpha=0}$$

$$= \left[T_1\left\{(T_2+T_3)^2 + \frac{\partial T_2}{\partial \alpha} + \frac{\partial T_3}{\partial \alpha}\right\}\right]_{\alpha=0}$$

Substituting the values of T_1, T_2, T_3, $\frac{\partial T_2}{\partial \alpha}$ and $\frac{\partial T_3}{\partial \alpha}$ in the limit $\alpha \to 0$ and writing $\hat{x} = \frac{x - \mathcal{E}_0(c)}{\sigma_0(c)}$, we have

$$\left.\frac{\partial^2}{\partial\alpha^2} \; I^c_\alpha \; (x)\right|_{\alpha = 0} = \frac{1}{\sqrt{2\pi}\sigma_0^3(c)} \; \exp \; (- \hat{x}^2/2) \, *$$

$$\Big\{ He_4 \; (\hat{x}) \; \zeta_c^{\,2} \; \sigma_K^{\,2} \; (c) + 2 \; He_3 \; (\hat{x}) \langle K \rangle^c \; \zeta_c \; \sigma_K \; (c) \; +$$

$$He_2 \; (\hat{x}) \; \left[\; (\langle K \rangle^c)^2 + \sigma_K(c) \right] \Big\}$$

where He_n $(\hat{x})$ are Hermite polynomials. Now

$$\left.\frac{\partial^2 F_\alpha \; (E)}{\partial \alpha^2}\right|_{\alpha = 0} = \int_{-\infty}^{E} \left.\frac{\partial^2}{\partial \alpha^2} \; I^c_\alpha \; (x) \right|_{\alpha = 0} dx$$

Carrying out this integral using a standardized variable $\hat{x}$ and writing $\hat{E}c = \dfrac{E - \xi_0 \; (c)}{\sigma_0 \; (c)}$, we have

$$\left.\frac{\partial^2 F_\alpha \; (E)}{\partial \alpha^2}\right|_{\alpha = 0} = - \frac{1}{\sigma_0 \; (c)} \; I^c(E) \Big\{ \zeta_c^{\,2} \, \sigma_K^{\,2}(c) \; He_3 \; (\hat{E}c) \; +$$

$$2 \langle K \rangle^c \; \zeta_c \; \sigma_K(c) \;\; He_2 \; (\hat{E}c) + \langle K^2 \rangle^c \; He_1 \; (\hat{E}c) \Big\} \quad .. \qquad .. \; (23)$$

Now, the second term in the expression for $S_2(E)$ is

$$- \frac{\partial}{\partial E} \left\{ \frac{1}{I^c(E)} \left(\left.\frac{\partial F_\alpha \; (E)}{\partial \alpha}\right|_{\alpha=0} \right)^2 \right\}$$ where, again for ease of

calculation we have considered only one configuration. This can be written as

$$\frac{1}{\left[I^c(E)\right]^2} \left(\frac{\partial F_\alpha(E)}{\partial \alpha}\bigg|_{\alpha=0} \right)^2 * \frac{\partial}{\partial E} I^c(E) - \frac{2}{I^c(E)} \left(\frac{\partial F_\alpha(E)}{\partial \alpha}\bigg|_{\alpha=0} \right) * \frac{\partial}{\partial E}\left(\frac{\partial F_\alpha}{\partial \alpha}\bigg|_{\alpha=0} \right)$$

$$= (S_1(E))^2 \frac{\partial}{\partial E} I^c(E) + 2\, S_1(E) \frac{\partial}{\partial E}\left(\frac{\partial F_\alpha}{\partial \alpha}\bigg|_{\alpha=0} \right) \quad \ldots \quad \ldots (24)$$

This expression can be simplified by substituting the values of various terms by using equations (12), (20) and (21). Finally putting together all the terms from (24) and (23) in (22) and summing over all configurations we get

$$S_2(E) = \sum_c \frac{I^c(E)}{I(E)} \left\{ \frac{1}{2\sigma_0(c)} (\zeta_c^2 \sigma_K^2(c)\, He_3(\hat{E}c) + \right.$$

$$2\langle K\rangle^c \zeta_c\, \sigma_K(c)\, He_2(\hat{E}c) + \langle K^2\rangle^c\, He_1(\hat{E}c)) +$$

$$1/2 \sum_c \frac{I^c(E)\ \ \hat{E}c}{I(E)\ \ \sigma_0(c)} * \left(\sum_c \frac{I^c(E)}{I(E)} (\langle K\rangle^c + \zeta_c\, \sigma_K(c)\, He_1(\hat{E}c))\right)^2$$

$$-\sum \frac{I^c(E)}{I(E)} (\langle K\rangle^c + \zeta_c\, \sigma_K(c)\, \hat{E}c\ ) \sum_c \frac{I^c(E)}{I(E)\ \sigma_0(c)} *$$

$$(\langle K\rangle^c\, \hat{E}c + \zeta_c\, \sigma_K(c)\, He_2(\hat{E}c))$$

This is a very useful result as we shall see later in the next section. A large variety of effective interactions for s-d and f-p shell have been studied by quantitatively analysing their quadrupole and pairing properties[41]. This has been done by generating an empirical interaction as a linear combination of the quadrupole and pairing operators, and by comparing the effective interactions via their correlation coefficients with this empirical interaction. A comparison is also made between the low lying states of the spectrum generated by the effective interaction and those obtained by various empirical interactions. We have used a somewhat similar approach to correct the estimates of the ground state energies thus obtained. We notice that the expressions for $S_1(E)$ and $S_2(E)$ depend on the parameters of the original Hamiltonian H, the perturbing Hamiltonian αK and the correlation coefficient between the two in the corresponding space. Thus knowing the estimates of ground state energy E_0 made by an empirical interaction hamiltonian H, the parameters of the perturbing hamiltonian and the correlation coefficient between the two operators, S_1 (E) and $S_2(E)$ can be calculated to give corrections to the estimates of E_0. Analytic expressions in scalar and configuration spaces and the results of calculations are given in the next section.

D. CORRECTION TO GROUND STATE ENERGY ESTIMATE

Given an effective interaction Hamiltonian H_F and an empirical interaction represented by H_M; since the empirical interaction is an approximation to the effective interaction, we can write $H_F = H_M + \alpha K = H_M + H_p$ where $K = H_p$ corresponds to the Hamiltonian of the perturbing interaction.

If E_0 is the ground state energy estimate obtained by using the empirical interaction, then S_1 (E_0) and S_2 (E_0) will provide the 1st order and 2nd order corrections to it, which have their origin in the neglect of the perturbing Hamiltonian

H_P. As is evident from their expressions, we need the correlation coefficient ζ_{MP} between the empirical and the perturbing hamiltonians H_M and H_P respectively. This can be obtained from the definition of correlation coefficient[41] in a given space α.

$$\zeta_{MP} = \frac{\langle \tilde{H}_M \; \tilde{H}_P \rangle^{\alpha}}{[\langle \tilde{H}_M^2 \rangle^{\alpha} \langle \tilde{H}_P^2 \rangle^{\alpha}]^{\frac{1}{2}}}$$

where $\tilde{H} = H - \langle H \rangle$ is the traceless part of H. The centroids and widths of the operators H_M and H_P are $\mathcal{E}_M$, σ_M and $\mathcal{E}_P$, σ_P respectively. Further, we can assume without loss of generality that $\mathcal{E}_P = \mathcal{E}_M$. Therefore

$$\zeta_{MP} = \frac{\langle \tilde{H}_M \; \tilde{H}_P \rangle}{\sigma_M \; \sigma_P} = \frac{\langle \tilde{H}_M \; \tilde{H}_F \rangle - \langle \tilde{H}_M \; \tilde{H}_M \rangle}{\sigma_M \; \sigma_P}$$

Now $\langle \tilde{H}_M \; \tilde{H}_F \rangle$ can be written in terms of the correlation coefficient ζ_{MF} between H_M and H_F which is known and maximised[41].

$$\therefore \quad \zeta_{MP} = \frac{\zeta_{MF} \; \sigma_M \; \sigma_F}{\sigma_M \; \sigma_P} - \frac{\sigma_M^2}{\sigma_M \; \sigma_P}$$

We also note that H_M and H_F have the same widths i.e. $\sigma_M = \sigma_F$ by a condition which demands that they have the same norms[41].

$$\therefore \; \zeta_{MP} = \frac{\sigma_M}{\sigma_P} \left(\zeta_{MF} - 1 \right) \quad .. \qquad .. \; (25)$$

Now S_1 (E) in scalar space is given by

$$S_1 \; (E_0) = \langle H_P \rangle + \zeta_{MP} \frac{\sigma_P}{\sigma_M} \; (E_0 - \mathcal{E}) \quad .. \qquad .. \; (26)$$

Where we have made the following substitutions

$$\langle K \rangle = \langle H_P \rangle = \langle (H_F - H_M) \rangle = 0$$
$$\sigma_K = \sigma_P, \quad \sigma_0 = \sigma_M \text{ in (11)} ..$$

Assuming $\mathcal{E} = \mathcal{E}_M = \mathcal{E}_P = 0$ and substituting the value of ζ_{MP} from (25) in (26) we have $S_1 (E_0) = -(1- \zeta_{MF}) E_0$

Since ζ_{MF} is always less than 1 and E_0 is - ve, $S_1 (E_0)$ gives a +ve correction to the ground state energy E_0. Again from equation (11), $S_2 (E_0) = (1-\zeta^2_{MP}) (E_0 - \mathcal{E})\sigma_P^2 / 2 \sigma_M^2$

Following similar arguments as for $S_1 (E_0)$ and observing that $\sigma_P^2 = \langle (\tilde{H}_F - \tilde{H}_M)^2 \rangle = 2 \sigma_F^2 (1- \zeta_{MF})$ we get

$S_2 (E_0) = E_0/2 \ (1 - \zeta^2_{MF})$, which, as can be clearly seen, is a -ve correction to the ground state E_0. The total correction is given by the sum of $S_1 (E_0)$ and $S_2 (E_0)$ and is found to be

$$S_1 (E_0) + S_2 (E_0) = - E_0/2 \ (1- \zeta_{MF})^2 \quad .. \qquad .. (27)$$

which is +ve. These are the expressions for scalar space. Similar analytical expressions can very easily be obtained for configuration spaces also.

Starting from the definition of correlation coefficient, we have in configuration spacee

$$\zeta_{MP}(c) = \frac{1}{\sigma_P(c)} (\zeta_{MF}(c) \ \sigma_F(c) - \sigma_M(c)) \qquad .. (28)$$

where all the quantities are to be evaluated in configuration space. More over $\sigma_M(c) \neq \sigma_F(c)$ contrary to the case of scalar space. This is so because the condition of equal norms is imposed on the overall density and not the partial densities into which it is subdivided. Therefore the configuration centroids $\mathcal{E}_M(c)$ and $\mathcal{E}_F(c)$, corresponding to H_M and H_F are also different Consequently, we have to evaluate $\sigma_P(c)$ explicitely.

$$\sigma_P^2(c) = \langle \widetilde{H}_P^2 \rangle^c = \langle ((H_F - H_M) - (\langle H_F \rangle - \langle H_M \rangle))^2 \rangle^c$$

$$= \langle (H_F^2 + H_M^2 - 2H_F H_M + (\langle H_F \rangle)^2 + (\langle H_M \rangle)^2 - 2\langle H_F \rangle\langle H_M \rangle$$

$$- 2 H_F \langle H_F \rangle + 2 H_M \langle H_F \rangle + 2 H_F \langle H_M \rangle - 2 H_M \langle H_M \rangle) \rangle^c$$

Now writing $H_F = \widetilde{H}_F + \mathcal{E}_F(c)$, $H_M = \widetilde{H}_M + \mathcal{E}_M(c)$

and performing the average over all configurations, we get

$$\sigma_P^2(c) = \sigma_F^2(c) + \mathcal{E}_F^2(c) + \sigma_M^2(c) + \mathcal{E}_M^2(c) - 2\,\zeta_{MF}(c)\,\sigma_F(c)\,\sigma_M(c) - 2\,\mathcal{E}_F(c)\,\mathcal{E}_M(c) \quad \ldots (29)$$

Substituting $\zeta_{MP}(c)$ from (28) for ζ_c in (21) and making the substitutions $\langle K \rangle^c = \langle H_P \rangle^c = \langle H_F - H_M \rangle^c = \mathcal{E}_F(c) - \mathcal{E}_M(c)$

$\sigma_K(c) = \sigma_P(c)$, $\sigma_0(c) = \sigma_M(c)$ we have,

$$S_1(E) = \sum_c \frac{I^c(E)}{I(E)} \left(\mathcal{E}_F(c) - \mathcal{E}_M(c) + \zeta_{MP}(c)\,\sigma_P(c) \left(\frac{E - \mathcal{E}_M(c)}{\sigma_M(c)} \right) \right) \quad \ldots (30)$$

Similarly S_2 (E) can be deduced from (22) and we have

$$S_2(E) = \sum_c \frac{I^c(E)}{I(E)} \left(\frac{1}{2\,\sigma_M(c)} \left(\zeta_{MP}^2(c)\, \sigma_P^2(c)\, He_3(\hat{E}c) + \right.\right.$$

$$2\,(\epsilon_F(c) - \epsilon_M(c))\,\zeta_{MP}(c)\,\sigma_P(c)\;He_2(\hat{E}c) + \langle H_P^2\rangle^c\;He_1(\hat{E}c)\,)\,)$$

$$+ 1/2 \sum_c \frac{I^c(E)}{I(E)}\,\frac{\hat{E}c}{\sigma_M(c)}) * \left(\sum_c \frac{I^c(E)}{I(E)} \,(\, \epsilon_F(c) - \epsilon_M(c) + \right.$$

$$\left. \zeta_{MP}(c)\,\sigma_P(c)\; He_1\,(\hat{E}c))\right)^2 - 1/2 \sum_c \frac{I^c(E)}{I(E)} \,(\epsilon_F(c) - \epsilon_M(c) +$$

$$\zeta_{MP}(c)\,\sigma_P(c)\;\;\hat{E}c) * \sum_c \frac{I^c(E)}{I(E)} \,(\,(\,\epsilon_F(c) - \epsilon_M(c))\;\;\hat{E}c +$$

$$\zeta_{MP}(c)\,\sigma_P(c)\;\;He_2\,(\hat{E}c)), \qquad \hat{E}c = \frac{E - \epsilon_M(c)}{\sigma_M(c)} \qquad .. \quad (31)$$

Equations (30) and (31) can be further simplified by substituting $\zeta_{MP}(c)$ from (28).

We have used the PW interaction as the effective interaction H_F, in the spectroscopic space of (s-d) shell with 4 particles. Kota et. al. (1980)[41] have constructed 5 empirical interactions in various spaces. Here we just give a brief description of these interactions. The common feature of these interactions is that the 2 - body part of each empirical interaction has been expressed as a linear combination of the quadrupole and the pairing operators.

The first empirical interaction, represented by H_{s1} is given as H_{s1} = ESPE + a(m) H_Q + b (m) H_P where ESPE are the external single particle energies (same as those of effective interaction), a (m) and b(m) are coefficients depending only on the number of particles m and the averages in scalar space, H_Q and H_P are the 2 - body parts of quadrupole and pairing operators.

When the same procedure is followed by taking averages over all states with fixed m and fixed isospin (T), the values of a and b depend on m and T. In this case the empirical interaction is denoted by

$$H_{st1} = \text{ESPE} + a(m,T)\, H_Q + b(m,T)\, H_P.$$

Now if we take into account the induced single particle energies (ISPE), we get another empirical interaction

$$H_{s2} = \text{ESPE} + \text{ISPE} + a\, \tilde{\tilde{H}}_Q + b\, \tilde{\tilde{H}}_P$$

where $\tilde{\tilde{H}}_Q$ and $\tilde{\tilde{H}}_P$ represent the unitary rank 2 parts of the quadrupole and pairing operators respectively. In this case ESPE and ISPE are the same as those of the effective interaction. If the calculations are done in scalar T space, then we have to take into account the isospin induced single particle energies. For this purpose, we have the followihg empirical interaction.

$$H_{st2} = \text{ESPE} + \text{isospin ISPE} + a\,(m,T)\, \tilde{\tilde{H}}_Q + b\,(m,T)\, \tilde{\tilde{H}}_P$$

Here $\tilde{\tilde{H}}_Q$ and $\tilde{\tilde{H}}_P$ are the tensor rank - 2 parts of H_Q and H_P respectively, with respect to the group U (Ω) ⓧ U (2). ($\Omega = \sum_i \Omega_i$, Ω_i = 1/2 N_i, N_i = degenracy of the spherical orbit i).

In scalar isospin space, T = 0 and T = 1 parts of the irreducible rank - 2 operator propagate independently. This property has been exploited in the definition of

$$H_{st3} = \text{ESPE} + \text{isospin ISPE} + a\, \tilde{\tilde{H}}_Q^{\,T=1} + b\, \tilde{\tilde{H}}_P^{\,T=1} + c\tilde{\tilde{H}}_Q^{\,T=0}$$

For all the empirical interactions the values of the coefficients a and b are calculated by maximising the correlation coefficient $\zeta(H_F, H_M)$ in the corresponding spaces, along with the conditions $\sigma_F = \sigma_M$ where σ corresponds to the width of the corresponding operators.

Using these interactions (Kota et. al. (1980)), their correlation coefficients with respect to various effective interactions in the s-d and f-p shell have been calculated and maximised. Estimates of ground state have also been given by making use of the empirical interactions so generated. We have used their results for PW interaction for our calculations in scalar and configuration spaces.

The PW interaction gives rise to a binding energy of - 40.6 ~~Me~~ MeV while the five empirical interactions[41] (in the order H_{s1}, H_{s2}, H_{st1}, H_{st2}, H_{st3}) estimate it at - 45.8, - 43.8, - 43.2, - 47.0 and - 46.1 (all in MeV) respectively. The corresponding maximised correlation coefficients ζ_{MF} are found to be 0.799, 0.846, 0.806, 0.855 and 0.858 respectively. Using the equation (27) we have directly calculated the total correction to the ground state estimates given by each empirical interaction in scalar space. The results are given in the Table V.

However, for the calculation in configuration space, we have used only two of the five empirical interactions described above. The first one is H_{s2}. It is generated in such a way that it has the same external and induced single particle energies as those of the effective PW interaction.

$$H_{s2} = ESPE + ISPE + a\,\tilde{\tilde{H}}_Q + b\,\tilde{\tilde{H}}_P \qquad .. (32)$$

$\tilde{\tilde{H}}_Q$ and $\tilde{\tilde{H}}_P$ are irreducible rank - 2 ($\nu = 2$) parts of the quadrupole and pairing operators respectively. The $\nu = 2$, 2 body matrix elements (TBME) corresponding to any hamiltonian are given by

$$V^{JT}_{ijkl}\,(\nu = 2) = \tilde{V}^{JT}_{ijkl} - \frac{1}{N-2}\,(\lambda_i + \lambda_j)\,\delta_{ik}\,\delta_{jl} \quad \text{where}$$

$$\tilde{V}^{JT}_{ijkl} = V^{JT}_{ijkl} - V_c\,\delta_{ik}\,\delta_{jl}$$

V^{JT}_{ijkl} are the TBME and V_c are the centroid of the TBME, given by

$$V_c = \frac{\sum_{i \leq j} V^{JT}_{ijij} [JT]}{N (N-1)/2} \quad ; \quad [JT] = (2J + 1)\ (2T + 1),$$

$N = \sum_i N_i$, $N_i = 2\ (2j_i + 1\ )$, i,j,k,l are the sperical orbits, N_i are their degeneracies. λ_i correspond to the induced single particle energies and are given by

$$\lambda_i = \frac{1}{N_i} \sum_{iJT} V^{JT}_{ijij}\ [JT]\ (\ 1 + \delta_{ij}) -$$

$$\frac{1}{N} \sum_{klJT} V^{JT}_{klkl}\ [JT]\ (\ 1 + \delta_{ij}),$$

The coefficients a and b in equation (32) are calculated by maximising ζ_{MF} in the corresponding spectroscopic space along with the condition that $\sigma_F = \sigma_M$. However we have used the values of a and b corresponding to the PW interaction given in reference 41 directly. They are - 0.107 and 0.160 respectively. ESPE and ISPE are the external single particle energies and contribution due to the induced single particle energies λ_i of the effective PW interaction respectively. Thus, first we generate ν= 2 part of the Q.Q and pairing hamiltonians. Then by adding the ESPE and ISPE of PW interactions, we get new TBME whose ν = 2 part is a sum of ν= 2 parts of Q.Q and pairing operators and ESPE and ISPE are those of the PW interaction.

The second empirical interactior that we have used is H_{st3}.

The coefficients a,b and c are calculated by the same procedure as mentioned earlier. However for PW interaction we have adopted them directly from the results in reference 41; they are − 0.075, 0.316 and − 0.113 respectively. ESPE are the external single particle energies and isospin ISPE corresponds to the contribution of isospin induced single particle energies, which are given as

$$\lambda_i^T = \frac{1}{\Omega_i} \sum_{i,J} V^{JT}_{ijij} [J] (1 + \delta_{ij}) -$$

$$\frac{1}{\Omega} \sum_{k,l,J} V^{JT}_{klkl} [J] (1 + \delta_{ij})$$

T is the isospin of the 2 − particle state, $\Omega_i = 1/2\, N_i$, and $\Omega = \sum_i \Omega_i$. ESPE and ISPE here again correspond to those of the effective interaction.

The configuration centroids and widths $\mathcal{E}(c)$, $\sigma(c)$ for effective interaction, each empirical interaction and the configuration correlation coefficients $\zeta_{MF}(c)$ were evaluated by using already existing computer programs[43]. Using equations (30), (31) we calculated S_1 (E_0) and S_2 (E_0) and the difference Δ between the ground states given by the effective interaction and the new calculated results. The results are tabulated in table V.

$E_{g.s}$ OLD corresponds to the ground state energie obtained by approximating the effective PW interaction by 5 model interactions[41], and $\triangle$ OLD is the difference between the $E_{g.s}$ given by the PW interaction and those given by the five empirical interactions. On the other hand $E_{g.s}$ NEW are the binding energies obtained as corrections to $E_{g.s}$ OLD by using the inverse energy weighted sum rule theory developed in the previous section. $\triangle$ NEW correspond to the corresponding difference between the binding energy of PW interaction and those obtained from the empirical interactions. The last two columns in the table V give similar results for the configuration space. We regret that due to non availability of data, we could not calculate the correction to ground state energies for the remaining three interactions. However the results we have obtained seem to be very encouraging. As is obvious from the table, $\triangle$ the difference between $E_{g.s}$ of effective and empirical interactions has reduced successively from - 3.2 to -2.7 in scalar space and from - 2.7 to - 0.83 in configuration space. Similarly, for the last interaction, from - 5.5 to - 5.0 and - 5.0 to - 2.1.

Thus we see that spectral distribution methods when applied to perturbation theory, give very good results for corrections to estimates of ground state energy given by various empirical

TABLE - 5

Corrections to ground state energy estimates obtained by applying spectral distribution methods to Rayleigh Schrodinger perturbation theory. Results are presented for scalar and configuration spaces. The effective interaction used is the PW interaction with binding energy - 40.6 MeV.

TABLE - 5

GROUND STATE ENERGY CORRECTIONS USING $S_1(E)$ AND $S_2(E)$ IN					
SCALAR SPACE				CONFIGURATION SPACE	
$E_{g.s}$ OLD	Δ OLD	$E_{g.s}$ NEW	Δ NEW	$E_{g.s}$ NEW	Δ NEW
- 45.8	- 5.2	- 44.9	- 4.3		
- 43.8	- 3.2	- 43.3	- 2.7	- 41.4	- 0.83
- 43.2	-- 2.6	- 42.4	- 1.8		
- 47.0	- 6.4	- 46.5	- 5.9		
- 46.1	- 5.5	- 45.6	- 5.0	- 42.7	- 2.1

interactions. The results improve considerably when the calculations are done in the configuration space.