CHAPTER - 2

INVERSE ENERGY WEIGHTED SUM-RULES

The spectral distribution methods (SDM)/4,22/ which make use of moments and averages of operators in a model space offer a useful technique to study most of the nuclear properties in a given spectroscopic space. These methods have been extensively used to study averaged properties of the nucleus like level densities, spin and isospin cutoff factors, averaged spectra, averaged strength distributions, averaged expectation values of various operators, etc.

In SDM, one usually starts by defining a distribution of states with respect to energy in terms of its few low-order moments, and proceeds to calculate smoothened forms for operator averages via moments defined for such a distribution. A rather simple approximation would be to work in the scalar space defined by distributing a finite number of particles in a set of single particle states, and take operator averages in the complete space. This however, is zeroth approximation as the detailed structure is averaged. Accuracy can be improved by either taking into account higher order moments, or decomposing the space according to some unitary symmetry, to include finer details. It turns out that these methods are quite successful in calculating ground state energies/3/ and ground state occupancies /17/. A detailed study using Wildenthal's universal s-d interaction performed recently by Sarkar et. al. /23/ confirms the claim of validity of SDM even in the ground state region, which lies far away from the scalar centroid.

Here, we deal with corrections to the ground-state binding energy when the effective hamiltonian is approximated by various model hamiltonians based on linear combinations of pairing and Q.Q operators/24/. Such a correction involves taking care of the difference between H_{eff} and H_{model} perturbatively, via inverse energy weighted sum-rules. This work has been partially done by Ms. Pramila Shenoy /20/, who obtained expressions for the first and the second order terms in the scalar and configuration spaces. This chapter briefly reviews her work, and in addition gives complete result for five model hamiltonians in configuration space.

The first section gives scalar result for the first, second and third order correction terms to the binding energy. This result has already been derived by Halemane /19/, who gave expressions for a variety of inverse energy weighted sums. We give an alternate and comparatively transparent derivation of Halemane's result. Arguments are then extended to the configuration space.

The next section deals with explicit expressions for correction terms in the scalar and configuration spaces, which are obtained as parametric derivatives of the perturbed eigenvalue E_α of the perturbed hamiltonian. The unperturbed eigenvalue density is assumed to have a gaussian shape characterised by its centroid and width. The perturbation merely causes a slight shift in the centroid and the width of the density function and does not affect the normal nature of the eigenvalue density. In the scalar space, expressions are derived for first four correction terms, while the derivation is limited upto the second term in the case of the configuration space.

These expressions are then used to derive corrections to the ground state binding energy of a nucleus obtained using the model hamiltonians H_{model}, which approximate an effective interaction H_{eff}. A brief discussion on the five model interactions used here for approximating the effective hamiltonian is also included in this section.

The last section gives the binding energy corrections upto the second order for the five model hamiltonians in scalar and configuration spaces, followed by discussion.

A Inverse Energy Weighted Sum-rules

Sum-rules in SDM are encountered in two different ways. One set of sum-rules is obtained when an excitation operator O acts between two eigenstates of the hamiltonian H. This gives rise to strength function R(E,E') between initial and the final state energies E and E' respectively. Moments of the strength which can be expressed as expectation values of operator $O^{+}H^{p}O$ as a function of energy E give rise to different sum-rule quantities, determined by the index p. $O^{+}O(E)$ corresponds to the non-energy weighted sum of the strength with the starting state energy E and with respect to intermediate energy states. Similarly $O^{+}HO(E)$ or the linear-energy weighted sum gives the centroid of the strength distribution. $O^{+}H^{2}O(E)$ (quadratically-energy weighted sum) gives an idea about the spread of the strength with respect to energy of the intermediate states. These sums are used to study single nucleon transfer processes and are discussed in a later chapter. Secondly, the sum-rules arise when a hamiltonian is perturbed by a small operator αK, α being only a multiplicative parameter. In this case, the expectation values of K and K^{2} as a function of energy are related to the width of the eigenfunctions of H at E, when expressed in terms of eigenfunctions of K; such calculations have been reported earlier by Potbhare /25/. So far, not much attention has been paid to inverse energy weighted sums. This is partly due to the notion that one has to deal with Green's functions and complete solutions of the problem in order to deal with inverse energy weighted sums. It is clear that these cannot be expressed in terms of linear polynomial traces, for the energy term in the denominator indicates a non-linear expansion. Recently, however, Halemane /19/ applied SDM to Rayleigh-Schroedinger perturbation theory and obtained expressions for a variety of inverse energy weighted sums. We now give a simpler procedure for deriving these sums.

The eigenvalue density of H in a finite dimensional space is always discrete. However, as the spectral distribution methods deal only with few lower order moments, a density of states $\rho(E)$ characterised by these is assumed continuous. Ratcliff /16/ gave a procedure to generate a smoothened spectrum from such assumed continuous density function. The spectrum so obtained is an averaged spectrum, free from level to level fluctuations. This procedure is described in detail in the fourth chapter. The averaged position of E_n, the n^{th} level starting from the ground state is given by

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

where D is the dimensionality of the space and $F(E_n)$ is the distribution function at energy E_n. If a small operator αK is added to H, the perturbation will shift the eigenvalues. The new set of eigenvalues $E_{n,\alpha}$ can be obtained similarly using $\rho_\alpha(x)$ characterised by moments of $H + \alpha K$:

$$D * \int_{-\infty}^{E_{n,\alpha}} \rho_\alpha(x)dx = D * \int_{-\infty}^{E_n} \rho(x)dx = n-1/2 = p_n . \qquad (2)$$

The above relation can be written down for a strictly rigid spectrum, i.e. by assuming that no crossing of levels takes place. Using Rayleigh-Schroedinger's perturbation theory, the eigenvalue $E_{n,\alpha}$ of the perturbed hamiltonian is expressed as

$$E_{n,\alpha} = E_{n,0} + \alpha S_1(E_{n,0}) + \alpha^2 S_2(E_{n,0}) + \alpha^3 S_3(E_{n,0}) + \cdots \tag{3}$$

and so on. $S_1(E_{n,0})$ is the expectation value of K as a function of energy $E_{n,0}$ and $S_2(E_{n,0})$ is the first inverse energy weighted sum. $S_3(E_{n,0})$ corresponds to the next (quadratically) inverse energy weighted sum and so on. Since we shall deal with a particular eigenvalue only, the suffix 'n' is dropped. From equation 1, we have

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

$$= \frac{\partial E_\alpha}{\partial \alpha} \rho_\alpha(E_\alpha) + \int_{-\infty}^{E_\alpha} \frac{\partial}{\partial \alpha} \rho_\alpha(x)\,dx \tag{4}$$

so that

$$\frac{\partial E_\alpha}{\partial \alpha} = -\frac{1}{\rho_\alpha(E_\alpha)} \int_{-\infty}^{E_\alpha} \frac{\partial}{\partial \alpha} \rho_\alpha(x)\,dx \tag{5}$$

In the limit $\alpha \rightarrow 0$, as the integration limit does not depend upon α, the integration over x can be interchanged with differentiation with respect to α, yielding

$$\left.\frac{\partial E_\alpha}{\partial \alpha}\right|_{\alpha=0} = S_1(E_0) = K(E_0)$$

$$= -\frac{1}{\rho_0(E_0)} \left[\frac{\partial}{\partial \alpha} \left[\int_{-\infty}^{E_0} \rho_\alpha(x)\,dx\right]_{\alpha=0}\right]$$

$$= -\frac{1}{\rho_0(E_0)} \left[\frac{\partial}{\partial \alpha} \left[F_\alpha(E_0)\right]_{\alpha=0}\right] \tag{6}$$

where $F_\alpha(E_0)$ is the distribution function at $E = E_0$. The suffix '0' indicates unperturbed values. This result was originally given by French and Chang /26/.

Higher order corrections, namely $S_2(E_0)$, $S_3(E_0)$ etc. can be obtained similarly, by further differentiation of $\partial E_\alpha/\partial\alpha$ with respect to α. On differentiating equation 5 twice with respect to α, one obtains:

$$S_2(E_0) = \frac{1}{2} \frac{\partial^2}{\partial\alpha^2} E_\alpha \Big|_{\alpha=0}$$

$$= - \frac{1}{2\rho_0(E_0)} \left[\frac{\partial^2}{\partial\alpha^2} F_\alpha(E_\alpha) \Big|_{\alpha=0} - \frac{\partial}{\partial E_0} \left\{ \frac{1}{\rho(E_0)} \left(\left(\frac{\partial}{\partial\alpha} F_\alpha(E_0) \right) \Big|_{\alpha=0} \right)^2 \right\} \right] \tag{7}$$

and

$$S_3(E_0) = - \frac{1}{6} \frac{\partial^3}{\partial\alpha^3} E_\alpha \Big|_{\alpha=0}$$

$$= - \frac{1}{6\rho_0(E_0)} \left[\left(\frac{\partial^3}{\partial\alpha^3} F_\alpha(E_0) \right) \Big|_{\alpha=0} - 6 \frac{\partial}{\partial E_0} \left(S_1(E_0)\, S_2(E_0)\, \rho(E_0) \right) + \frac{\partial^2}{\partial E_0^2} \left(S_1^2(E_0)\, \rho(E_0) \right) \right] \tag{8}$$

Detailed derivations for $S_2(E_0)$ and $S_3(E_0)$ are given in appendix (I-A).

.B Correction to Perturbed Eigenvalues

(a) Scalar Space Correction

The result in the scalar space can be immediately applied whenever the strong action of the central limit theorem (CLT) renders the eigenvalue density function into a gaussian defined by its centroid ϵ and width σ. The change in the centroid merely shifts the eigenvalue spectrum while the change in width corresponds to the scale change. We have

$$\epsilon = \langle H \rangle, \quad \epsilon(\alpha) = \langle H \rangle + \alpha \langle K \rangle$$
$$\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2 \; ; \; \sigma_k^2 = \langle K^2 \rangle - \langle K \rangle^2$$
$$\sigma^2(\alpha) = \sigma^2 + 2\alpha\zeta\sigma\sigma_k + \alpha^2\sigma_k^2 . \tag{9}$$

ζ in the above set of equations is the correlation coefficient between H and K. The scale change parameter λ is defined by

$$\lambda = (\sigma(\alpha)/\sigma - 1) = (1 + 2\alpha\zeta\sigma_k/\sigma + \alpha^2\sigma_k^2/\sigma^2)^{1/2} - 1 . \tag{10}$$

Geometrically, the total change in an eigenvalue will have contributions from change due to centroid shift and that due to scale change, which is related to the change in width. The second change is proportional to the distance of the eigenvalue from the centroid of the eigenvalue density, which is $(E_0 - \epsilon)$. With these two shifts, the perturbed eigenvalue E_α can be written as:

$$E_\alpha = E_0 + \alpha\langle K \rangle + \lambda(E_0 - \epsilon) . \tag{11}$$

We must remember that the above changes are valid only in the CLT limit. This expression for perturbed eigenvalue E_α can be differentiated n-times to obtain the nth order correction as:

$$S_n(E_0) = (1/n!)\,\partial^n E_\alpha / (\partial\alpha)^n \Big|_{\alpha=0} . \tag{12}$$

The first four correction terms turn out to be :

$$S_1(E_0) = \langle K \rangle + (E_0-\varepsilon)\, \sigma_k/\sigma \;,$$

$$S_2(E_0) = 1/2(1-\zeta^2)\,(E_0-\varepsilon)\, \sigma_k{}^2/\sigma^2 \;,$$

$$S_3(E_0) = -1/2\,(1-\zeta^2)\,(E_0-\varepsilon)\, \sigma_k{}^3/\sigma^3 \;, \tag{13}$$

and $$S_4(E_0) = -1/8(1-\zeta^2)\,(1-5\zeta^2)\,(E_0-\varepsilon)\, \sigma_k{}^4/\sigma^4 \;.$$

A better approximation can be obtained by incorporating higher order moments of the density function. This could be done by using a Cornish-Fisher expansion around a gaussian density, which gives expression for perturbed eigenvalue as:

$$x_\alpha = x_0 + \gamma_{1\alpha}/\,6(x_0^2-1) + \gamma_{2\alpha}/\,24(x_0^3-3x_0) + \gamma_{1\alpha}^{2}/\,36(4x_0^3-7x_0) \;, \tag{14}$$

where $x_0 = (E_0-\varepsilon)\,/\sigma$,

$$\gamma_{1\alpha} = \mu_{3\alpha}/\sigma^3(\alpha) = \langle(\hat{H}+\alpha\hat{K})^3\rangle/\langle(\hat{H}+\alpha\hat{K})^2\rangle^{3/2} \;,$$

$$\gamma_{2\alpha} = \mu_{4\alpha}/\sigma^4(\alpha) - 3 = (\hat{H}+\alpha\hat{K})^4\,/\langle(\hat{H}+\alpha\hat{K})^2\rangle^{2} - 3 \;,$$

$$\hat{H} = H - \langle H \rangle \text{ and } \hat{K} = K - \langle K \rangle \;.$$

$\gamma_{1\alpha}$ and $\gamma_{2\alpha}$ are the first and the second shape parameters respectively, which correspond to the skewness and excess of the eigenvalue distribution. Differentiating X_α (as given by equation 14) with respect to α, and taking CLT limit ($\gamma_1, \gamma_2 \to 0$), the first order correction term with higher order averages is given as

$$S_1(E_0) = \partial x_\alpha / \partial \alpha \Big|_{\alpha=0} \overset{CLT}{\dashrightarrow} \langle \hat{H}\hat{K} \rangle x_0 - 1/2 \langle \hat{K}\hat{H}^2 \rangle (x_0^2-1)$$
$$- 1/6 (\langle \hat{K}^3\hat{H} \rangle - 3 \langle \hat{K}\hat{H} \rangle) * (x_0^3-3x_0) \quad . \tag{15}$$

The above expression involves traces of products of three or more operators, which become cumbersome to calculate. Therefore we do not make use of equation 15.

(b) Extension to configuration space

Despite the assurance of working of the CLT in region of interest, the scalar space results are a rough approximation, this being an inherent property of averaging methods. Since, taking into account higher moments is tedious, it is desirable to partition the space according to some known symmetry to improve the accuracy of the result. Following that, the space is now decomposed according to configurations; each configuration is specified by a configuration density defined by its centroid and width. The overall state density $\rho(E)$ is then expressed as a sum of intensities of all configurations into which the space has now been subdivided:

$$\rho(E) = 1/D \sum_c d_c \rho^c(E) = \sum_c I^c(E)/D \, , \tag{16}$$

where d_c is the configuration dimensionality and $D = \sum_c d_c$ is the total dimensionality. Each term in the above summation corresponds to the intensity of the configuration in the eigenvalue distribution at energy E. It becomes necessary to deal with intensities in the case of configuration partitioning, since configuration symmetry is not necessarily a good symmetry. We assume that each configuration density is a gaussian, given by

$$\rho^{c}(E) = \frac{1}{(2\pi)^{1/2}\sigma_0(c)} \exp\left\{ - \left(E-\varepsilon_0(c)\right)^{2} / \, 2\sigma_0(c)^2 \right\} , \qquad (17)$$

where $\varepsilon_0(c)$ and $\sigma_0(c)$ are the configuration centroid and width respectively for unperturbed H. The perturbation αK added to H acts on each configuration differently so that each configuration centroid and width gets perturbed:

$$\varepsilon_\alpha(c) = \varepsilon_0(c) + \alpha \langle K \rangle^{c}$$

$$\sigma_\alpha^2(c) = \sigma_0^{\,2}(c) + 2\,\zeta_c \sigma_k(c)\sigma_0(c) + \alpha^2 \sigma_k^{\,2}(c)$$

Suffix 0 indicates unperturbed values which correspond to H . The perturbed configuration density $\rho_\alpha^{c}(E_\alpha)$ can be obtained by substituting the expressions for the perturbed centroid, perturbed width and E_α into configuration density expression of equation (17). Making use of equation (6) and (7), the first and the second order correction terms in the configuration space are obtained as[†]

[†] expressions for correction terms are derived in appendix I-B

$$S_1(E_0) = \Big[\sum_c (d_c/D)\rho^c(E_0)\,\{ \langle K\rangle^c + \zeta_c\sigma_k(c)\, x_c \}\Big] / \rho(E_0) \qquad (18)$$

and

$$S_2(E_0) = \frac{1}{2\rho(E_0)}\Bigg[\sum_c (d_c/D)\frac{\rho^c(x_c)}{\sigma_0(x_c)} \{ \zeta_c^2\, \sigma_k^2(c)\, He_3(x_c)$$

$$+ 2\langle K\rangle^c\sigma_k(c)\zeta_c\, He_2(x_c) + [\, (\langle K\rangle^c)^2 + \sigma_k^2(c)\,]\, x_c\}\Bigg]$$

$$+ \frac{1}{2(\rho(E_0))^3}\Bigg[\sum_c (d_c/D)\frac{x_c}{\sigma_0(c)}\rho^c(x_c)\Bigg]\Bigg[\sum_c (d_c/D)\rho^c(x_c)[\langle K\rangle^c + \zeta_c\sigma_k(c)x_c]\Bigg]^2$$

$$- \frac{1}{(\rho(E_0))^2}\Bigg[\sum_c (d_c/D)\rho^c(x_c)\,\{\langle K\rangle^c + \zeta_c\sigma_k(c)\, x_c\}\Bigg]$$

$$\ast\ \Bigg[\sum_c (d_c/D)\frac{\rho^c(x_c)}{\sigma_0(c)}\{ \langle K\rangle^c x_c + (x_c^2 - 1)\,\zeta_c\sigma_k(c) \}\Bigg], \qquad (19)$$

where $x_c = (E_0 - \varepsilon_0(c)) / \sigma_0(c)$.

Here $He_i(x)$ are the Hermite polynomials in x, and c in the above equations indicates that the corresponding quantity is calculated in configuration space. Note that in general, ζ_c cannot be called the correlation coefficient as configuration partitioning does not necessarily correspond to a good symmetry. However, it has the same structure and hence the same nomenclature is used:

$$\zeta_c = \langle(K-\langle K\rangle^c)\ (H-\langle H\rangle^c)\rangle^c/\sigma_k(c)\sigma_0(c) \qquad (20)$$

C Application to ground state energy

A substantial amount of study in nuclear structure centres around the two highly schematic quadrupole and pairing operators due to their association respectively with the long-ranged and short-ranged parts of the nuclear interaction. A large amount of experimental evidence in this respect has prompted us to use a linear combination of these two operators as an empirical approximation to the effective hamiltonian. It is possible to obtain ground state energies for Q.Q and pairing operators analytically. In some cases, exact energy values can be found without resorting to shell model calculations. If a part of the effective hamiltonian can be treated exactly, the remaining part can be treated perturbatively.

A nuclear hamiltonian defined by its single particle energies and two-body matrix elements can be decomposed according to its different unitary ranks giving the total H as a linear combination: $H = H^{(0)} + H^{(1)} + H^{(2)}$, where the superfix denotes the unitary rank. $H^{(0)}$ is the averaged part of the nuclear hamiltonian, $H^{(1)}$ is the single particle energy part and $H^{(2)}$ has terms related to two-body nucleon-nucleon interaction. There exist two types of single particle energies, namely the external single particle energy (ESPE) and the interaction-dependent induced single particle energy (ISPE). The ESPE is generally taken from the spectra of a lone nucleon above a closed shell. For example, energy levels of ^{17}O provide the ESPE's for most of the s-d shell interactions. These may be denoted as ϵ_i. The ISPE denoted by λ_i are obtained through two-body matrix elements of the effective interaction. The total single particle energy for the i-th orbit = $\epsilon_i + \lambda_i$: In spherical orbit formalism, the ISPE are given by

$$\lambda_i = \frac{m-1}{N-2} \quad \frac{1}{N_i} \sum_{jJT} W^{JT}_{ijij} \, [J][T](1+\delta_{jj}) \; - \; \frac{1}{N} \sum_{ijJT} W^{JT}_{ijij} \, [J][T](1+\delta_{ij}) \; , \qquad (21)$$

where N_i = number of single particle states in the i-th orbit, $N = \sum_i N_i$ denotes the total number of single particle states and W^{JT}_{jjkl} is the antisymmetrized two body matrix element in the JT space. In the above equation, if the summation is carried over only angular momentum J instead of JT, the single particle energy retains the isospin T dependence. One thus gets isospin ISPE as

$$\lambda_i^{T} = \left(1 / \Omega_j\right) \sum_{jJ} W^{JT}_{ijij} \, (2J+1)(1+\delta_{ij}) - \left(1/\Omega\right) \sum_{k,l,J} W^{JT}_{klkl} \, (2J+1)(1+\delta_{ij}) , \tag{22}$$

where $\Omega_i = (1/2)N_i$ and $\Omega = \sum_i \Omega_i$. While constructing model hamiltonians, we can choose to keep some part of the model hamiltonian same as that of the effective interaction hamiltonian. Following are the model hamiltonians (H_{model}) constructed by Kota et al/6/.

(1) HS1 = ESPE + a(m) H_Q + b(m) H_P

Here, the external single particle energy of the model hamiltonian is same as that of the effective interaction. H_P and H_Q are two-body matrix elements of the pairing and quadrupole operators respectively. Averaging is done in scalar space, over all states with fixed particle number m, hence a and b depend upon m.

(2) HST1 = ESPE + a(m,T) H_Q+b(m,T) H_P

This interaction is similar to HS1, the only difference being that averaging is done in the scalar space over fixed particle number m and also fixed isospin T. This gives an (m,T) dependence to the coefficients of H_Q and H_P.

(3) HS2 = ESPE + ISPE + $a\overset{\approx}{H}_Q$ $+b\overset{=}{H}_P$

As indicated, in this approximation, apart from ESPE, the ISPE are chosen to be the same as that of the effective interaction. $\overset{\approx}{H}_Q$ and $\overset{=}{H}_P$

refer to the unitary rank-2 parts of H_Q and H_P respecively. Since the entire particle number dependence is absorbed in the ISPE, the matrix elements of H_Q and H_P and therefore the coefficients a and b are independent of particle number m.

(4) HST2 = ESPE + Isospin ISPE + a $(m,T)\ \overset{\approx}{H}_Q$ + b $(m,T)\overset{\approx}{H}_P$.

In this model hamiltonian, more information is incorporated by taking the isospin ISPE from the effective interaction. $\overset{\approx}{H}_Q$ and $\overset{\approx}{H}_P$ are the tensor rank-2 part of H_Q and H_P respectively, with respect to the group $U(\Omega) \otimes U(2)$. Once again the coefficients are a function of particle number m and isospin T.

(5) HST3 = ESPE + isospin ISPE + a $\overset{\approx}{H}_Q^{T=1}$ + a $\overset{\approx}{H}_P^{T=1}$ + c $\overset{\approx}{H}_Q^{T=0}$.

Single particle energy is same as that of HST2 here and advantage has been taken of the fact that the irreducible rank-2 parts of operators H_Q and H_P propagate independently. Therefore, T = 0 and T = 1 part of the operators can be separated from each other and their correlation coefficients with respect to H_{eff} can be individually maximised to obtain corresponding coefficients for constructing the model hamiltonian. Hence they are propagated separately. Pairing operator does not have T = 0 component. For the three components $H_Q^{T=1}$, $H_P^{T=1}$ and $H_Q^{T=0}$, we would have three coefficients a, b and c respectively. The coefficients turn out to be independent of (m,T).

Coefficients of H_Q and H_P for different model interactions can be obtained by maximising the correlation between H_{eff} and the corresponding part of H_{model}. Detailed expressions for these are given by Kota et. al. /24/.

Consider an effective hamiltonian H_F, which is approximated by a model hamiltonian H_M. The difference between them is small, and is therefore treated perturbatively:

$$H_F = H_M + \alpha K = H_M + H_{per} , \qquad (23)$$

where $H_{per} = \alpha K$ is the perturbation hamiltonian, α being the perturbative parameter. The correlation coefficient between H_F and H_M is given by

$$\zeta(H_F, H_M) = \zeta_{FM} = \langle \hat{H}_F \hat{H}_M \rangle / \sigma_F \sigma_M \qquad (24)$$

where $\hat{H} = H - \langle H \rangle$. Once the centroids are subtracted out, the correlation coefficients depend only upon the direction and widths of the two hamiltonians. Therefore we can assume without the loss of generality that the hamiltonians are zero centered in the space, i.e.

$$\langle H_F \rangle = \langle H_M \rangle = 0 = \langle H_F - H_M \rangle . \qquad (25)$$

To compare the model hamiltonian with the effective hamiltonian, we choose that these two have the same widths in the scalar space, so that

$$\sigma_F = \sigma_M . \qquad (26)$$

The hamiltonian H_{per} may be assumed to have a width σ_{per}. The correlation coefficient between the effective and perturbation hamiltonian is denoted by ζ_{HF}. It is found that

$$\zeta_{HF} = \sigma_M / \sigma_{per} \ (\zeta_{MF} - 1); \ \sigma^2_{per} = 2\sigma^2_F \ (1 - \zeta_{MF}). \qquad (27)$$

Substituting these values into equations(13), the scalar space corrections to the binding energy turn out to be

$$\begin{aligned}
S_1(E_g) &= -\ (1-\zeta_{MF})\ E_g \\
S_2(E_g) &= 1/2\ E_g\ (1-\zeta^2_{MF}) \\
S_3(E_g) &= 1/2\ (1-\zeta_{MF})^2\ (1+\zeta_{MF})E_g \\
S_4(E_g) &= 1/8(1+\zeta_{MF})^2(3-5\zeta_{MF})(1-\zeta_{MF})^2\ E_g \qquad (28) \\
S_1(E_g)+S_2(E_g) &= -1/2(1-\zeta_{MF})^2\ E_g \\
S_3(E_g)+S_4(E_g) &= 1/8\ (1-\zeta^2_{MF})(1+\zeta_{MF})(7-5\zeta_{MF})E_g.
\end{aligned}$$

In configuration space, expressions for the first and second order corrections follow from equations (18) and (19). In this space, no approximations can be afforded with respect to configuration centroids and widths, since each value is different for each configuration. We can still have equal norms by demanding that the scalar width remain same for H_F and H_M. However, the correction terms involve centroids and widths of all the three operators namely H_F, H_M and H_{per}. The final expressions for first and second order correction to the ground state energy are:

$$S_1(E) = \sum_c \frac{I^c(E)}{\rho(E)} \left\{ \varepsilon_F^c(E) - \varepsilon_M^c(E) + \zeta_{MP}^c(E)\, \sigma_{per}^c(E)\, \tilde{x}_c \right\} \tag{29}$$

$$\begin{aligned} S_2(E) = \frac{1}{2\rho(E)} \Bigg[\sum_c \frac{I^c(E)}{\sigma_M^c(E)} & \Big\{ \zeta_{MP}^c(E)\, (\sigma_{per}^c(E))^2\, He_3(\tilde{x}_c) \\ & + 2\, (\varepsilon_F^c(E) - \varepsilon_M^c(E))\, \zeta_{MF}^c(E)\, \sigma_{per}^c(E)\, He_2(\tilde{x}_c) \\ & + [\, (\varepsilon_F^c(E) - \varepsilon_M^c(E))^2 + (\sigma_{per}^c(E))^2\,]\, He_1(\tilde{x}_c) \Big\} \Bigg] \\ + \frac{1}{2\rho^3(E)} \Big[\sum_c I^c(E) & \Big\{ (\varepsilon_F^c(E) - \varepsilon_M^c(E)) + \zeta_{MP}^c(E) \sigma_{per}^c(E)\, \tilde{x}_c \Big\} \Big]^2 \Big[\sum_c \frac{I^c(E)}{\sigma_M^c(E)} \tilde{x}_c \Big] \\ - \frac{1}{(\rho(E))^2} & \Big[\sum_c I^c(E) \Big\{ \varepsilon_F^c(E) - \varepsilon_M^c(E) + \zeta_{MP}^c(E) \sigma_{per}^c(E)\, \tilde{x}_c \Big\} \Big] \\ * & \Big[\sum_c \frac{I^c(E)}{\sigma_M^c(E)} \Big\{ \tilde{x}_c (\varepsilon_F^c(E) - \varepsilon_M^c(E)) + \zeta_{MP}^c(E)\, \sigma_{per}^c(E)\, He_2(\tilde{x}_c) \Big\} \Big] \end{aligned} \tag{30}$$

where $I^c(E) = d_c\, \rho^c(E)/D$; $D = \sum_c d_c$, $\rho(E) = \sum_c I^c(E)$

and $\tilde{x}_c = (E - \varepsilon_M^c(E)) \,/\, \sigma_M^c(E)$

$He_i(\tilde{x}_c)$ are the i-th order Hermite polynomials in $\tilde{x}_c$.

D Results and Discussion

Calculations are carried out for five model interactions namely HS1, HS2,HST1, HST2 and HST3 to obtain correction to the ground state binding energy of ^{20}Ne which contains four particles above ^{16}O. core. The effective interaction chosen is the PW interaction of the s-d shell, that gives a binding energy of 40.6 Mev for ^{20}Ne. Table 2.1 gives a, b and c coefficients for all five model hamiltonians, which are calculated using available computer programmes.

The first and the second order corrections to the ground state binding energy are given for both scalar and configuration spaces. For the scalar space, it turns out that these two are large. For example, in the case of HS1, for E_g = -45.8 MeV, τ =0.799, S_1=9.21 MeV and S_2 = -8.28 MeV. The third and fourth order corrections are extremely small. These values are respectively

S_3 = 1·66 MeV and S_4 = -0·75 MeV. The CLT approximation is therefore justified, as higher order corrections would be still smaller. The first two corrections calculated for scalar and configuration spaces are displayed in Table 2.2. The second column shows binding energy of the five model interactions. These values for ^{20}Ne are directly taken from ref./6/. Column 3 gives the corrected scalar binding energy. Rest of the columns correspond to configuration space corrections.

The root mean square derivation can be calculated as

$$\Delta_{RMS} = \Big(\sum_{H_M} [(E_g(H_M) + \Delta E_g) - E_g(H_F)]^2 \Big)^{\frac{1}{2}} \qquad (31)$$

This value turns out to be 4.22 MeV for scalar space and 2·05 MeV for

Table 2.1: Coefficients for quadrupole and pairing operators for ^{20}Ne

Haml.	a*(Q.Q)	b*(pair)	c*(Q.Q)	ζ_{H_M, H_F}
HS1	-0.1266	0.1916		0.799
HS2	-0.1070	0.1600		0.846
HST1	-0.1166	0.3060		0.806
HST2	-0.0977	0.2574		0.855
HST3	-0.0750	0.3160	-0.113	0.857

Table 2.2: First and second order corrections to the ground state binding energy of ^{20}Ne

Haml.	$E_g(H_M)$	Scalar space			Configuration space		
		$S_1(E_g)$	$S_2(E_g)$	$E_g(H_M)+\Delta E_g$	$S_1(E_g)$	$S_2(E_g)$	$E_g(H_M)+\Delta E_g$
HS1	-45.8	9.21	-8.28	-44.9	12.94	-3.64	-36.5
HS2	-43.2	8.38	-7.57	-43.4	5.99	-2.27	-39.5
HST1	-43.8	6.74	-6.22	-42.4	7.03	-3.37	-40.1
HST2	-47.0	6.82	-6.32	-46.5	9.17	-2.99	-40.8
HST3	-46.1	6.55	-6.08	-45.6	8.12	-4.45	-42.5
H_F	-40.6						

configuration space. Clearly, configuration space gives better results than the scalar space. The first order correction $S_1(E)$ (which is positive) has nearly the same magnitude for both scalar and configuration spaces. The second order correction $S_2(E)$ (which is negative) is smaller for configuration space, indicating a faster convergence of the inverse energy weighted sums in the configuration space.