Pramāṇa – J. Phys., Vol. 32, No. 4, April 1989, pp. 507–513. © Printed in India.

Inverse energy weighted sum-rules

V K B KOTA†, V POTBHARE*, P SHENOY* and N TRESSLER*

† Physical Research Laboratory, Navrangpura, Ahmedabad 380009, India
* Physics and Applied Physics Departments, MS University of Baroda, Baroda 390002, India

Abstract. A new derivation of the inverse energy-weighted sum-rules is given by applying the spectral distribution methods to the Rayleigh-Schrodinger perturbation theory. The scalar space result is then extended to the configurations. This is applied to obtain corrections to the ground-state energy estimates when the effective interaction is approximated by a model Hamiltonian obtained by taking linear combinations of various parts of the pairing and the Q.Q operators.

Keywords. Spectral-distribution-methods; inverse-energy-weighted sum-rules; ground-state-energy; effective-interactions.

PACS Nos 21·10; 21·60

1. Introduction

Spectral distribution methods (Kota and Kar 1987; French and Kota 1982) (SDM), which make use of moments and averages of various operators in a given spectroscopic space, have been well established and used quite extensively to study average properties like level densities, spin cut-off factors, averaged-spectra (fluctuation part removed), averaged-expectation values, averaged-strength distributions etc. There are some reservations against applying these methods in the ground-state domain, as this region is too far removed from the centre of the distribution (many times more than three widths away from the centroid). Nevertheless, it turns out that these methods have been quite successful in calculating ground-state energies (Chang *et al* 1971) and ground-state occupancies (Potbhare and Pandya 1976), much better than other microscopic theories. A detailed study using Wildenthal's universal $s-d$ shell interaction, performed recently by Sarkar *et al* (1986), confirms the claim of applicability of SDM in the ground-state domain. Here, we deal with correction to the ground-state energy when the effective hamiltonian is approximated by various model hamiltonians based on linear combinations of pairing and Q.Q operators (Kota *et al* 1980). Such a correction involves taking care of the difference between H_{eff} and H_{model}, perturbatively via inverse energy-weighted sums. In the next section, we derive the inverse energy-weighted sum-rule in the scalar space. This was first derived by Halemane (1981); we provide here an alternative derivation. In the third section, this result is extended to configuration space and then its application for ground-state energy correction is given in the last section.

2. Inverse energy-weighted sum-rules

Sum-rules in SDM are encountered in two different ways. First, if an excitation operator O acts on an eigenstate of a hamiltonian H, with energy E; then the expectation value of O^+O as a function of E, that is $O^+O(E)$ corresponds to the non-energy weighted sum of strength with respect to the intermediate eigenstates E' and with starting state energy E. Thus $O^+O(E)$, the non-energy weighted sum is the total strength of the excitation operator, averaged with respect to all starting states with energy E. Similarly, the linear energy-weighted sum $O^+HO(E)$, the expectation value of O^+HO as a function of E, relates to the centroid of the strength distribution. The $O^+H^2O(E)$ (quadratically energy-weighted sum) has information about the spread of the strength with respect to the energy of the intermediate states. These sums have been used to study single nucleon transfer processes (non-energy-weighted sum $\Rightarrow$ occupancy, linear energy-weighted sum $\Rightarrow$ effective single particle energy of orbit from or to which a particle is transferred). Secondly, the sum-rules arise when a hamiltonian is perturbed by a small operator αK, here α being only a multiplicative parameter. In this case, the expectation value of K as a function of energy is related to the width of the eigenfunction of H at E, when expressed in terms of the eigenfunctions of K; such calculations have earlier been reported by Potbhare (1977). So far, not much attention has been paid to the inverse energy-weighted sums, partly due to the notion that one has to deal with Green's function and complete solutions of the problem in order to deal with inverse-energy-weighted sums. Recently, however, Halemane (1981) applied the SDM to Rayleigh-Schrodinger perturbation theory and obained expressions for varieties 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 $\rho(E)$ characterized by these is assumed continuous. Ratcliff (1971) gave a procedure to generate a smoothened spectrum from such assumed continuous density function, the spectrum so obtained is the averaged spectrum, free from level-to-level fluctuations. The averaged position of E_n, the nth level starting from the ground-state is given by,

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

d here 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 $E_{n,\alpha}$ can be obtained similarly using $\rho_\alpha(x)$, characterized by the moments of $(H + \alpha K)$,

$$d * \int_{-\infty}^{E_{n,0}} \rho_{\alpha=0}(x)\mathrm{d}x = d * \int_{-\infty}^{E_{n,\alpha}} \rho_\alpha(x)\mathrm{d}x = n - 1/2 = p_n. \tag{1a}$$

The procedure adopted here is statistical in nature and hence is applicable when the spectrum is rigid (that is, it does not involve crossing of levels or large level motion due to collectivity). Series expansion of $E_{n,\alpha}$ in powers of α is given by the

Rayleigh-Schrodinger perturbation theory

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

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

Thus S_1 corresponds to the expectation value of K and S_2 is the first inverse energy weighted sum. The SDM provide smoothened expressions for the coefficients $S_i(E)$. Differentiating (1a) with respect to α (from now on we drop the state index n)

$$\frac{dp}{d\alpha} = 0 = \frac{\partial E}{\partial \alpha} \rho_\alpha(E_\alpha) + \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx, \tag{3}$$

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

In the limit $\alpha \to 0$, as the integration limits do not depend upon α, interchanging the integration over x and differentiation with respect to α, we get

$$\frac{\partial E_\alpha}{\partial \alpha}\Big|_{\alpha=0} = S_1(E_0) = K(E_0) = -\frac{1}{\rho(E_0)} \left[\frac{\partial}{\partial \alpha} \int_{-\infty}^{E_0} \rho_\alpha(x) dx \right]_{\alpha=0}$$

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

$F(x)$ here is the distribution function and suffix 0 indicates the unperturbed values. This result was originally given by Chang and French (1973). Differentiating (4) again with respect to α, we obtain,

$$\frac{\partial^2 E_\alpha}{(\partial \alpha)^2} = -\frac{1}{\rho_\alpha(E_\alpha)} \int_{-\infty}^{E_\alpha} \frac{\partial^2}{(\partial \alpha)^2} \rho_\alpha(x) dx + \frac{1}{\rho_\alpha^2(E_\alpha)} \frac{\partial \rho_\alpha(x)}{\partial \alpha}\Big|_{x=E_\alpha} * \int_{-\infty}^{E_\alpha} \frac{\partial \rho_\alpha(x)}{\partial \alpha} dx$$

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

Here, one has to be careful in keeping all terms which depend upon α. For example, $\partial \rho_\alpha(E_\alpha)/\partial \alpha$ can be written as,

$$\frac{\partial \rho_\alpha(E_\alpha)}{\partial \alpha} = \frac{\partial}{\partial \alpha} \left\{ \rho_\alpha(E_0) + \frac{\partial \rho_\alpha(x)}{\partial x}\Big|_{x=E_0} (E_\alpha - E_0) \right.$$

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

Substituting (7) into (6) and then taking the limit as $\alpha \to 0$, we obtain the inverse energy-weighted sum $S_2(E)$ as

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

$$= -\frac{1}{2\rho(E_0)} \left[\left(\frac{\partial^2}{(\partial \alpha)^2} F_\alpha(E_0) \right)_{\alpha=0} - \frac{\partial}{\partial E_0} \left\{ \frac{1}{\rho(E_0)} \left(\frac{\partial F_\alpha(E_0)}{\partial \alpha}\Big|_{\alpha=0} \right)^2 \right\} \right]. \tag{8}$$

This result was given by Halemane (1981). We have given a new and comparatively transparent derivation of the same using the Ratcliff's procedure. Further differentiation of (6) with respect to α would provide us expressions for $S_m(E)$, $(m > 2)$.

This 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 CLT also allows us to assume that the perturbed eigenvalue density due to small perturbation αK is gaussian too; however with centroid $\varepsilon(\alpha)$ and width $\sigma(\alpha)$. The change in the centroid merely shifts the eigenvalue spectrum while the width change corresponds to the scale change.

$$\varepsilon = \langle H \rangle, \quad \sigma^2 = \langle H^2 \rangle - \langle H \rangle^2, \quad \sigma_K^2 = \langle K^2 \rangle - \langle K^2 \rangle,$$
$$\varepsilon_\alpha = \langle H \rangle + \alpha \langle K \rangle, \quad \sigma^2(\alpha) = \sigma^2 + 2\alpha\zeta\sigma\sigma_K + \alpha^2\sigma_K^2,$$

where ζ is the correlation coefficient between H and K. The scale change parameter λ is defined by

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

Taking into account these two changes, it is clear using the geometric picture that eigenvalue E_0 is shifted to E_α due to perturbation

$$E_\alpha = E_0 + \alpha\langle K \rangle + \lambda(E_0 - \varepsilon). \tag{9}$$

Expanding the parameter λ as a power series in α gives

$$E_\alpha = E_0 + \alpha\{\langle K \rangle + \zeta\sigma_K/\sigma * (E_0 - \varepsilon)\} + \alpha^2/2 * (E_0 - \varepsilon)(1 - \zeta^2)\sigma_K^2/\sigma^2. \tag{10}$$

Thus in the CLT limit we have,

$$S_1(E_0) = K(E_0) = \langle K \rangle + \zeta\sigma_K/\sigma * (E_0 - \varepsilon),$$
$$S_2(E_0) = 1/2(1 - \zeta^2)(E_0 - \varepsilon)\sigma_K^2/\sigma^2. \tag{11}$$

3. Extension to configurations

The arguments based on the centroid shift and scale change for calculating $S_1(E)$ and $S_2(E)$ are easily applicable in the scalar space. Usually, one partitions the space according to some symmetry group, in order to increase the accuracy of the results. If we decompose the space according to configurations (Chang *et al* 1971), the overall state density $\rho(E)$ is then expressed as the sum of intensities of all configurations into which the space has now been subdivided.

$$\rho(E) = 1/D \sum_c d_c * \rho^c(E) = \sum_c I_c(E) \tag{12}$$

where d_c is the configuration dimensionality and $D = \sum_c d_c$ is the total dimensionality. Each term in the summation above corresponds to the intensity of the configuration in the eigenvalue distribution at energy E. We assume that each configuration density is a gaussian,

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

where $\varepsilon_0(c)$ and $\sigma_0(c)$ are the configuration density centroid and width respectively for unperturbed H. The introduction of perturbation αK to H shifts and scales each configuration differently, according to

$$\varepsilon_\alpha(c) = \varepsilon_0(c) + \alpha\langle K\rangle^c$$
$$\sigma_\alpha^2(c) = \sigma_0^2(c) + 2\zeta_c\sigma_K(c)\sigma_0(c) + \alpha^2\sigma_K^2(c).$$

Suffix 0 indicates unperturbed values which refer to H. Introducing these into the general expressions for $S_1(E)$ and $S_2(E)$ (equations (5) and (8) given above), though tedious, is quite straightforward. We merely indicate the final result here

$$S_1(E) = \frac{\sum_c d_c/D\,\rho^c(E)\{\langle K\rangle^c + \zeta_c\sigma_K^c x_c\}}{\rho(E)} \tag{13}$$

$$x_c = (E - \varepsilon_0(c))/\sigma_0(c)$$

$$\begin{aligned} S_2(E) = {} & \frac{1}{2\rho(E)}\left[\sum_c \frac{d_c}{D}\frac{\rho^c(x)}{\sigma_0(x)}\{\zeta_c^2\sigma_K^2(c)\mathrm{He}_3(x_c)\right. \\ & \left. + 2\langle K\rangle^c\sigma_K(c)\zeta_c\mathrm{He}_2(x_c) + [(\langle K\rangle^c)^2 + \sigma_K^2(c)]\mathrm{He}_1(x_c)\}\right] \\ & + \frac{1}{2[\rho(E)]^3}\left[\sum_c \frac{d_c}{D}\frac{x_c}{\sigma_0(c)}\rho^c(x_c)\right]*\left[\sum_c \frac{d_c}{D}\rho^c(x_c)[\langle K\rangle^c + \zeta_c\sigma_K(c)x_c]\right]^2 \\ & - \frac{1}{[\rho(E)]^2}\left[\sum_c \frac{d_c}{D}\rho^c(x_c)(\langle K\rangle^c + \zeta_c\sigma_K(c)x_c)\right] \\ & *\left[\sum_c \frac{d_c}{D}\frac{\rho^c(x_c)}{\sigma_0(c)}\{\langle K\rangle^c x_c + (x_c^2 - 1)\zeta_c\sigma_K(c)\}\right]; \end{aligned} \tag{14}$$

where He_i are the Hermite polynomials, and c in the above equations indicates that the corresponding quantity is calculated in configuration c. Note that in general, ζ_c cannot be called the correlation coefficient as the configuration partitioning does not correspond to good symmetry; however, it has the same structure and hence the same nomenclature is used;

$$\zeta_c = \langle(K - \langle K\rangle^c)(H - \langle H\rangle^c)\rangle^c/\sigma_K(c)\sigma_0(c).$$

4. Applications

Kota *et al* (1980) gave several model Hamiltonians H_M approximating the effective interaction H_F by linear combinations of various parts of the Q.Q operator and the pairing operator. It is clear that such a model interaction cannot completely represent H_F, as a part of the H_F will always be orthogonal to H_M. Hence, the ground-state energy calculated using H_M will not be the same as the true ground-state energy. We are now in a position to correct the ground-state energy estimate obtained using H_M, by taking into account the difference between H_F and H_M;

$$H_F = H_M + H_P = H_M + K.$$

Table 1. Ground-state energies for ^{20}Ne (in MeV)

Interaction	$E_g(H_M)$	$E_g(H_M)+\Delta E_g$(scalar)	$E_g(H_M)+\Delta E_g$(conf.)
HS1	−45·8	−44·9	−36·5
HS2	−43·8	−43·3	−40·1
HST1	−43·2	−42·4	−39·5
HST2	−47·0	−46·5	−40·8
HST3	−46·1	−45·6	−42·5
H_F	−40·6	—	—

The operator K is treated as a perturbation to the model Hamiltonian H_M. The scalar space result for such a correction is very easy to obtain;

$$S_1(E_g)+S_2(E_g)=-E_g/2(1-\zeta_{MF}^2)=\Delta E_g,$$

where E_g is the ground-state energy as given by H_M, ζ_{MF} is the correlation coefficient between H_M and H_F. Similar result using configuration space has been obtained in terms of averages of various combinations of H_M and H_F in each configuration. The ground-state energy corrections using these expressions have been displayed in table 1 for the case of ^{20}Ne in $d-s$ shell space using the PW interaction as the effective interaction, with ^{17}O single-particle energies.

The interactions HS1, HS2, HST1, HST2 and HST3 are various model interactions (Kota *et al* 1980). The ground-state energies in column 2 have been obtained using the shell-model programme; the third column gives the ground-state energies using the scalar space result while the last column corresponds to the corrected ground-state energies using the configuration space expressions for ΔE_g. It is immediately clear by looking at table 1 that the corrected ground-state energies are closer to the H_F ground-state energy and further that the configuration space result is much better than the scalar space result. Also the deviation from true ground-state is the largest in the case of HS1; the interaction derived using the least information input from the effective interaction.

In conclusion, we would like to point out that, we have a new derivation (8) of the expressions that are statistical in nature, for the inverse energy-weighted sums that appear in the Rayleigh Schrodinger perturbation theory. These expressions (especially (14) and its extensions) are useful in a wide variety of problems. As a simple example, we have applied them and calculated the ground-state energy corrections when the effective interaction is approximated by a model Hamiltonian.

Acknowlegement

We thank J B French for the valuable input that has come from him which lead to the derivation of equation (14).

References

Chang F S and French J B 1973 *Phys. Lett.* **B44** 131
Chang F S, French J B and Thio T H 1971 *Ann. Phys.* **66** 137

French J B and Kota V K B 1982 *Annu. Rev. Nucl. Part. Sci.* **32** 35
Halemane T R 1981 *J. Math. Phys.* **22** 2961
Kota V K B and Kar K 1987 Univ. of Rochester Preprint UR-1058
Kota V K B, Pandya S P and Potbhare V 1980 *Nucl. Phys.* **A349** 397
Potbhare V 1977 *Nucl. Phys.* **A289** 373
Potbhare V and Pandya S P 1976 *Nucl. Phys.* **A265** 253
Ratcliff K F 1971 *Phys. Rev.* **C3** 117
Sarkar S, Kar K and Kota V K B 1987 *Phys. Rev.* **C36** 2700