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Effective operators and the truncation of shell model configuration space

Y K GAMBHIR and G BASAVARAJU
Department of Physics, Indian Institute of Technology, Bombay 400 076

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Abstract. An alternative derivation of the projection method for constructing effective operators in the truncated shell model space is presented. The results of explicit numerical calculations in three different nuclear regions are discussed. Non-hermiticity of the effective Hamiltonian and various hermitisation procedures are investigated in detail.

Keywords. Shell mode; truncation of configuration space; effective operators; non-hermiticity.

1. Introduction

The need to limit the configuration space in the shell model calculations is well known. The effects of the neglected configurations are taken into account in an approximate manner through the use of effective operators (like Hamiltonian, E_2, M_1, etc.). Two main approaches, the energy dependent (Eden and Francis 1955; Bloch and Horowitz 1958; MacFarlane 1969) formalism and the energy independent formalism, have been followed in constructing the effective Hamiltonian. In the former approach the energy of the exact state appears explicitly. This undesirable energy dependence of the effective Hamiltonian can be avoided by using an approximate averaging procedure (MacFarlane 1969) which is valid only in restricted cases. The latter approach, either in terms of folded diagrams (Brandow 1967 and 1970; Oberlechner *et al* 1970; Johnson and Baranger 1971; Kuo *et al* 1971) or in an equivalent algebraic formulation (Des Cloisezux 1960; Schucan and Weidenmuller 1972 and 1973; Hofmann *et al* 1974; Harvey 1976) involves the energy of the exact state, only through the normalisation of that state. Recently, Kassis (1977) has shown following the wave operator formalism, that both the energy dependent and the energy independent formalisms are equivalent and that one can be derived from the other simply by algebraic manipulation.

In these formalisms the effective Hamiltonian is given in the form of a series expansion. For the cases where the neglected configurations involve the single particle (SP) states in the same major shell, such a series expansion of effective Hamiltonian may not be satisfactory because of small unperturbed energy differences appearing in the denominators of the various terms of the series. Therefore, a projection method has been followed for such cases. In this method an effective operator is constructed by requiring that its matrix element between those parts of the exact (true) states which lie in the truncated space i.e. between the projected states,

exactly reproduces the value of the matrix element of the original operator between the exact states. The projected states apart from the normalisation, then clearly are the eigenstates of the effective Hamiltonian. Because of the non-orthogonality of the projected states, the effective Hamiltonian is no longer hermitian. This undesirable feature can be removed by a suitable hermitisation procedure.

In the present paper we give first an alternative derivation of projection method by introducing a correlation matrix (U) in the wave operator formalism. We then consider the truncation of the configuration space involving one or more single particle valence levels. The effective operators which include the effects of the neglected configurations are constructed in terms of the operators in the full space. Explicit expressions for the effective operators are presented in a simple form suitable for numerical computation. In addition, these expressions bring out very clearly the factors contributing to the renormalisation of the effective operators due to the truncation of configuration space. Only the matrix elements (ME) of U which link the truncated space to the omitted space, appear in these expressions. The estimation of many-body correlations introduced by the truncation requires only these M.E. of U. For the case of two particles the present formulation, like the projection method, is equivalent to summing up all order diagrams of the perturbation theory. The non-hermiticity of the effective Hamiltonian is examined in detail. Different prescriptions for hermitisation of the effective Hamiltonian, so that it can be used directly in the many particle shell model calculations, are discussed. The present formulation which is very much pertinent to shell model, is quite general and is applicable to any quantum mechanical problem involving truncation of configuration space.

2. Formalism

In the full space D the problem is defined through the following equations:

$$H \mid \psi^\alpha \rangle = E^\alpha \mid \psi^\alpha \rangle, \tag{1a}$$

$$H = H_0 + V, \tag{1b}$$

$$H_0 \mid N \rangle = E_N \mid N \rangle, \tag{1c}$$

$$\mid \psi^\alpha \rangle = \sum_{N \subset D} a_N^\alpha \mid N \rangle, \tag{1d}$$

$$a_N^\alpha = \langle N \mid V \mid \psi^\alpha \rangle / (E_N - E^\alpha). \tag{1e}$$

Here the symbols have their usual meaning. In the projection method the effective Hamiltonian H_{eff} is required to satisfy

$$H_{\text{eff}} \mid \phi^\alpha \rangle = E^\alpha \mid \phi^\alpha \rangle, \tag{2a}$$

$$P \mid \psi^\alpha \rangle = \mid \phi^\alpha \rangle = \sum_{i \subset d} a_i^\alpha \mid i \rangle, \tag{2b}$$

where P is the projection operator for the model space d. We have denoted A-nucleon basis state by $|N\rangle$ in the full space D and by $|i\rangle$ in the model space d, respectively, we shall reserve $|\mathcal{I}\rangle$ to denote A-particle basis state in the excluded space.

In terms of the wave operator Ω, the problem defined by equations (2a) and (2b) is equivalent to:

$$H_{\text{eff}} = H_0 + V_{\text{eff}}, \tag{3a}$$

$$V_{\text{eff}} = V\Omega, \tag{3b}$$

$$|\psi^\alpha\rangle = \Omega\,|\phi^\alpha\rangle. \tag{3c}$$

In general any effective operator $\hat{O}_{\text{eff}}$ in d is related to the operator $\hat{O}$ in D through

$$\hat{O}_{\text{eff}} = \overleftarrow{\Omega}\,\hat{O}\,\overrightarrow{\Omega}. \tag{4}$$

In (4) the arrows on the top of Ω indicate the direction of operation of Ω. It is easy to show (Harvey 1976) that the expression (3b) for V_{eff} (H_{eff}) is consistent with (4). Evidently, the whole problem reduces to the determination of Ω, which immediately gives H_{eff} (V_{eff}) or $\hat{O}_{\text{eff}}$. In the perturbation theory Ω is given by

$$\Omega = 1 + \frac{Q}{E^\alpha - H_0} V\,\Omega, \tag{5}$$

with $Q=1-P$. In the second order perturbation theory, Ω is replaced by unity in the r.h.s. of (5). The expression (5) for Ω can be rewritten in terms of Rayleigh-Schrödinger form which does not involve E^α explicitly.

We do not intend to evaluate Ω upto a certain order of perturbation theory. Instead, we use (3c) to obtain Ω to solve the problem defined by (2a) and (2b). The difference between the exact state $|\psi^\alpha\rangle$ and the model state $|\phi^\alpha\rangle$ stems entirely through the excitations of the model space to the omitted space. Therefore, in terms of a real operator U representing that part of Ω which introduces the correlations and hence links the model space d with the omitted space, the expression (3c) for $|\psi^\alpha\rangle$ becomes

$$\begin{aligned}|\psi^\alpha\rangle &= (1+U)\,|\phi^\alpha\rangle \\ &= |\phi^\alpha\rangle + U\,|\phi^\alpha\rangle.\end{aligned} \tag{6}$$

The second quantised form of U is given by

$$U \to \sum_{\substack{i \subset d \\ \mathcal{I} \not\subset d}} \langle \mathcal{I}\,|\,u\,|\,i\rangle\, \mathcal{V}^+_{\mathcal{I}}\, \mathcal{V}_i, \tag{7}$$

where the operator $\mathscr{V}^+$ ($\mathscr{V}$) creates (destroys) A-nucleon basis state. Using the knowledge of the exact state $|\psi^\alpha\rangle$ the matrix elements of U can be obtained through the relations (1c), (2b), (6) viz.

$$|\psi^\alpha\rangle = \sum_{N \subset D} a_N^\alpha |N\rangle = |\phi^\alpha\rangle + \sum_{\substack{i \subset d \\ \mathscr{J} \not\subset d}} \langle \mathscr{J} | u | i \rangle \mathscr{V}^+_{\mathscr{J}} \mathscr{V}_i |\phi^\alpha\rangle$$

$$= |\phi^\alpha\rangle + \sum_{\substack{i \subset d \\ \mathscr{J} \not\subset d}} \langle \mathscr{J} | u i \rangle a_i^\alpha |\mathscr{J}\rangle. \tag{8}$$

Equating the coefficients of $|\mathscr{J}\rangle$ in (8), yields

$$a_{\mathscr{J}}^\alpha = \sum_{i \subset d} \langle \mathscr{J} | u | \rangle a_i^\alpha, \tag{9}$$

for each $\mathscr{J}$ and for all α. This set of equations is sufficient to determine all the ME of the correlation matrix U connecting the omitted space and the model space. The remaining ME of U may be left arbitrary as these do not enter in the calculation of V_{eff} (equation (10)) or $\hat{O}_{\text{eff}}$ (equation (11)).

The expression for the ME of V_{eff} (H_{eff}) in the model space d in terms of U, is then given by

$$\langle i | V_{\text{eff}} | j \rangle = \langle i | V | j \rangle + \sum_{\mathscr{J} \not\subset d} \langle i | V | \mathscr{J} \rangle \langle \mathscr{J} | u | j \rangle, \tag{10}$$

or

$$\langle i | H_{\text{eff}} | j \rangle = \langle i | H | j \rangle + \sum_{\mathscr{J} \not\subset d} \langle i | V | \mathscr{J} \rangle \langle \mathscr{J} | u | j \rangle. \tag{11}$$

It is clear from (10) that

$$\langle i | H_{\text{eff}} | j \rangle \neq \langle j | H_{\text{eff}} | i \rangle,$$

and therefore H_{eff} is no longer hermitian. Using (9) it is easy to show that the expression (11) for H_{eff} is identical with the corresponding expression given by the projection method. It is clear from (11) that the correction to the Hamiltonian due to truncation involves only those ME of the interaction V and the operator U which connect the model space d and the omitted space. Analogous expression for $\hat{O}_{\text{eff}}$ is

$$\langle i | \hat{O}_{\text{eff}} | j \rangle = \langle i | \hat{O} | j \rangle + \sum_{\mathscr{J} \not\subset d} (\langle \mathscr{J} | u | i \rangle \langle \mathscr{J} | \hat{O} | j \rangle$$

$$+ \langle \mathscr{J} | u | j \rangle \langle i | \hat{O} | \mathscr{J} \rangle) + \sum_{\mathscr{J}\mathscr{J}' \not\subset d} \langle \mathscr{J} | u | i \rangle \langle \mathscr{J}' | u | j \rangle \langle \mathscr{J} | \hat{O} | \mathscr{J}' \rangle. \tag{12}$$

The form of (12) is explicit and simple to enable the calculation of $\hat{O}_{\text{eff}}$ in the model space d. On the other hand, the corresponding expression of the projection method is very formal and hence is not suitable for numerical calculation.

In the derivation of (11) and (12) nowhere have been the explicit form of the wave functions used. Therefore, the present formulation is quite general and is applicable to any quantum mechanical problem involving truncation of configuration space.

The basic aim of all approaches discussed above is to obtain two-body effective Hamiltonian $\left(H_{\text{eff}}^{(2)}\right)$ which can be used in many-particle shell model calculations in the truncated space. This requires at most the solution of two-particle shell model problem in the full space, which is quite feasible in almost all the cases. The justification for the use of $V_{\text{eff}}^{(2)}\left(=H_{\text{eff}}^{(2)}-H_0\right)$ as two-body effective interaction in the many-particle shell model calculations demands that many-body correlations introduced by the truncation should be small. These many body correlations can be estimated by comparing the ME of H_{eff} (equation (11)) with the corresponding ME calculated with the standard shell model techniques employing $V_{\text{eff}}^{(2)}$ as two-body effective interaction. This problem is under investigation.

As stated earlier $H_{\text{eff}}^{(2)}$ obtained by the projection method is no longer hermitian and therefore has to be hermitised before it can be used in the many-particle shell model calculations. Barret *et al* (1975) in their studies confined to the $2s$-$1d$ region have defined the hermitised two-body effective Hamiltonian $\left(\bar{H}_{\text{eff}}^{(2)}\right)$ as

$$\bar{H}_{\text{eff}}^{(2)}=\tfrac{1}{2}\left(H_{\text{eff}}^{(2)}+H_{\text{eff}}^{(2)+}\right). \tag{13}$$

A slightly different procedure has been followed by Gupta (1973), in which the lowest projected state and all the lowest exact eigenvalues corresponding to the dimensionality of the model space d are reproduced. The remaining eigenvectors orthonormal to this projected state are then constructed by the Schmidt-orthogonalisation procedure. In addition to these procedures, we use here a third prescription in which $\bar{H}_{\text{eff}}^{(2)}$ is defined as

$$\langle i|\,\bar{H}_{\text{eff}}^{(2)}|j\rangle=\left(\langle i|\,H_{\text{eff}}^{(2)}|j\rangle\,\langle j|\,H_{\text{eff}}^{(2)}|\,i\rangle\right)^{\frac{1}{2}}. \tag{14}$$

The numerical calculations, the discussion of which will follow, reveals that the prescription followed by Gupta (1973) is not satisfactory, in particular for the cases where the number of retained configurations is more than two, while the averaging procedure of Barret *et al* (1975) is satisfactory in almost all the cases except where the non-hermiticity is quite large. On the other hand, the prescription defined by (14) is consistently better in all the cases,

3. Results and conclusions

Explicit numerical calculations in the $2s$-$1d$ region with ^{16}O core, in the $2p$-$1f$ region with ^{40}Ca core and in the space of $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ and $1g_{9/2}$ with ^{56}Ni core are carried

out. The results of truncation of two-particle configurations containing $1d_{3/2}$ single-particle level in the $2s$-$1d$ region, $2p_{1/2}$ and/or $1f_{5/2}$ SP levels in the $2p$-$1f$ region and $1g_{9/2}$ state for the case of ^{56}Ni core, are discussed. Two sets of interaction matrix elements are used in the $2s$-$1d$ region. The first is a phenomenological set of Chung and Wildenthal (1977) determined by directly fitting the relevant observed spectra. The second is a microscopic set reported by Vary and Yang (1977). It is derived from the Reid soft-core potential and it also includes $3p$-$1h$ and $4p$-$2h$ core excitations. The SP unperturbed energies used are taken from the ^{17}O spectrum, these are 0·0, 0·87 and 5·08 MeV for $1d_{5/2}$, $2s_{1/2}$ and $1d_{3/2}$ respectively. The non-hermiticity defined as

$$\frac{\langle i|H_{\text{eff}}^{(2)}|j\rangle - \langle j|H_{\text{eff}}^{(2)}|i\rangle}{\langle i|H_{\text{eff}}^{(2)}|j\rangle + \langle j|H_{\text{eff}}^{(2)}|i\rangle}, \tag{15}$$

is found to be small in general, maximum being 10·8% for $J=1$, $T=0$ state with the interaction ME of Chung and Wildenthal. As the non-hermiticity is small and the maximum number of configurations retained is not more than two, the various procedures described earlier for obtaining $\bar{H}_{\text{eff}}^{(2)}$ lead to almost identical results and reproduce equally well the exact eigenvalues and the projected states. A representative result for this region is given in table 1. The eigenvalues of $\bar{H}_{\text{eff}}^{(2)}$ obtained by the hermitisation procedures of Gupta (1973), Barret *et al* (1975) and equation (14) are listed in the columns labelled as E_a, E_b and E_c respectively. The corresponding results of the second order perturbation theory are also listed in the column E_{2PT}, for comparison. The overlaps of the respective eigenvectors with the normalised projected states are given in the parentheses.

In the $2p$-$1f$ region, the interaction ME reported by Kuo and Brown (1968) calculated from the Hamada-Johnston potential and corrected for core-excitations with $3p$-$1h$ intermediate states are used. The calculations are also performed with the interaction ME obtained by one of us (Gambhir, unpublished), using Tabakin non-local separable potential. This set of ME includes, in the perturbation theory, the second order Born term as well as the appropriate core polarisation corrections with

Table 1. Eigenvalues of $\bar{H}_{\text{eff}}^{(2)}$ for $J=1$, $T=0$ state in the $2s-1d$ region. E_a, E_b, E_c and E_{2PT} correspond respectively to the results obtained by the procedures of Gupta (1973), Barret *et al* (1975), equation (14) and by the second order perturbation theory. The overlaps of the respective eigenvectors with the projected states are given in parentheses.

Interaction ME of Chung and Wildenthal				Interaction ME of Vary and Yang (1977)			
E_a*	E_b	E_c	E_{2PT}	E_a*	E_b	E_c	E_{2PT}
−5·03	−5·04	−5·03	−3·23	−4·74	−4·75	−4·74	−2·65
(1·000)	(0·999)	(0·999)	(0·996)	(1·000)	(0·999)	(0·999)	(0·999)
−1·04	−1·03	−1·04	−0·88	−0·99	−1·00	−0·99	−0·75
(0·995)	(0·999)	(0·999)	(0·982)	(0·997)	(0·999)	(0·999)	(0·992)

*These eigenvalues are identical to the lowest eigenvalues in the full space.

$3p$-$1h$ intermediate states. The SP unperturbed energies used are 0·0, 2·1, 3·9 and 6·5 MeV for $1f_{7/2}$, $2p_{3/2}$, $2p_{1/2}$ and $1f_{5/2}$ respectively consistent with Kuo and Brown (1968). The non-hermiticity in this region is found to be less than 30% except for $J=1$, $T=0$ state where it is 62% for Kuo-Brown (KB) interaction ME and is 53% for the Tabakin (TB) interaction ME. The large non-hermiticity for $J=1$, $T=0$ state arises due to the fact that the first excited $J=1,T=0$ state in the full space has less than 50% component belonging to the model space d. In this sense (Barret *et al* 1975) this excited state can therefore be considered as an ' intruder ' state. The results of $\bar{H}^{(2)}_{\text{eff}}$ obtained by the averaging procedure of Barret *et al* (1975) and by (14) are almost identical because of small ($\leqslant 30\%$) non-hermiticity, except for $J=1$, $T=0$ where the procedure of (14) reproduces better the exact eigenvalues and the projected states. These results however, differ from the corresponding results of $\bar{H}^{(2)}_{\text{eff}}$ obtained by the procedure of Gupta (1973), in particular for the cases where the number of retained configurations exceeds two. The results for $J=1$, $T=0$ and $J=2$, $T=1$ are shown in table 2.

In the case of ^{56}Ni core the Tabakin interaction ME appropriate to this space and the SP energies 0·0, 0·78, 1·08 and 3·5 MeV for $2p_{3/2}$, $1f_{5/2}$, $2p_{1/2}$ and $1g_{9/2}$ respectively, are used. The non-hermiticity is found to be small ($\leqslant 10\%$). The results for $J=2$, $T=1$, as a representative case in this region are shown in table 3. Again the

Table 2. Eigenvalues of $\bar{H}^{(2)}_{\text{eff}}$ for $J=1$, $T=0$ and $J=2$, $T=1$ states in $2p-1f$ region. For details see caption of table 1.

J, T	Interaction ME of Kuo and Brown (1968)				Interaction ME of Gambhir (unpublished)			
	E_a*	E_b	E_c	E_{2PT}	E_a*	E_b	E_c	E_{2PT}
1, 0	−1·82	−2·09	−1·82	−1·14	−1·82	−1·97	−1·82	−1·42
	(1·000)	(0·963)	(0·977)	(0·996)	(1·000)	(0·982)	(0·989)	(0·999)
	1·47	1·75	1·48	3·19	1·85	1·99	1·85	3·08
	(0·856)	(0·963)	(0·946)	(0·808)	(0·928)	(0·982)	(0·973)	(0·908)
2, 1	−1·05	−1·06	−1·05	−1·04	−1·02	−1·02	−1·02	−1·01
	(1·000)	(1·000)	(1·000)	(1·000)	(1·000)	(1·000)	(1·000)	(1·000)
	1·21	1·21	1·21	1·25	1·16	1·16	1·16	1·21
	(0·987)	(1·000)	(1·000)	(1·000)	(0·983)	(1·000)	(1·000)	(1·000)
	3·69	3·69	3·69	3·83	3·58	3·58	3·58	3·70
	(0·9990)	(1·000)	(1·000)	(0·999)	(0·988)	(1·000)	(1·000)	(0·999)

Table 3. Eigenvalues of $\bar{H}^{(2)}_{\text{eff}}$ for $J=0$, $T=1$ state for the case of ^{56}Ni core. For details see caption of table 1.

E_a*	E_b	E_c	E_{2PT}
−2·69	−2·69	−2·69	−2·61
(1·000)	(1·000)	(1·000)	(1·000)
0·50	0·50	0·50	0·57
(0·940)	(1·000)	(1·000)	(0·999)
2·24	2·24	2·24	2·25
(0·941)	(1·000)	(1·000)	(1·000)

procedures of Barret *et al* (1975) and (14) lead to identical results and reproduce well the exact eigenvalues and the projected states. On the other hand, the procedure of Gupta (1973) leads to poor results in many cases. This probably is due to the non-uniqueness of the procedure for constructing the orthonormal states.

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