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Effective interactions in the $s d$ and $p$ shells ${ }^{1}$

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#### Abstract

Using matrix-inversion techniques effective interactions for the sd and $p$ shells are determined in the complete space $0 \hbar \omega+2 \hbar \omega$. The derived interactions are used to determine the spectra of $\mathrm{A}=18-20$ and $\mathrm{A}=5-15$ nuclei and compare them with experiment.


## 1. INTRODUCTION

One of the purposes of nuclear theory is the derivation of effective interactions appropriate for shell model calculations. Since the pioneer work of Kuo and Brown (1966), there has been a large amount of studies in this field trying to deduce effective interactions using several methods and techniques.

In this paper, we describe a method based on matrix-inversion techniques to derive effective interactions appropriate for shell model calculations in the sd and p shells (Skouras and Varvitsiotis $1990 \mathrm{a}, \mathrm{b}$ ). In this method the energy matrices are constructed in the space of $0 \hbar \omega+2 \hbar \omega$ excitations and convergence studies are made for the effective interaction after the elimination of the unlinked graphs in the above space.

This work falls in three parts. First, the elimination of unlinked graphs in the space of $0 \hbar \omega+2 \hbar \omega$ excitations is shown in sect.2, which leads to the linked plus folded diagram expansion. The summation of the above expansion is performed in sect. 3 and finally the results of the calculation are given in sect.4.

## 2. ELIMINATION OF UNLINKED DIAGRAMS IN $O \hbar \omega+2 \hbar \omega$ SPACE

The energy matrices are constructed for the $\mathrm{A}=16-18$ and $\mathrm{A}=4-8, \mathrm{~A}=14-16$ systems in a space that includes all $0 \pi \omega+2 \hbar \omega$ excitations. The Hamiltonian for a system of A nucleons has the form

$$
\begin{equation*}
H=\sum_{i=1}^{A} t_{i}+\sum_{i<j}^{A} V(i, j) \tag{1}
\end{equation*}
$$

1 Presented by J.C. Varvitsiotis
where $t$ denotes the kinetic energy, $V$ the two body interaction while $A$ the number of the nucleons in the nucleus. The Hamiltonian (1) can be written as

$$
\begin{equation*}
H=H_{0}+H_{1} \tag{2}
\end{equation*}
$$

where

$$
\begin{equation*}
H_{0}=\sum_{i=1}^{1}\left(t_{i}+U_{i}\right), \quad H_{1}=\sum_{i<1}^{1} V(i, j)-\sum_{i=1}^{1} U(i) \tag{3}
\end{equation*}
$$

and $U$ an one body potential. We also define the projection operators

$$
\begin{equation*}
P=\sum_{a=1}^{\mu}|\alpha\rangle\langle\alpha|, \quad Q=\sum_{i=1}^{M}|i\rangle\langle i|, \tag{4}
\end{equation*}
$$

where $P$ projects onto the $0 \hbar \omega$ model space while $Q$ onto the $2 \hbar \omega$ space. By Greek letters $\alpha, \beta, \gamma, \ldots$ are labeled the model space states while by $\mathrm{i}, \mathrm{j}, \mathrm{k}, \ldots$ the $2 \hbar \omega$ states. $\mu, \mathrm{M}$ denote the dimensions of the $0 \hbar \omega$ and $2 \hbar \omega$ spaces respectively.

We consider now the Rayleigh-Schroedinger expansion for a degenerate system

$$
\begin{equation*}
V_{e f f}^{R \cdot S}=\sum_{k=1}^{\infty} S_{k} \tag{5}
\end{equation*}
$$

Since all energy denominators in the calculation are equal, the first few terms of the above series are written as

$$
\begin{gather*}
S_{1}=E_{1}  \tag{6a}\\
S_{2}=E_{2}  \tag{6b}\\
S_{3}=E_{3}  \tag{6c}\\
S_{4}=E_{4}-\frac{2 E_{3} E_{1}}{D}+\frac{E_{2} E_{1}^{2}}{D^{2}}-\frac{E_{2}^{2}}{D} \tag{6d}
\end{gather*}
$$

e.t.c, where
$E_{1}=P H_{1} P, \quad E_{n}=\frac{P H_{1} Q\left(Q H_{1} Q\right)^{n-2} Q H_{1} P}{D^{n-1}}, n \geq 2, \quad D=E_{0}-E_{Q}$
The terms of the Rayleigh-Schroedinger series (5) that produce unlinked diagrams in a space restricted to $2 \hbar$ wexcitations appear in fourth and higher orders and are those that contain two or more factors $E_{k}$ with $k>1$ (Mavromatis and Skouras 1979, Skouras and Varvitsiotis 1990a,b). For example, the term $-E_{2}^{2} / D$ of the fourth order in a double closed shell system contains the product graphs of fig. 1


Fig. 1 Product graph 5 contained in- $E_{2}^{2} / D$ term of fourth-order. The dash line denotes a minus and an extra denominator $D$.
which in a complete space calculation are canceled by the unlinked graphs of fig. 2 .


Fig. 2 Fourth-order unlinked diagrams that appear in the closed core system.

The graphs of fig. 2 are coming from the leading term $E_{4}$ of (6d) and don't appear in the present calculation since they invoive higher than $0 \hbar \omega+2 \hbar \omega$ excitations. By removing from Rayleigh-Schroedinger expansion (5) all the terms that contain more than one factor $E_{\mathrm{k}}$ with $k>1$, the series

$$
\begin{equation*}
Y=\sum_{k=0}^{\infty} Y_{k+2} \tag{7}
\end{equation*}
$$

results, where

$$
\begin{gather*}
Y_{2}=E_{2}  \tag{8a}\\
Y_{3}=E_{3}-\frac{E_{2} E_{1}}{D}  \tag{8b}\\
Y_{4}=E_{4}-\frac{2 E_{3} E_{1}}{D}+\frac{E_{2} E_{1}^{2}}{D^{2}} \tag{8c}
\end{gather*}
$$

e.t.c. Hence, the series (7) in the $0 \hbar \omega+2 \hbar \omega$ space includes only linked graphs in agreement with the formal theory of effective interactions (Brandow 1967). The summation of series (7) in the above space is the subject of the next section.

## 3. SUMMATION OF LINKED PLUS FOLDED DIAGRAMS EXPANSION IN $0 \hbar \omega+2 \hbar \omega$ SPACE

A summation to all orders of expansion (7) is obtained in a space that is the direct product of the $P$ and $Q$ spaces of sect.2. This space denoted by $P \otimes$ Qhas dimension $\mu \times$ Mand the following quantities are defined into it
a) An operator $Z$ :

$$
\begin{equation*}
Z_{l a, \beta \beta}=\frac{\left(Q H_{1} Q\right)_{i j} \delta_{a \beta}-\left(P H_{1} P\right)_{\alpha \beta} \delta_{i j}}{D} \tag{9}
\end{equation*}
$$

b) The $\mu^{2}$ row vectors $\Psi_{\beta}^{\alpha}(\alpha, \beta=1,2, \ldots, \mu)$ :

$$
\begin{equation*}
\left(\Psi_{\beta}^{\alpha}\right)_{1 \gamma}=\delta_{\beta \gamma}\left(P H_{1} Q\right)_{a 1} \tag{10}
\end{equation*}
$$

c) The column vector $\Phi$ :

$$
\begin{equation*}
\Phi_{i \gamma}=\left(Q H_{1} P\right)_{i \gamma} \tag{11}
\end{equation*}
$$

We also define the model space quantities

$$
\begin{equation*}
\left(R_{n}\right)_{a \beta}=\frac{(-)^{n}}{D^{n+1}} \Psi_{\beta}^{\alpha}(I-Z)^{-(n+1)} \Phi, \quad n=0,1,2, \ldots \tag{12}
\end{equation*}
$$

where $I$ denotes the unit matrix in the $P \otimes Q$ space. The quantities $R_{n}$ can be expressed in the form of a series:

$$
\begin{equation*}
R_{n}=\frac{(-)^{n}}{D^{n}} \sum_{l=0}^{\infty}\binom{n+i}{n} y_{l+2}, n=0,1,2, \ldots \tag{13}
\end{equation*}
$$

where

$$
\begin{equation*}
\left(Y_{1+2}\right)_{\alpha \beta}=\frac{\Psi_{\beta}^{\alpha} Z^{l} \Phi}{D} \tag{14}
\end{equation*}
$$

The quantities $R_{n}$ are the basic units in our method to derive the effective interaction. For a Q space restricted to $0 \hbar \omega+2 \hbar \omega$ excitations, each $R_{n}$ includes linked plus folded valence diagrams and linked core diagrams (Skouras and Varvitsiotis 1990a). By considering the difference

$$
\begin{equation*}
r_{n}^{\prime}=R_{n}^{\prime}-R_{n}^{c} \tag{15}
\end{equation*}
$$

we obtain the valence one-body graphs, where j and c denote an orbital in the model space of ${ }^{17} \mathrm{O}$ and the core state respectively. For the two-particle system, we obtain the valence graphs by considering

$$
\begin{equation*}
\langle i j ; J T| r_{n} \mid k l ; J T>=\langle i j ; J T| R_{n} \mid k l ; J T>-\delta_{i k} \delta_{j l}\left(r_{n}^{i}+r_{n}^{j}+R_{n}^{c}\right) \tag{16}
\end{equation*}
$$

where $\mathrm{i}, \mathrm{j}, \mathrm{k}$ and l denote orbitals of the sd shell.

We correspond now the quantity $r_{0}$ to the Q-box of Krenciglowa and Kuo (1974) and the quantities $r_{n} \quad(n>0)$ as the derivatives of the Q -box. Hence, the effective interaction is given by the expansion

$$
\begin{equation*}
V_{e f f}=F_{0}+F_{1}+F_{2}+\ldots \tag{17}
\end{equation*}
$$

where

$$
\begin{equation*}
F_{0}=r_{0}, \quad F_{1}=r_{1} r_{0}, \quad F_{2}=r_{2} r_{0}^{2}+r_{1}^{2} r_{0}, \quad \text { e.t.c } \tag{18}
\end{equation*}
$$

## 4. RESULTS

In this section we present the results for the effective interactions for the $s d$ and $p$ shells using the method of sect.3. The results for the sd shell have been obtained with the choice of 1.7 fm for the oscillator parameter ( $\hbar \omega=14.42 \mathrm{Mev}$ ) and using for the two body interaction V in (1) the "Sussex" matrix elements of Elliot et al(1968). At first, we have to determine the quantities $R_{n}$ defined in (12). As (12) shows, the exact determination of these quantities involves the inversion of matrix $\mathbf{Z}$. However, the dimension of $\mathbf{Z}$, as for example in the $(\mathrm{J}, \mathrm{T})=(2,1)$ state of $\mathrm{A}=18$ with dimension 17880 , exceeds in several cases the capabilities of our computing system. Hence, we determine the quantities $R_{n}$ approximately by summing the first fifty terms of expansion (13) in all cases where matrix inversion is not possible.

The next step contains the calculation of the operators $F_{n}$ defined by (18) and the convergence study of expansion (17). The results are shown in table 1 for ${ }^{17} \mathrm{O}$ and the $\mathrm{J}=0$ state of ${ }^{18} \mathrm{O}$ and contain contributions up to $F_{6}$ term. In table 1 the results for ${ }^{17} \mathrm{O}$ include the zero-order contribution and give the energies of ${ }^{17} \mathrm{O}$ states relative to ${ }^{16} \mathrm{O}$. The energy of ${ }^{16} \mathrm{O}$ is also included in table 1 calculated by considering only the contribution of $F_{0}$ term. As it is clear from table 1 , for the ${ }^{17} \mathrm{O}$ case there is a rapid convergence of expansion (17). Hence, the energy of ${ }^{17} \mathrm{O}$ states is almost completely attributed by the first two terms $F_{\mathrm{o}}$ and $F_{1}$. In the ${ }^{18} \mathrm{O}$ case the convergence of expansion (17) is much slower, although such convergence clearly exists. The largest difference between the results of columns 5 and 6 of table 1 , appears in the $<(5 / 2)^{2} ; J=0\left|V_{\text {eff }}\right|(3 / 2)^{2} ; J=0>$ matrix element and represents only $4 \%$. For this reason we consider only up to $F_{0}$ terms in the determination of the effective interaction.

It is well known (Brandow 1967) that due to the inclusion of folded graphs the operator $H_{\text {eff }}$ defined by

$$
\begin{equation*}
H_{e f f}=H_{0}+V_{e f f} \tag{19}
\end{equation*}
$$

is not Hermitian. Following the procedure described by Brandow (1968) and Des Cloizeaux (1960), one can find a symmetric $H_{\text {eff }}$ having the same eigenvalues in the space of two-particle states with the original non-symmetric $H_{\text {aff }}$ The two-body matrix elements of the symmetric operator $H_{\text {off }}$ for all ( $\mathbf{J}, \mathrm{T}$ ) states of the $\mathrm{A}=18$ system (Skouras and Varvitsiotis 1990a) are found
to be in remarkable agreement with Kuo's matrix elements (Kuo 1967) and with those obtained by Preedom and Wildenthal (1972). This agreement shows that our matrix elements obtained without the use of any adjustable parameters, may be suitable for shell model calculations in the beginning of the sd shell. A first test was done by using our interaction to determine the spectra of the $A=19$ and $A=20$ nuclei. The results of this shell model calculation are shown in figures 3 and 4 and are in reasonable agreement with experiment (Ajzenberg-Selove 1983).

As mentioned in the beginning of this paper, we also use our method to determine the effective three-body interaction in the space of $0 \hbar \omega+2 \hbar \omega$ excitations. In the case of 0 p shell the dimensions of the energy matrices are not extremely large (the biggest dimension is 1868). Hence, the quantities $R_{n}$ are determined directly by matrix inversion. We use two types of two-body interactions. The first is the "Sussex" interaction of Elliot et al (1968) while the other is a G-matrix (Skouras and Varvitsiotis 1990b) derived from the Reid soft-core potential (Reid 1968). We distinguish the results obtained using these two interactions by $V_{\text {eff }}^{(\mathcal{S})}$ and $V_{o f}^{(R)} 7$ respectively. In table 2 we present the results for the matrix elements of the three-body effective interaction. In this table there are several three-body matrix elements with magnitude between 0.5 and 1 Mev . This notice suggests that three-body forces will have an important effect on the spectra of nuclei with several valence particles in the 0p shell. Actually, in the calculation of the spectra of the 0 p shell nuclei we find (Skouras and Varvitsiotis 1990b) the three-body interaction to produce significant differences in the excitation energies. These differences are of the order of several Mev near the end of the 0 p shell. We also observe that generally, the three-body effects bring the calculated spectra to closer agreement with experiment. This behaviour is clear in fig. 5 where the spectrum of ${ }^{10} \mathrm{~B}$ is shown. The introduction of the three-body component of $V_{\mathrm{of} f}$ pushes up for example the $(1,0)$ state from 0.13 Mev to 2.44 Mev and better agreement with experiment is obtained.

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## Table 1

Convergence oi $V$., , in terms of additional folded graphs

| ME | Number of folds ${ }^{\top}$ |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | 0 | 1 | 2 | 3 | 4 | 5 | 6 |
| 160 | .95.02 |  |  |  |  |  |  |
| 170 |  |  |  |  |  |  |  |
| 5/2 | $-1.448$ | -1.431 | -1.432 | -1.432 | -1.432 | -1.432 | -1.432 |
| $3 / 2$ | 4.508 | 4.543 | 4.542 | 4.542 | 4.542 | 4.542 | 4.542 |
| 1/2 | -1.895 | -1.783 | -1.785 | -1.787 | -1.786 | -1.786 | -1.786 |
| 180 |  |  |  |  |  |  |  |
| 5.5 | -2.424 | -2.132 | -2.297 | -2.192 | -260 | -2.215 | -2.246 |
| 5.3 | -2.119 | -2.913 | -2.381 | -2733 | . 2501 | -2.657 | -2549 |
| 5.1 | -1.487 | -1.476 | -1.419 | -1.467 | -1.434 | -1.456 | -1.440 |
| 3.5 | -2.971 | -3.040 | -3.030 | -3.029 | -3.031 | -3.030 | -3.031 |
| 3.3 | -1.378 | -1.158 | -1.187 | -1.191 | -1.184 | -1.189 | -1.185 |
| 3.1 | -1.088 | -1.035 | -1.039 | -1.041 | -1.039 | -1.040 | -1.040 |
| 1.5 | -1.366 | -1.278 | -1.302 | -1.288 | -1.298 | -1.291 | -1.296 |
| 1.3 | -i. 168 | -1.157 | -1.098 | -1.149 | -1.113 | -1.138 | -1.120 |
| 1.1 | -1.457 | -1.545 | -1.541 | -1.544 | -1.540 | -1.543 | -1.541 |

${ }^{+}$Each coiumn oi resuiks represenes the cocal resultes up to thas orcer. For ${ }^{160}$ and ${ }^{7} \mathrm{O}$ o the comanbution of $H$, has been adied in the colvina oi $F$.

Table 2
List of 3-bociy matrix eiements

| ME | $V^{(s)}$ | $V^{(R)}$ | ME | $V^{(s)}$ | $V\left(\begin{array}{l}\text { (1) }\end{array}\right.$ | ME | $V(\$)$ | $V_{1, f}^{(R)}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1,1 | 0.518 | 0.624 | 6,8 | 0.219 | 0.155 | 12.12 | 0.307 | 0.213 |
| 1.2 | 0.054 | 0.129 | 6.9 | 0.208 | 0.101 | 12.13 | 0.085 | 0.026 |
| 1.3 | -0.418 | -0.268 | 6,10 | 0.489 | 0.385 | 12.14 | -0.063 | -0.030 |
| 1,4 | -0.464 | -0.264 | 7,7 | 0.128 | 0.194 | 13,13 | 0.032 | 0.121 |
| 1.5 | $-0.715$ | $-0.172$ | 7.8 | -0.070 | -0.076 | 13,14 | 0.726 | 0.320 |
| 2.2 | -0.305 | -0.387 | 7,9 | 0.278 | 0.300 | 14,14 | 0.239 | 0.464 |
| 2.3 | -0.139 | -0.385 | 7,10 | . 0.266 | -0.137 | 15,15 | -0.187 | -0.064 |
| 2.4 | -0.143 | -0.105 | 8.8 | 0.071 | 0.050 | 15,16 | 0.167 | 0.113 |
| 2.5 | 0.296 | 0.406 | 8.9 | -0.008 | 0.045 | 16,16 | -0.371 | -0.147 |
| 3,3 | -0.646 | -0.744 | 8,10 | -0.163 | -0.021 | 17,17 | 0.363 | 0.625 |
| 3,4 | $-0.017$ | -0.086 | 9,9 | 0.277 | 0.254 | 18,18 | - -0.060 | 0.032 |
| 3.5 | 0.364 | 0.568 | 9,10 | -0:131 | $-0.023$ | 18,19 | 0.023 | 0.019 |
| 4,4 | 0.895 | 0.916 | 10.10 | 0.273 | 0.309 | 18,20 | 0.175 | 0.052 |
| 4.5 | -0.296 | -0.101 | 11.11 | -0.001 | 0.012 | 19,19 | 0.131 | 0.119 |
| 5,5 | -0.839 | -0.719 | 11.12 | $-0.083$ | -0.043 | 19,20 | -0.209 | -0.087 |
| 6.6 | 0.153 | 0.148 | 11.13 | 0.120 | 0.070 | 20,20 | 0.214 | 0.148 |
| 6.7 | 0.054 | 0.069 | 11.14 | 0.341 | 0.224 | 21.21 | 0.063 | 0.075 |



Fig.3. Energy spectra of the $A=19$ nuclei


Fig.4. Energy spectra of the $A=20$ nuclei


Calc.
${ }^{\circ} \mathcal{B}$
Fig.5. Energy spectrum of ${ }^{10_{B}}$
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