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Spin–tensor analysis of a new empirical shell-model interaction for the 1s–0d shell nuclei

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Abstract. New empirical two-body matrix elements derived from the spectra of 1s–0d shell nuclei are compared with previous empirical results and with the G-matrix elements obtained from the Reid soft-core and Paris potentials. A spin–tensor decomposition of the matrix elements is made and comparisons are presented for the separated central, tensor, spin–orbit and antisymmetric spin–orbit components.

The derivation of the residual two-body interaction for the shell model from the free nucleon–nucleon interaction remains one of the most fundamental problems in nuclear physics. Considerable progress has been made in calculating the finite-nucleus reaction, or G, matrix. However, the renormalisation of the bare G matrix, which is required by the inevitable use of a truncated shell-model space, involves many uncertainties [1]. In the present work we compare theoretical effective two-body matrix elements, determined in calculations which start with the properties of the nucleon–nucleon interaction, with the properties of empirical matrix elements which are determined from fits of many-body shell-model eigenvalues to binding-energy data in the sd shell. This study is motivated in part by the need to determine empirical effective interactions for heavier mass regions which are as successful as those presently determined for the 1s–0d shell. We hope that by thoroughly analysing the empirical sd-shell interactions in the context of theoretical values, the essential features of the empirical results can be translated to the larger shell-model spaces typically necessary for heavier nuclei.

The important physical aspects of the residual interaction can be more readily discerned by transforming the representation of the two-body matrix elements from the j–j coupling scheme, which is the representation generally needed for shell-model calculations, to the L–S coupling scheme, and following this by a spin–tensor decomposition of these elements. The essence of the spin–tensor decomposition method employed has been described by Kirson [2] and Yoro [3]. The two-body interaction can be written in the form

$$V = \sum V_k = \sum U^k \cdot S^k \tag{1}$$

where the operators U and S are irreducible tensors of rank k in space and spin coordinates, respectively. By combining the j–j to L–S and spin–tensor decompositions,

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one can relate the L–S coupled matrix elements of V_k to the j–j coupled matrix elements:

$$\langle abLSJT|V_k|cdL'S'JT\rangle = (2k+1)\begin{Bmatrix} L & S & J \\ S' & L' & k \end{Bmatrix}\sum_{J'}(-1)^{J'+k}(2J'+1)\begin{Bmatrix} L & S & J' \\ S' & L' & k \end{Bmatrix} \times\langle abLSJ'T|V|cdL'S'J'T\rangle \tag{2}$$

where

$$\langle abLSJ'T|V|cdL'S'J'T\rangle = [(1+\delta_{ab})(1+\delta_{cd})]^{-1/2}\sum_{j_{a'},j_{b'},j_{c'},j_{d'}}[(2j_{a'}+1)(2j_{b'}+1)(2j_{c'}+1)(2j_{d'}+1)]^{1/2} \times\begin{Bmatrix} l_{a'} & \frac{1}{2} & j_{a'} \\ l_{b'} & \frac{1}{2} & j_{b'} \\ L & S & J' \end{Bmatrix}\begin{Bmatrix} l_{c'} & \frac{1}{2} & j_{c'} \\ l_{d'} & \frac{1}{2} & j_{d'} \\ L' & S' & J' \end{Bmatrix} \times[(1+\delta_{\alpha'\beta'})(1+\delta_{\gamma'\delta'})]^{1/2}\langle\alpha'\beta'J'T|V|\gamma'\delta'J'T\rangle \tag{3}$$

where $\alpha=(n_a, l_a, j_a)$ and $a=(n_a, l_a)$, etc. The two-body matrix elements are normalised and antisymmetrised. The nomenclature we use in this study for the separated components is explained in table 1.

We concentrate in this study on effective two-body matrix elements for the 1s–0d model space. The empirical effective matrix elements we analyse are the latest results of Wildenthal (W) [4], together with the earlier Chung–Wildenthal 'particle' (CWP), Chung–Wildenthal 'hole' (CWH) [5, 6] and Preedom–Wildenthal (PW) [7] results. The W matrix elements incorporate a mass dependence of $(A/18)^{-0.3}$ and our comparisons are made for $A=18$. These empirical values are compared with the calculated bare (BK) and renormalised (RK) G-matrix elements of Kuo which are based on the Hamada–Johnston nucleon–nucleon potential [8], and with the more recent results of Shurpin, Kuo and Strottman (SKS) for the renormalised G-matrix elements based on the Reid soft-core (SKSR) and the Paris (SKSP) nucleon–nucleon potentials [9]. The renormalised Kuo calculations include only the lowest second-order corrections, whereas the SKS calculations use the folded-diagram technique and include up to fourth-order correction terms. (We use the 'C4' matrix elements of [9] and treat the non-hermiticity by averaging the matrix elements of type V_{ik} and V_{ki}.)

In the comparisons it should be remembered that the RK matrix elements were used as the starting parameters in the fitting procedure in which the empirical matrix elements were

Table 1. Nomenclature for the separated interaction components.

k	S	S'	Spin–tensor components
0	0	0	C = central
	1	1	
1	0	1	ALS = antisymmetric spin–orbit
	1	0	
	1	1	LS = spin–orbit
2	1	1	T = tensor

obtained. In the studies which determined the PW and CW matrix elements only about ten linear combinations of parameters were well determined from the fits to experimental binding energies, whereas in the determination of the W interaction in which many more energies were considered, 47 parameters were allowed to vary. This is the reason that, as shown in the comparison, the PW and CW matrix elements which were not well determined remain close to the RK values. The W matrix elements are considerably more independent of their origins.

In order to get a completely independent set, as well as to obtain an estimate of the errors in the empirical matrix elements, we have repeated the fit based on the 440 binding and excitation energy data which was used to obtain the W interaction [4], and allowed all 63 two-body matrix elements and three single-particle matrix elements to vary. We will refer to this set as the Brown–Richter–Wildenthal (BRW) matrix elements. The values of the W and BRW matrix elements ae essentially the same.

Our results are illustrated by the comparisons of the various matrix elements for the central, tensor, antisymmetric spin–orbit and spin–orbit components of the interaction, shown respectively in figures 1–4. The matrix elements in each case are labelled by numbers corresponding to the quantum numbers in table 2.

Figure 1, which displays the results for the central components of the interaction, is divided into three panels. In each of the panels the BRW matrix elements are shown by

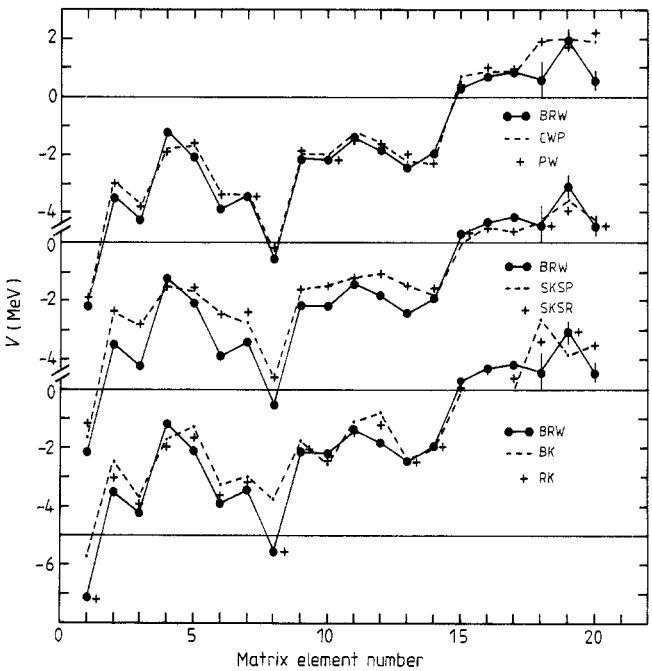

Figure 1. Matrix elements for the central interaction. The number on the x axis refers to the label for the quantum numbers for the matrix elements given in table 2. In the top panel the empirical Brown–Richter–Wildenthal (BRW) matrix elements (with error bars) are compared with the empirical Chung–Wildenthal 'particle' (CWP) matrix elements and Preedom–Wildenthal (PW) matrix elements. In the middle panel the BRW matrix elements are compared with the renormalised G-matrix elements calculated by Shurpin, Kuo and Strottman from the Paris (SKSP) potential and Reid soft-core (SKSR) potential. In the bottom panel the BRW matrix elements are compared with the bare Kuo (BK) and renormalised Kuo (RK) G-matrix elements based on the Hamada–Johnston potential.

Table 2. Quantum numbers of the $L-S$ coupled matrix elements.

										Number[a]			
l_a	l_b	l_c	l_d	L	L'	S	S'	J^b	T	C	ALS	LS	T
2	2	2	2	0	0	1	1	1	0	1	—	—	—
2	2	2	2	2	0	1	1	1	0	—	—	—	1
2	2	2	2	2	2	1	1	3	0	2	—	1	2
2	2	2	2	4	2	1	1	3	0	—	—	—	3
2	2	2	2	4	4	1	1	5	0	3	—	2	4
2	2	2	0	0	2	1	1	1	0	—	—	—	5
2	2	2	0	2	2	1	1	3	0	4	—	3	6
2	2	2	0	4	2	1	1	3	0	—	—	—	7
2	2	0	0	0	0	1	1	1	0	5	—	—	—
2	2	0	0	2	0	1	1	1	0	—	—	—	8
2	0	2	0	2	2	1	1	3	0	6	—	4	9
2	0	0	0	2	0	1	1	1	0	—	—	—	10
0	0	0	0	0	0	1	1	1	0	7	—	—	—
2	2	2	2	1	0	0	1	1	0	—	1	—	—
2	2	2	2	3	2	0	1	3	0	—	2	—	—
2	2	2	0	1	2	0	1	1	0	—	3	—	—
2	2	2	0	3	2	0	1	3	0	—	4	—	—
2	2	0	0	1	0	0	1	1	0	—	5	—	—
2	2	2	2	2	1	1	0	1	0	—	6	—	—
2	2	2	2	4	3	1	0	3	0	—	7	—	—
2	2	2	0	2	2	1	0	2	0	—	8	—	—
2	0	2	0	2	2	1	0	2	0	—	9	—	—
2	2	2	2	0	0	0	0	0	1	8	—	—	—
2	2	2	2	2	2	0	0	2	1	9	—	—	—
2	2	2	2	4	4	0	0	4	1	10	—	—	—
2	2	2	0	2	2	0	0	2	1	11	—	—	—
2	2	0	0	0	0	0	0	0	1	12	—	—	—
2	0	2	0	2	2	0	0	2	1	13	—	—	—
0	0	0	0	0	0	0	0	0	1	14	—	—	—
2	2	2	2	1	1	1	1	2	1	15	—	5	11
2	2	2	2	3	1	1	1	2	1	—	—	—	12
2	2	2	2	3	3	1	1	4	1	16	—	6	13
2	2	2	0	1	2	1	1	2	1	—	—	7	14
2	2	2	0	3	2	1	1	3	1	—	—	8	15
2	0	2	0	2	2	1	1	3	1	17	—	9	16
2	2	2	2	2	1	0	1	2	1	—	10	—	—
2	2	2	2	4	3	0	1	4	1	—	11	—	—
2	2	2	0	2	2	0	1	2	1	—	12	—	—
2	2	2	2	1	0	1	0	0	1	—	13	—	—
2	2	2	2	3	2	1	0	2	1	—	14	—	—
2	2	2	0	1	2	1	0	2	1	—	15	—	—
2	2	2	0	3	2	1	0	2	1	—	16	—	—
2	2	0	0	1	0	1	0	0	1	—	17	—	—
2	0	2	0	2	2	1	0	2	1	—	18	—	—
2	2	2	2	1	1	0	0	1	0	18	—	—	—
2	2	2	2	3	3	0	0	3	0	19	—	—	—
2	0	2	0	2	2	0	0	2	0	20	—	—	—

[a] These are the numbers used to label the matrix elements in figures 1–4.

[b] In cases for which there is more than one possible J value for a given set of quantum numbers, the matrix element corresponding to the largest J value is used for the comparisons. The matrix elements for other J values are trivially related to each other by the relative values of the first $6-j$ symbol in equation (2).

circles with error bars and are connected by a full line. BRW is compared in the top panel with the PW and CWP matrix elements, in the middle panel with the SKS matrix elements obtained from the Reid soft-core potential (SKSR) and the Paris potential (SKSP) and in the bottom panel with the renormalised (RK) and bare (BK) matrix elements of Kuo.

From this comparison of the central matrix elements we see that all empirical values are well determined except for those with $(S, T)=(0, 0)$ (numbers 18, 19 and 20). The latter have relatively large error bars. The differences between the empirical BRW, PW and CWP matrix elements are surprisingly small in view of the overall superiority of BRW over PW and CWP in reproducing sd-shell binding energies and excitation energies and in view of the significantly greater ranges of data used at each stage of the empirical studies.

The differences between the G-matrix elements obtained from the Reid (SKSR) and Paris (SKSP) potentials are small compared with the differences between the original Kuo (RK) and the new (SKSR) results based on the Reid potential. In the Kuo calculation the renormalisation corrections are important in improving agreement with BRW. The renormalisation terms (the bare values are not shown) are not as large in the more complete SKS calculation as in the earlier Kuo results. However, compared with RK the SKS results are in worse agreement with BRW. The repulsive $(S, T)=(0, 0)$ and $(1, 1)$ SKS matrix elements are in reasonable agreement with BRW, but the important attractive $(S, T)=(0, 1)$ and $(1, 0)$ SKS matrix elements are too weak when compared with BRW.

In figure 2 the tensor components of the various two-body interactions are compared in the same scheme. It will be noted that in the upper panel two of the $T=0$ matrix elements (numbers 3 and 10) are rather poorly determined, even taking into account the magnitude of the uncertainties reflected in the BRW error bars. There is generally greater fluctuation

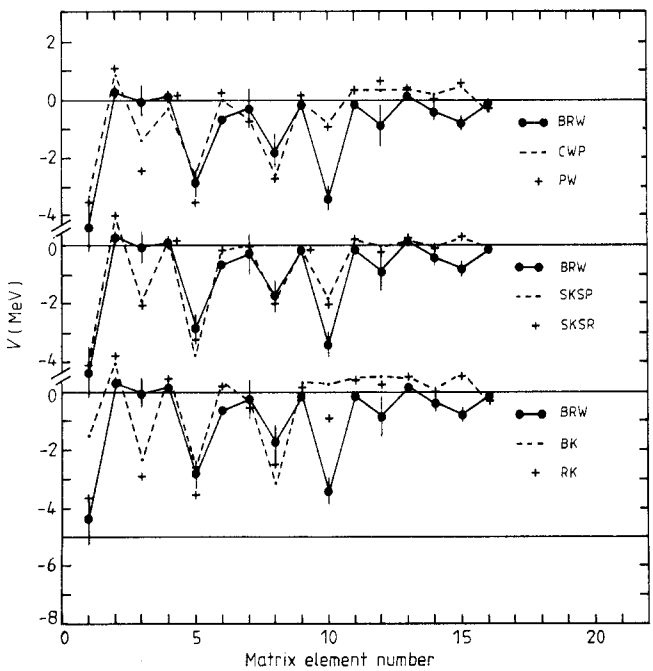

Figure 2. Matrix elements for the tensor interaction. The conventions are the same as in figure 1.

among the empirical values than for the central components. In the middle panel there is reasonable agreement between the SKS and BRW values, with the exception of the two poorly determined $T=0$ matrix elements noted above and some of the quite small $T=1$ matrix elements (numbers 11–17).

It is interesting to note that although the Reid and Paris potentials differ most in the tensor force [9], the tensor components of the effective interactions derived from the potentials are virtually identical. In the bottom panel the effect of renormalisation on the bare Kuo values is generally small, but where it is significant it improves the agreement with the BRW values in some instances (e.g. matrix elements 1, 8 and 10) but has the opposite effect for others (e.g. matrix elements 3 and 5).

In figure 3 the various antisymmetric spin–orbit (ALS) components are compared. In the top panel we see that there is considerable scatter among the values of the $T=1$ components of the three empirical interactions which cannot be explained in terms of the uncertainties resulting from the fitting procedure. There is also considerable uncertainty in the $T=0$ values in view of the sizes of the error bar relative to the rather small ALS values. In the middle panel it is noteworthy that the SKS values for the Reid and Paris potentials are again very similar and the agreement with the BRW values is generally not very good.

In the lower panel the values corresponding to the bare G matrix should be zero because the free nucleon–nucleon interaction conserves parity and contains no ALS component as a consequence. The small values found for the Kuo bare matrix elements are probably due to numerical inaccuracies in calculating the G matrix. Renormalisation introduces a small but significant ALS component into the effective interaction. This example emphasises the fundamental difference between the free-nucleon interaction and the effective interaction in a many-body system. The effect of the renormalisation

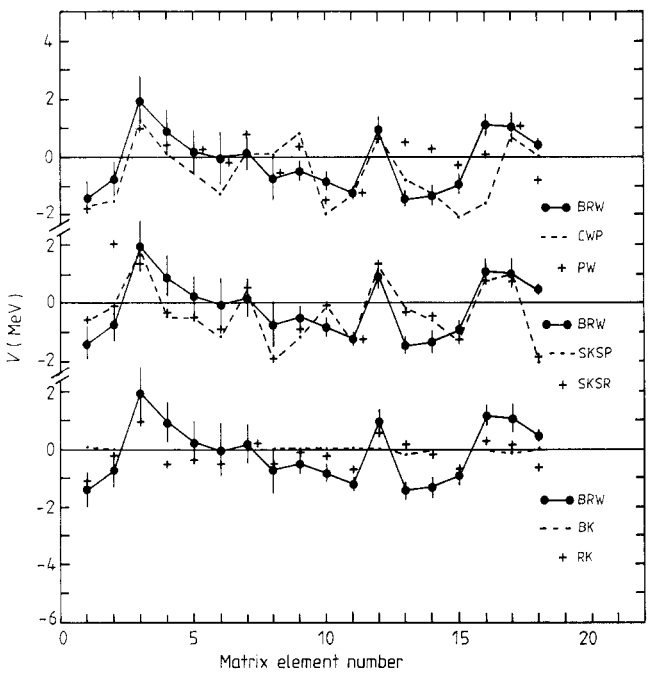

Figure 3. Matrix elements for the antisymmetric spin–orbit interaction. The conventions are the same as in figure 1.

is generally to produce better agreement with the BRW values. Most of the $T=1$ renormalised values (numbers 10–18) are too small compared with BRW.

In figure 4 the spin–orbit components of the matrix elements are displayed and compared with each other. In the upper panel we see that the spin–orbit components for the empirical interactions are relatively well determined in the $T=1$ cases (numbers 5–9) while there is a noticeable variation among the $T=0$ values (numbers 1–4). The SKS values for the Reid and Paris potentials are again quite similar, but in most cases differ significantly from the BRW values. The effect of renormalisation on the bare Kuo G-matrix values can be seen to be almost negligible in the lower panel. Except for matrix elements 3, 4 and 7, the agreement with the BRW values is quite reasonable.

It has been seen from the comparisons of the SKSP and SKSR matrix elements that the various spin–tensor components of the Paris potential generally agree closely with those of the Reid soft-core potential. The Paris potential is theoretically derived from meson theory (with the exception of the short-range part, $r < 0.8$ fm, which is constructed to fit the N–N scattering phase shifts), whereas the Reid soft-core potential is purely phenomenological. Our results support the findings of Shurpin *et al* [9] that there is little to choose between these two potentials in the context of their resultant two-body matrix elements.

It is also evident that effective interactions based on these potentials differ significantly from the empirically determined interactions like the BRW interaction and hence cannot be expected to yield energy spectra of the same quality. The spin–tensor analysis has also shown in which cases renormalisation of the bare Kuo G-matrix elements is significant, and that the renormalisation generally produces better agreement with the BRW interaction. From comparisons such as the above we hope to obtain an improved method of calculating effective interactions to be used in nuclear-structure calculations.

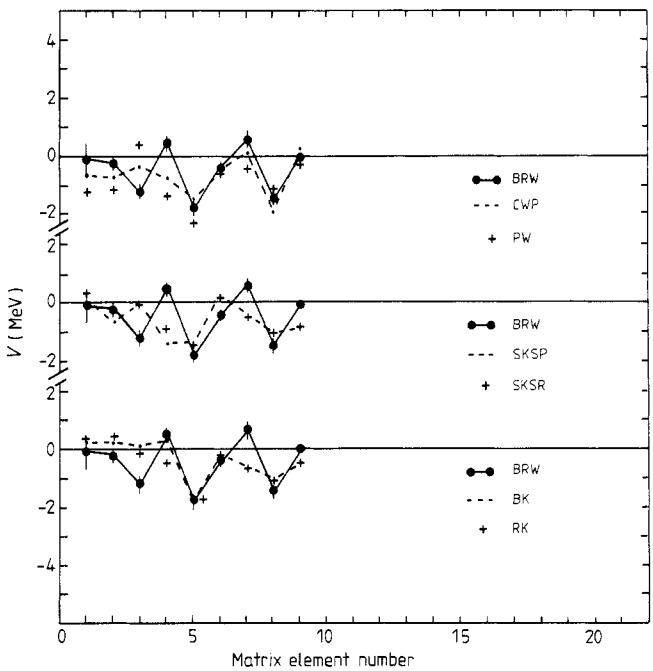

Figure 4. Matrix elements for the spin–orbit interaction. The conventions are the same as in figure 1.

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