Three-body interactions in the $1f_{7/2}$ shell?

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Abstract. It is shown that the three-body forces in the $1f_{7/2}$ shell, for which recently evidence was claimed on the basis of spectroscopic properties of the Ca isotopes and $N = 28$ isotones, can be most naturally explained as an effective interaction due to excluded higher-lying shells, in particular the $2p_{3/2}$ orbit.

Three-body interactions play an important role in nuclear many-body theories. They may be part of the “bare” interaction. They may also arise from the renormalization of the “bare” two-body interaction, yielding the effective interaction which may be used in the shell model. This is obtained by replacing the effects of admixtures of highly excited configurations by a modification of the “bare” interaction.

On the other hand, shell-model calculations, during the last 60 years, have been successfully using almost exclusively two-body effective interactions. It should be realized, however, that three-body interactions may contribute to single-nucleon energies which are usually taken from experiment. They may well include contributions of interactions of two core nucleons and a valence nucleon.

Also matrix elements of two-body interactions which are used in shell-model calculations are usually determined from experiment. They may include contributions due to the interaction of a core nucleon with two valence nucleons. Even if three-body interactions are weak, the large number of core nucleons makes their possible contribution significant. Still, no explicit evidence for effective three-body interactions between valence nucleons has been observed.

This feature is clearly seen in spectra of several $j^n$ configurations of identical nucleons. Experimentally observed level spacings in these proton or neutron configurations are well reproduced by the use of two-body effective interactions with rather pure shell-model wave functions. Only a few levels seem to be perturbed.

In lighter nuclei, the $1f_{7/2}$ shell of neutrons is expected in calcium nuclei with $Z = 20$ and neutron number $N$ from 21 to 28. The $1f_{7/2}$ proton shell should be found in nuclei with $N = 28$ and $Z = 21–28$. Shell-model calculations assuming $1f_{7/2}$ configurations were carried out [1, 2, 3, 4]. It turned out that the situation is rather complicated. All levels of these configurations are observed in experiment. Ground states of nuclei (binding energies) seem to agree with predictions based on two-body effective interactions. Spacings of many excited states, however, strongly deviate from such predictions.

These deviations were interpreted many years ago as due to mixing of $(1f_{7/2})^n$ states with states of configurations which are rather close in energy, in particular, states in which one $1f_{7/2}$ nucleon is raised into the $2p_{3/2}$ orbit. The position of the neutron $2p_{3/2}$ in $^{44}$Ca is only 2 MeV above the $7/2^-$ ground state. The position of the proton $2p_{3/2}$ state is about 3 MeV above the...
Additional quantum numbers which may be necessary to characterize the states. The author claims to show the “manifestation of three-body forces in shell-model space which is too restricted. Recently, however, a paper was published [15], in which arise from interactions with close configurations. In other words, they are due to a choice of functions in the functions in terms of coefficients of fractional parentage (c.f.p.) [17]. Every antisymmetric wave function in the shell which includes two-body as well as three-body ones [12, 13].

In a long and very detailed paper [14], Poves and Zuker considered not only the $1f_{7/2}$ states of identical nucleons. They analyzed the complete $1f_{7/2}$ shell of protons and neutrons, from $^{40}$Ca to $^{56}$Ni. They checked the agreement obtained by using various interactions suggested by many-body theory and modified them to obtain better agreement with experiment. They considered perturbations from nearby configurations due to two-body interactions. This way, they obtained the effective interactions in the $1f_{7/2}$ shell which includes two-body as well as three-body interactions. The agreement of results obtained by using the effective interaction which they derived for the $1f_{7/2}$ shell, with experiment was good.

The results of ref. [14] clearly indicated that effective three-body interactions in $1f_{7/2}$ shell arise from interactions with close configurations. In other words, they are due to a choice of shell-model space which is too restricted. Recently, however, a paper was published [15], in which the author claims to show the “manifestation of three-body forces in $f_{7/2}$-nuclei”. Although the report by Poves and Zuker is quoted in ref. [15], no mention is made of the fact that in ref. [14] it was shown how configuration mixing leads to three-body interactions. In ref. [14] the latter were actually used for calculating successfully energy levels. The author of ref. [15] contrasts the two approaches and states that “the three-body effective interaction has a somewhat different manifestation which can be experimentally identified.”

We do not intend to consider the $1f_{7/2}$ shell in detail. Our aim was to reiterate the fact that configuration mixing, due to two-body interactions leads to three-body effective interactions [16]. We were unaware of ref. [14] and hence, we used earlier calculations, in which such mixings were considered [5, 6, 7, 8]. We took non-diagonal matrix elements of the two-body interactions, obtained in these references and computed the resulting three-body interactions. The results show that the three-body interaction obtained by Volya [15] is rather similar to those following from configuration mixing.

Using the non-diagonal matrix elements of the two-body interaction from refs. [5, 6, 7, 8], we calculate matrix elements of the three-body effective interaction. These matrix elements completely define the three-body interaction. We make use of the expansion of $(1f_{7/2})^n$ wave functions in terms of coefficients of fractional parentage (c.f.p.) [17]. Every antisymmetric wave function in the $j^n$ configuration may be expanded as

\[
\Psi(j^n aJ) = \sum_{a_0 J_0} [j^{n-1}(a_0 J_0)jJ] j^n aJ \Psi(j^{n-1}(a_0 J_0)j_J J),
\]

where $[j^{n-1}(a_0 J_0)jJ] j^n aJ$ are coefficients of fractional parentage (c.f.p.) and $a$, $a_0$ are additional quantum numbers which may be necessary to characterize the states. The $j^{n-1}$ wave functions on the r.h.s. of (1) are antisymmetric in $n-1$ particles to which $j_n$ of the $n$th particle is coupled to yield the total $J$. Each of them may not be fully antisymmetric but their linear combination (1) is.

The c.f.p. are very convenient for calculating matrix elements of various operators. To calculate matrix elements of two-body or three-body interactions, use is made of the fact that
both states are fully antisymmetric and the interaction is symmetric in all \( n \) particles. Hence, the contribution of each of the \( n!/k!(n-k)! \) \( k = 1, 2, \ldots < n \) terms of the \( k \)-body interaction to the matrix element is the same. Thus, we obtain

\[
\langle j^n aJ | \hat{V} | j^n bJ \rangle = \frac{n!}{k!(n-k)!} \langle j^n aJ | \hat{V}_{12, k} | j^n bJ \rangle
\]

\[
= \frac{n!}{k!(n-k)!} \sum_{a_0 b_0 j_0} \langle j^{n-1} a_0 J_0 | \hat{V}_{12, k} | j^{n-1} b_0 J_0 \rangle
\]

\[
\times \langle j^{n-1} (a_0 J_0) j J | j^n aJ \rangle \langle j^{n-1} (b_0 J_0) j J | j^n bJ \rangle
\]

\[
= \frac{n}{n-k} \sum_{a_0 b_0 j_0} \langle j^{n-1} a_0 J_0 | \hat{V} | j^{n-1} b_0 J_0 \rangle
\]

\[
\times \langle j^{n-1} (a_0 J_0) j J | j^n aJ \rangle \langle j^{n-1} (b_0 J_0) j J | j^n bJ \rangle.
\]

(2)

This procedure may be further applied until the \( j^3 \) or \( j^2 \) configuration is reached.

We first consider the \( j^2 \) configuration and the effect of mixing with an excited \( jj' \) configuration. The contribution to the energy in second-order perturbation theory is given by

\[
\sum_{j'} \frac{|\langle j^2 J_0 | \hat{V} | jj' J_0 \rangle|^2}{E(j^2 J_0) - E(jj' J_0)}
\]

(3)

where the matrix elements of the two-body interaction \( \hat{V} \) are taken between antisymmetric and normalized states \( \langle j^2 J_0 \rangle \) and \( | jj' J_0 \rangle \). The expression (3) is the matrix element of an additional two-body interaction in the \( | j^2 J_0 \rangle \) state.

To obtain matrix elements of the three-body interaction, the \( j^3 \) configuration should be considered. Antisymmetrized and normalized states of the excited configuration may be obtained as

\[
\Psi(j^3(J_1)j_1\dot{J}) = \frac{1}{\sqrt{3}}(\Psi(j^2(J_1)j_2\dot{J}) - \Psi(j^2(J_1)j_3\dot{J}) - \Psi(j^2(J_1)j_3\dot{J})).
\]

(4)

In calculating the matrix element between the state (4) and the state \( \Psi(j^3 J) \), the two-body interaction \( \hat{V}_{12} + \hat{V}_{13} + \hat{V}_{23} \) may be replaced by \( 3\hat{V}_{12} \). Using c.f.p. we obtain for it the expression

\[
-\sqrt{3} \sum_{J_0} \langle j^2(J_0) j J | j^3 aJ \rangle \langle j^2(J_0) j_3 J | \hat{V}_{12} j^2(J_1) j_1' J \rangle
\]

\[
-\sqrt{3} \sum_{J_0} \langle j^2(J_0) j J | j^3 aJ \rangle \langle j^2(J_0) j_3 J | \hat{V}_{12} j^2(J_1) j_2' J \rangle.
\]

(5)

To evaluate the second term in (5), we use a change of coupling transformation ((10.11) in ref. [17]) and obtain for the excited state the expression

\[
| j_1 j_3 (J_1) j_2' J \rangle = \sum_{J_2} (-1)^{j+j'+J_1+J_2} \hat{J}_1 \hat{J}_2 \left\{ \begin{array}{c} j \\ j' \\ J_1 \end{array} \right\} | j_1 j_2' (J_2) j_3 J \rangle,
\]

(6)

with \( \hat{J} = \sqrt{2J+1} \). Using (6), the integration over \( j_3 \) may be carried out. It yields the only term with non-vanishing contribution which has \( J_2 = J_0 \). The second term in (5) is thus equal to

\[
-\sqrt{3}(-1)^{j+j'+J_1} \sum_{J_0} \hat{J}_0 \hat{J}_1 | j^2(J_0) j J \rangle \langle j^3 aJ \rangle \left\{ \begin{array}{c} j \\ j' \\ J_0 \end{array} \right\} \langle j_1 j_2 J_0 | \hat{V}_{12} | j_1 j_2' J_0 \rangle.
\]

(7)
where the state is the same for all states of the \( j \) we make an assumption on the energy denominator in (10). We make the approximation that it \( \epsilon \) using identities of Racah coefficients. We obtain, due to \( j \) in the

The first term in (5) yields a similar result

\[
\sqrt{3}(-1)^{j+j'+J_1} \sum_{J_0} \hat{J}_0 \hat{J}_1 [j^2(J_0) j J] j^3 a J \left\{ \begin{array}{ccc}
 j & J \cr j' & J_1 \cr j & j \end{array} \right\} \langle j_1 j_2 J_0 | \hat{V}_{12} | j j' J_0 \rangle. \tag{8}
\]

The two expressions may be combined yielding the result

\[
-\sqrt{6}(-1)^{j+j'+J_1} \sum_{J_0 J'_0} \hat{J}_0 \hat{J}_1 [j^2(J_0) j J] j^3 a J \left\{ \begin{array}{ccc}
 j & J_0 \cr j' & J_1 \cr j & j \end{array} \right\} \langle j_1 j_2 J_0 | \hat{V}_{12} | j j' J_0 \rangle,
\]

where the state \( | j j' J_0 \rangle \), as well as \( | j^2 J_0 \rangle \), is antisymmetric and normalized.

To obtain the contribution of second-order perturbation, (9) should be multiplied by a similar summation in which \( J_0 \) is replaced by \( J'_0 \). The result is thus equal to

\[
6 \sum_{J_0 J'_0} (2J_1 + 1) \sum_{J_0 J'_0} \hat{J}_0 \hat{J}_1 [j^2(J_0) j J] j^3 a J \left\{ \begin{array}{ccc}
 j & J_0 \cr j' & J_1 \cr j & j \end{array} \right\} \langle j_1 j_2 J_0 | \hat{V}_{12} | j j' J_0 \rangle \frac{\langle \hat{J}_1 | V_{12} | j^2 J_0 \rangle \langle j^2 J_0 | \hat{V}_{12} | j^2 J_0 \rangle}{E(J^3 a J) - E(J^2 a J)}.
\]

In order to obtain an effective three-body interaction which is valid for all \( j^n \) configurations, we make an assumption on the energy denominator in (10). We make the approximation that it is the same for all states of the \( j^n \) and \( j^{n-1} j' \) configurations. This assumption, which is probably more justified in atomic spectroscopy, was made in refs. [12, 13]. The energy denominator in (10) is thus replaced by \( E(J^3) - E(J^2 j') = \Delta E \) which is independent of \( a, J_1 \) and \( J \). It may be taken to be, according to perturbation theory, equal to the difference of single-nucleon energies \( \epsilon_j - \epsilon_{j'} \).

In this approximation, the summation over even values of \( J_1 \) in (10) may be carried out by using identities of Racah coefficients. We obtain, due to \( J_0 \) and \( J'_0 \) having even values,

\[
2 \sum_{J_1 \text{ even}} (2J_1 + 1) \left\{ \begin{array}{ccc}
 j & J_0 \cr j' & J_1 \cr j & j \end{array} \right\} \left\{ \begin{array}{ccc}
 j & J' \cr j' & J'_0 \cr j & j \end{array} \right\}
\]

\[
= \sum_{J_1} (2J_1 + 1) \left\{ \begin{array}{ccc}
 j & J_0 \cr j' & J_1 \cr j & j \end{array} \right\} \left\{ \begin{array}{ccc}
 j & J' \cr j' & J'_0 \cr j & j \end{array} \right\}
\]

\[
+ \sum_{J_1} (-1)^{J_1} (2J_1 + 1) \left\{ \begin{array}{ccc}
 j & J_0 \cr j' & J_1 \cr j & j \end{array} \right\} \left\{ \begin{array}{ccc}
 j & J' \cr j' & J'_0 \cr j & j \end{array} \right\}
\]

\[
= \frac{\delta_{J_0 J'_0}}{2J_0 + 1} + \left\{ \begin{array}{ccc}
 j & J \cr j' & J'_0 \end{array} \right\}.
\]

Using this result in (10) we obtain the second-order contribution given by

\[
3 \sum_{J_0 J'_0} \hat{J}_0 \hat{J}_1 [j^2(J_0) j J] j^3 a J [j^2(J'_0) j J] j^3 a J \left\{ \begin{array}{ccc}
 \delta_{J_0 J'_0} & J_0 \cr \delta_{J_0 J'_0} & J'_0 \end{array} \right\} \frac{\langle j^2 J_0 | \hat{V}_{12} | j^2 J_0 \rangle \langle j^2 J_0 | \hat{V}_{12} | j^2 J_0 \rangle}{\Delta E}.
\]

As explained above, (12) includes also matrix elements of an effective two-body interaction. Their contribution may be obtained by using (2) with \( n = 3 \) and \( k = 2 \). The matrix element in the \( j^2 \) configuration is given by (3) in which, according to our approximation, the energy
fits to the calcium isotopes and to the three-body interaction. The three-body matrix elements of Volya [15] result from separate terms with \( J \) momentum \( j \) and energy \( \epsilon \), therefore, there is no need for the additional label \( a \). There are six three-nucleon states considered. The additional two-body terms (13) are usually, however, absorbed into the other terms contribute to both (13) and (14). They must be cancelled when both interactions are considered. The two-body interaction is induced when the model space is restricted to \( J = 1 \) for various p3f7 interactions. Energies are in keV.

The contribution in second-order perturbation is contained in both (13) and (14). This contribution is always attractive (negative). This need not be the case for the three-body interaction (14). The reason is that in (11), terms with odd values of \( J \) are introduced. In terms with \( J_0 \neq J_0' \), it follows from (11) that \( \sum_{j_1} \sum_{j_1} J_0 J_0' \left( J_0 J_0' \right) J_1 = 0 \) and hence, the contribution of terms with odd-\( J \) values to the three-body terms vanishes. If, however, \( J_0 = J_0' \), these odd-\( J \) terms contribute to both (13) and (14). They must be cancelled when both interactions are considered. The additional two-body terms (13) are usually, however, absorbed into the other effective two-body interaction.

The above formalism can be applied to the \( 1f_{7/2} \) shell. Several interactions are available that include effects from the \( 2p_{3/2} \) shell. Two of them were derived on the basis of spectroscopic properties of the calcium isotopes [5, 6] and two more from those of the \( N = 28 \) isotones [7, 8]. In particular, the authors of these references give numerical values for the matrix elements involving the \( 2p_{3/2} \) shell which enter the expression (14) and for the difference in single-particle energies, \( \epsilon_{2p_{3/2}} - \epsilon_{1f_{7/2}} \). We refer to these interactions as p3f7, followed by the relevant reference.

We have used these interactions, without any modification, to calculate the effective three-body interaction which is induced when the model space is restricted to \( 1f_{7/2} \). The results are shown in Table 1. For \( j = 7/2 \) a three-nucleon state is completely specified by its total angular momentum \( J \) and there is no need for the additional label \( a \). There are six three-nucleon states with \( J = 3/2, 5/2, 7/2, 9/2, 11/2 \) and \( 15/2 \), and each of these states defines a component of the three-body interaction. The three-body matrix elements of Volya [15] result from separate fits to the calcium isotopes and to the \( N = 28 \) isotones, and they should thus be compared with corresponding matrix elements obtained with the p3f7 interactions from refs. [5, 6] and [7, 8].

Table 1. The \( T = 3/2 \) three-body interaction matrix elements in the \( 1f_{7/2} \) shell obtained by Volya and the effective three-body interaction matrix elements derived with the formula (14) for various p3f7 interactions. Energies are in keV.

| \( J \) | \( Z = 20 \) | \( N = 28 \) |
|---|---|---|
| | \( V_{\text{Vol}} \) [15] | \( V_{\text{3f7}} \) [5] | \( V_{\text{3f7}} \) [6] | \( V_{\text{Vol}} \) [15] | \( V_{\text{3f7}} \) [7] | \( V_{\text{3f7}} \) [8] |
| 3/2 | -559 (273) | -412 | -173 (89) | -128 (88) | -53 (29) | -115 |
| 5/2 | 2 (185) | -207 | -104 (48) | -18 (70) | -54 (26) | -57 |
| 7/2 | 53 (70) | 138 | 76 (58) | 55 (28) | 42 (24) | 37 |
| 9/2 | 272 (98) | 392 | 157 (96) | 122 (41) | 36 (34) | 110 |
| 11/2 | 51 (130) | 29 | 46 (91) | 102 (43) | 72 (77) | 6 |
| 15/2 | -24 (73) | 77 | 28 (27) | -53 (29) | 5 (5) | 23 |
respectively. The numbers in parentheses in Table 1 are the variances of the parameters in the fits, either given by Volya or computed from the errors on the matrix elements which are known for two of the interactions [6, 7].

There are substantial variations in the calculated effective three-body matrix elements. In particular, those derived from the $Z = 20$ p3f7 interactions are generally larger than those obtained with the $N = 28$ p3f7 interactions. This results from a combination of a larger difference $\epsilon_{2p3/2} - \epsilon_{1f7/2}$ and smaller two-body matrix elements $\langle(1f7/2)^2|\mathbf{V}|1f7/22p3/2J_0\rangle$ in the latter interactions.

There are certainly differences between these calculations and the results of Volya. However, in spite of these differences and uncertainties, it is clear that the matrix elements are correlated: with one exception, attractive (repulsive) matrix elements in the analysis of Volya turn out to be attractive (repulsive) in our analysis. The exception concerns the $J = 15/2$ interaction which is attractive in Volya’s analysis while it is repulsive for the p3f7 interactions.

We considered two approaches to the $1f7/2$ shell. A dogmatic one in which states of nucleons outside closed shells are taken to be pure $1f7/2$ states. In this approach, to obtain the observed energies, it is necessary to introduce three-body interactions. In the other approach, it is recognized that there are rather close configurations whose states may mix with $(1f7/2)^n$ states by two-body interactions. It was shown by Poves and Zuker [14] and repeated here, that the effect of such mixing in second-order perturbation theory leads to three-body effective interactions in the $(1f7/2)^n$ configuration.

It is true that the first requirement of any calculation is to reproduce well the energies of a system. This is due to the fact that the energy is stationary at the correct wave functions. Small deviations from the exact wave functions may have a large effect on other observables like electromagnetic moments and transitions. Looking at the magnetic moments, it is clear that states of actual nuclei are not well described by pure $(1f7/2)^n$ states. In pure $j^n$ configurations of identical nucleons, the $g$-factors of all states should be equal. In contrast to other shells, this is not the case for the $1f7/2$ shell. Introducing three-body interactions does not change any state with the exception of the two $J = 2$ and two $J = 4$ for $n = 4$ configurations.

Magnetic moments are very sensitive to certain small admixtures in the wave functions. Many years ago, Arima and Horie [18] showed that changes in them are proportional to the amplitude of admixtures similar to those discussed above. In such excitations, one $j = l + 1/2$ nucleon is raised into the $j' = l - 1/2$. In the present case, excitation of a $1f7/2$ nucleon into the $1f5/2$ orbit are important. Even an admixture of 1–2% is sufficient to obtain the magnetic moment of $^{43}\text{Ca}$ which is rather different from that of $^{41}\text{Ca}$. Examples of using configuration mixing to obtain the correct magnetic moments can be found for calcium isotopes in ref. [19] and for $N = 28$ isotones in ref. [20].

Other evidence for the impurity of $(1f7/2)^n$ states in actual nuclei follows from the results of various direct reactions. They exhibit definite admixtures of $l = 1$ components in wave functions. Admixtures of configurations affect energies of states as well as other observables. Large quadrupole moments and strong E2 transitions in light calcium isotopes may indicate appreciable admixtures of core-excited collective states. If energies of states are correctly obtained by using three-body forces with rather pure $(1f7/2)^n$ wave functions, no place for the necessary admixtures is available.

In ref. [15] it is stated that “while going beyond the single $j$-shell is imperative to account for the observed $g$-factors, the agreement between the experiment and the common large-scale shell model results is not perfect”. From this fact the author concludes that this “may be a hint for the presence of a three-body force.” We would like to remind the reader that such arguments may be valid in QED which is a very exact theory. They are certainly irrelevant in looking for deviations from calculations based on the shell model which is a drastic approximation to the exact theory of nuclear structure.
References
[1] Lawson R D and Uretsky J L 1957 Phys Rev 106 1369
[2] Talmi I 1957 Phys Rev 107 326
[3] Ginocchio J N and French J B 1963 Phys Lett 7 137
[4] McCullen J D, Bayman B F and Zamick L 1964 Phys Rev 134 B515
[5] Engeland T and Osmes E 1966 Phys Lett 20 424
[6] Federman P and Talmi I 1966 Phys Lett 22 469
[7] Auerbach N 1967 Phys Lett B 24 260
[8] Lips K and McEllistrem M T 1970 Phys Rev C 1 1009
[9] Eisenstein I and Kirson M 1973 Phys Lett B 47 315
[10] Quesne C 1970 Phys Lett B 31 7
[11] Zelevinsky V 2009 Yadernaya Fizika [Phys At Nucl] 72 1107
[12] Rajnak K and Wybourne B G 1963 Phys Rev 132 280
[13] Racah G and Stein J 1967 Phys Rev 156 58
[14] Poves A and Zuker A 1981 Phys Reports 70 235
[15] Volya A 2009 Eur Phys Lett 86 52001
[16] Van Isacker P and Talmi I 2010 Eur Phys Lett 90 32001
[17] See eg Talmi I 1993 Simple Models of Complex Nuclei. The Shell Model and Interacting Boson Model (Harwood, Academic, Chur)
[18] Arima A and Horie H 1954 Prog Theor Phys 12 623
[19] Taylor M J et al 2003 Phys Lett B 559 187
[20] Speidel K-H et al 2000 Phys Rev C 62 031301