Spin-dependent effective interactions for halo nuclei

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(Received 12 March 2003; published 24 July 2003)

We discuss the spin dependence of the effective two-body interactions appropriate for three-body computations. The only reasonable choice seems to be the fine and hyperfine interactions known for atomic electrons interacting with the nucleus. One exception is the nucleon-nucleon interaction imposing a different type of symmetry. We use the two-neutron halo nucleus \(^{11}\)Li as an illustration. We demonstrate that models with the wrong spin dependence are basically without predictive power. The Pauli forbidden core and valence states must be consistently treated.

DOI: 10.1103/PhysRevC.68.014002

PACS number(s): 21.45.+v, 21.60.Gx, 27.20.+n

INTRODUCTION

Quantum halos occur in several branches of physics, although mostly discussed in molecules and nuclei [1–4]. These structures are described in terms of a few weakly bound composite clusters. The corresponding two-body interactions should, in principle, be derived from the basic interactions between the particles within the clusters. However, to be practical, effective forces must be employed for at least two reasons. First the calculations simplify and second the inherent inaccuracy in the calculations from first principles is often much worse than in the few-body computations. Thus, the accuracy and interdependence of computed observables can be drastically improved by use of phenomenological effective interactions. This division between understanding the basic interactions and understanding the resulting many-body system is strikingly illustrated by nuclear structure that was described virtually independent from detailed knowledge of the nucleon-nucleon interaction [5].

In descriptions of nuclear halos, effective two-body interactions are indeed always constructed and used with only superficial connection to the fundamental forces [6–11]. This strategy is particularly well suited for the spatially extended halos where details of the potentials are unimportant. Only low-energy scattering properties are crucial for the gross structures. However, more quantities are both computed and measured with ever increasing accuracy [12–17]. At some point we are bound to exceed the validity limit of the models. Designing the models to maximum performance is very desirable. Their range of applicability can then be extended by careful choices of model space and form of the effective interactions.

Few-body computations with spin-dependent effective interactions have so far not been very abundant [18,8,9,19], but this is likely to change in the near future. It is then important to have a correct starting point which unavoidably is the two-body interaction. The purpose of this paper is to discuss the constraints on the spin dependence of the effective two-body interactions. We shall test by application to three-body nuclear halo systems where the effects are more indirect, to some extent even hidden, and only revealed by systematic computations.

SYMMETRY REQUIREMENTS

It was noted early in the history of nuclear physics that a spin dependence in the nucleon mean-field potential was necessary to reproduce the magic numbers [5]. The only rotationally invariant, parity conserving, spin-dependent quantity is the spin-orbit potential which is doing the job and therefore used in all realistic mean-field computations. In complete analogy, the nucleon-core effective interaction for zero core spin can then only have central and spin-orbit terms.

On the other hand, the nucleon-nucleon interaction has central, spin-spin, spin-orbit, quadratic spin-orbit, and tensor terms [20]. For an even-even nucleus they reduce to central and spin-orbit terms after applying the mean-field average as in all optical model computations [21]. However, for nonzero core spin all these spin-dependent forms are allowed in the construction of the nucleon-core effective potential. We shall, for simplicity, omit quadratic spin-orbit and tensor interactions. The first is usually small and the effect of the second is reproduced by an orbital angular momentum dependent central force if the nondiagonal part is neglected or does not contribute. In few-body physics this is consistent with the common choice of Hilbert space with only a few opposite parity relative states, e.g., \( s \) and \( p \) states.

This leaves us with central, spin-spin, and spin-orbit terms. The spin dependence of the effective two-body interaction must then be a combination of the three possible independent scalar quantities, i.e.,

\[
as_n \cdot s_n + b \ell \cdot s_n + c \ell \cdot s_c,
\]

where \( s_n \) and \( s_c \) are the spins of the two particles, \( \ell \) is the relative orbital angular momentum operator, and \( a, b, c \) are constants. The spin-symmetric combination,

\[
as_n \cdot s_c + b \ell \cdot (s_n + s_c),
\]

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has to be used for identical particles such as nucleons [20]. However, an asymmetric system such as the electron and the nucleus requires the combinations

\[ a(\ell + s_n) \cdot s_c + b \ell \cdot s_n, \]

where “\( n \)” now refers to the electron and \( s_c \) is the total angular momentum of the nucleus. The origin of the first term in Eq. (3) is the magnetic hyperfine interaction arising from the nuclear and electron spins [22].

Other combinations are clearly also possible, e.g.,

\[ a s_n \cdot s_c + b \ell \cdot s_n, \]

\[ (\ell + s_n) \cdot (\ell + s_c) = \ell \cdot \ell + s_n \cdot s_c + \ell \cdot (s_n + s_c), \]

where Eq. (5) is more symmetric but equivalent to Eq. (2) with the \( \ell \cdot \ell \) term included in the central potential.

For the nucleon-core interaction the absence of symmetry requirements is complicating the choice. One option could be to use Eq. (2) as in Refs. [23,19], where three-body systems with two nucleons outside a core of finite spin are investigated. With appropriate parameter adjustments the computed spectra obtained in Ref. [19] and the results involving both the ground state structure and breakup reactions are indeed quite reasonable [23].

When the combinations in Eq. (2) are used the total spin \( s = s_n + s_c \) of the neutron-core system is a conserved quantum number. When the core has a finite spin the two values of \( s = s_n \pm 1/2 \) decouple and separate through the spin-spin term. Each of these two spin values is then split up by the spin-orbit term according to the possible total two-body angular momenta \( j = (\ell + s)^2 \). However, \( s \) and \( j \) are not the usual mean-field quantum numbers, where every nucleon moves in an orbit characterized by the relative nucleon-core orbital \( \ell \) and nucleon total \( j_n = \ell \pm 1/2 \) angular momentum. Instead, \( j_n \) couples to \( s_c \) to give the total two-body angular momentum \( j \).

One serious problem with Eq. (2) arises because the nucleon angular momentum \( j_n \) is not conserved like the total spin. Therefore the usual mean-field spin-orbit partners with \( j_n = \ell \pm 1/2 \) are inevitably mixed in both two- and three-body systems. The essence of the difficulty is that the motion of the valence nucleons(s) outside the core is inconsistent with the (approximate mean-field) motion of the identical nucleons within the core. This is obviously a problem for a few-body description in terms of components with given \( j_n \) as needed when we want to bridge the gap to mean-field computations.

The problem is much worse if one and only one of the mixed spin-orbit partners is Pauli forbidden by core occupancy as the \( 2p_{3/2} \) orbit in \( ^{10}\text{Li} \) and \( ^{11}\text{Li} \). This may be disguised by parameter adjustments, but sufficiently many independent observables computed from the same parameter set would undoubtedly reveal the problem. Computations of relatively few observables may be quite reasonable, although uncontrolled and thus suspicious.

We need to restore the mean-field single-particle total angular momentum as a conserved quantum number. Therefore in subsequent calculations (see, for example, Ref. [24]) the spin-orbit interaction was changed and the spin dependence was instead given by Eq. (4). Now the dominating spin-orbit term conserves \( \ell \) and \( j_n \) as indicated by the usual notation \( \ell j_n \). The spin-spin term should then be a perturbation specifically designed to split the states with different total angular momenta arising from couplings of core \( (s_c) \) and nucleon \( (j_n) \) spins. This is a reasonable assumption when the single-particle spin-orbit splitting is much larger and essentially is maintained.

To achieve full consistency with the mean-field description, we have to replace Eq. (2) with Eq. (3), which conserves \( j_n \). It is interesting that this choice is appropriate for nucleon core, as well as for electron-nucleus interactions. In both cases the fine and hyperfine structures can apparently then be properly described as originating from the spin-spin and spin-orbit terms, respectively. The difference between Eqs. (3) and (4) is marginal for the present cases of interest, since the strength of the spin-spin term in both cases must be rather small. However, Eq. (3) is clearly preferable from a conceptual point of view where the connection to mean-field computations is necessary or at least very desirable.

It is worth emphasizing that Eqs. (2)–(5) are identical both for \( s \) waves and for zero core spin.

### Comparing Two-Body Properties

The interaction must, in general, be a combination of three terms as in Eq. (1) with appropriate individual radial form factors. The relative importance of the terms in Eq. (2) is illustrated for \( d \) waves in the upper part of Fig. 1. We define \( a = x \) and \( b = \sqrt{1-x^2} \) such that the parameter \( x \) controls the relative weight between the spin-spin and spin-orbit parts of these potentials. For \( x = \pm 1 \) only the spin-spin term enters, the total spin is conserved, and the state with \( s = 0 \) is separated from the three degenerated \( s = 1 \) states. When \( |x| \)
\[
V(x) = s_n \cdot s_c + B \ell \cdot s_n + x \ell \cdot s_c ,
\]

(7) which for \(x = 0\) and 1 reduce to Eqs. (4) and (3), respectively. We see that although \(j_n\) is not a conserved quantum number even for \(x = 0\), the eigenvalues remain almost constant all the way up to \(x = 1\). This result is a consequence of the small absolute size of the spin-spin interaction compared to the spin-orbit term. Under this realistic condition Eq. (4) is a good approximation to Eq. (3).

In the lower part of Fig. 2 we show the same kind of results for \(p\) waves and \(s_n = 3/2\). We start again with expression (6), but now with \(B = 20\). The positive value of \(B\) reverses the normal order of the spin-orbit splitting. Then for \(x = 1\), where \(j_n\) and \(j\) are good quantum numbers, the eigenvalues with smallest value of \(j_n\) are the lowest. This is a useful tool to exclude occupation of the Pauli forbidden \(p_{3/2}\) states achieved by shifting them to high energies. Again, we see that Eq. (3) \((x = 1)\) allows close lying, still spin-split, states with equal value of \(j_n\). In contrast, Eq. (2) \((x = 0)\) corresponds to two pure \(j_n = 3/2\) states and four other states which mix the \(p_{1/2}\) and the \(p_{3/2}\) orbits according to

\[
s_j = \begin{cases} 
1 & \text{if } j = 1, \\
2 & \text{if } j = 2, \\
1 & \text{if } j = 2, \\
2 & \text{if } j = 2,
\end{cases}
\]

(8a, 8b, 8c, 8d)

It is then clear that when Eq. (2) is used, the two low-lying \(p\) states necessarily contain part of the \(p_{1/2}\) states. They are forbidden by the Pauli principle for both \(^{10}\text{Li}\) and \(^{11}\text{Li}\). The dashed lines in the lower part of Fig. 2 show eigenvalues obtained from potential (7). Again we observe that Eq. (4) \((x = 0)\) is a good approximation to Eq. (3) \((x = 1)\), provided the spin-spin term only is a perturbation to the spin-orbit term.

**COMPARING THREE-BODY PROPERTIES**

Let us now investigate how the different choices of the nucleon-core interaction affect the full three-body calculation. We take \(^{11}\text{Li}\) \(\text{(Li}^4 + n + n)\) as an example with the Hilbert space consisting of \(s\) and \(p\) waves. Then \(s_n = 3/2\) and the lowest neutron \(s_{1/2}\) and \(p_{3/2}\) orbits are fully occupied in the \(^{9}\text{Li}\) core, and therefore not available for the valence neutrons due to the Pauli principle. The calculations are performed by solving the Faddeev equations with the hyperspherical adiabatic expansion method [25]. For the neutron-neutron interaction we use Eq. (2) supplemented by a central part. The
The potentials in Eqs. (9) (solid line) and (11) (dashed line) are used. The strengths of the Gaussians $V_{s}^{(\ell=0)}$, $V_{s}^{(\ell=1)}$, and $V_{s}^{(\ell=1)}$ are $-7.05$ MeV, $-1.6$ MeV, 260.25 MeV, 1.0 MeV, and 300 MeV, respectively, for potential (9) and $-5.95$ MeV, $-1.6$ MeV, $-27.125$ MeV, 1.5 MeV, and 5 MeV for potential (11). The range of the Gaussians is 2.55 fm in all the cases.

radial form factors are Gaussians, and their parameters are adjusted to reproduce low-energy nucleon-nucleon scattering data.

For the nucleon-core interaction we first use Eq. (3) plus a central part, i.e.,

$$V_{nc}^{(\ell)} = V_{c}^{(\ell)} + V_{s}^{(\ell)} s_{p} \cdot s_{n} + V_{s}^{(\ell)} \ell \cdot s_{n}.$$  

We use Gaussian radial form factors adjusted independently for $s$ and $p$ waves. To account for the Pauli principle for the $s_{1/2}$ and $p_{3/2}$ states, we start by using a simple shallow $s$ wave interaction without bound states and a large repulsive spin-orbit strength shifting the $p_{3/2}$ states to high energy as seen in the lower part of Fig. 2 for $x=1$.

As in Ref. [25], we choose a range for the $^{9}$Li-neutron interaction of 2.55 fm, and adjust the strengths of $V_{c}^{(\ell=1)}$ and $V_{s}^{(\ell=0)}$ to place the two low-lying spin-split $p_{3/2}$ resonances in $^{10}$Li at 0.3 and 0.5 MeV computed as poles of the $S$ matrix. These values are consistent with the available experimental data [26]. We finally use the strength of the central $s$-wave interaction to fit the experimental $^{11}$Li separation energy, and the strength of the $s$-wave spin-spin potential to place a low-lying virtual $s$ state in $^{10}$Li at 50 keV, as indicated by experiments.

The precise values of the parameters in the potentials are given in the caption of Fig. 3. The computed rms radius is 3.3 fm, and the $p$-wave content is slightly above 30%. Use of a weaker central $s$-wave interaction can increase the $p$-wave content up to around 40% in somewhat better agreement with the known experimental values. In this case an additional effective three-body potential is needed to maintain the two-neutron separation energy at the right value. However, this finetuning is not necessary for the present investigation.

The $^{10}$Li energy distribution is approximately obtained as the Fourier transform $\Psi(p_{x},p_{y})$ of the $^{11}$Li wave function, i.e.,

$$\frac{dn}{dE_{x}}(MeV^{-1}) = \mu_{s} p_{x} \left| \Psi(p_{x},p_{y}) \right|^{2} d^{3}p_{x} d\Omega_{p_{y}},$$  

where $p_{x}$ is the $^{9}$Li-neutron relative momentum whose direction is given by $\Omega_{p_{y}}$, $\mu_{s}$ is the $^{9}$Li-neutron reduced mass, $p_{y}$ is the relative momentum between the second neutron and the $^{10}$Li center of mass, and $E_{x} = p_{x}^{2}/2\mu_{s}$.

Let us carry out the same calculations, but now using Eq. (2). The $^{9}$Li-neutron interaction is given as

$$V_{nc}^{(\ell)} = V_{c}^{(\ell)} + V_{s}^{(\ell)} s_{p} \cdot s_{n} + V_{s}^{(\ell)} \ell \cdot (s_{n} \cdot s_{y})_{p}.$$  

The $p$ resonances are now characterized by the quantum numbers given in the lower part of Fig. 2 for $x=0$. We proceed as before, placing the two lowest $p$ resonances at the energies of 0.3 MeV and 0.5 MeV and using the spin-orbit strength to shift the remaining four states to higher energies. Again, the $s$-wave interaction is used to adjust to the experimental separation energy of 0.3 MeV. This procedure results in a rms radius of 3.4 fm, also consistent with the experimental data, but the $p$-wave content is now too small, less than 7%.

An increase of this $p$-wave content without changing the energies of the two lowest resonances can only be achieved by reducing the strength of the spin-orbit interaction. With the parameters given in the caption of Fig. 3, we then obtain a reasonable $^{11}$Li wave function, with the right separation energy, rms radius, and a $p$-wave content of 27%. Furthermore, as shown by the dashed curves in Fig. 3, the dominating radial wave function as well as the $^{10}$Li energy distribution obtained with the potential (11) resemble those obtained with Eq. (9).

However, some hidden differences remain. First, the $p_{3/2}$-occupation probability only amounts to 7% with the potential in Eq. (9) and around 13%, more than half of the total $p$-wave contribution, with potential (11). Second, by increasing the repulsion in the spin-orbit interaction in potential (9), this $p_{3/2}$ probability can be reduced without significant changes of the computed $^{11}$Li properties. However, with potential (11) it is not possible to reduce the $p_{3/2}$ probability and still keep the $p$-wave content at a realistic fairly high value. Third, with the potential in Eq. (9), the computed $^{10}$Li has only two low-lying resonances of $p_{1/2}$ character, while for Eq. (11) almost all the $p$ resonances are rather close lying, i.e., the five lowest energies (computed as poles of the $S$ matrix) are 0.3, 0.5, 1.0, 1.3, and 1.6 MeV.

Let us now maintain the realistic properties of the $^{11}$Li ground state and turn to the lowest $1^{-}$ excitation, i.e., the $1/2^{+}$ state. The only difference in the calculation is that the inclusion of the Faddeev components must be consistent.
with the new quantum numbers. The same potentials as for the ground state must be used, since precisely the same partial waves constitute both ground state and excited state configurations.

Now drastic differences appear. For the potential in Eq. (9), the computed $1/2^+$ state is unbound. Furthermore, a calculation with the complex scaling method reveals a $1/2^+$ resonance at 0.4 MeV with a width of 0.3 MeV. These values are consistent with the detailed calculations shown in Ref. [13]. However, when the potential in Eq. (11) is used, the $1/2^+$ state is bound by 1.3 MeV, i.e., even more bound than the ground state. We can then conclude that when only ground state properties are used to fit the potential parameters, the excited states are not automatically also correct even when they are spanned by the same Hilbert space.

For the $1^-$ excitations of $^{11}$Li, basically one $s$ and one $p$ state are simultaneously occupied unlike the ground state where both neutrons simultaneously are located in pairs of either $s$ or $p$ states. The $1/2^-$ resonance obtained with Eq. (9) does not contain contributions from the $p_{3/2}$ waves when a realistic spin-orbit splitting is applied. In contrast, this resonance obtained with Eq. (11) contains a $p_{3/2}$ contribution of about 10%. The wrong properties of the interactions may be parametrized away while still reproducing the ground state observables, but catastrophically wrong results may return for the other properties, for example, of $1^-$ excitations.

THE PAULI PRINCIPLE

The calculations shown in the preceding section contain an important simplification concerning the way the Pauli principle is taken into account. This has been done to make the conclusions clear and avoid the mixing with technical details that could easily obscure them. We shall now investigate if a better treatment of the Pauli principle, necessary for any realistic calculation, is modifying some of the previous results. In Ref. [27], an appropriate method to treat the Pauli principle in few-body calculations is described. The realistic two-body interactions able to bind a nucleon into a Pauli forbidden state are substituted by the corresponding phase equivalent potentials with exactly the same phase shifts, but without the Pauli forbidden bound states.

In Ref. [26], constraints on the neutron-$^9$Li were derived, which were consistent with the known $^{10}$Li spectrum and the $^{11}$Li properties. In particular, it was found that the interaction in Eq. (9) with Gaussian radial form factors with range equal to 2 fm, and strengths for $V_c^{(e=0)}$, $V_s^{(e=0)}$, $V_s^{(e=-1)}$, $V_s^{(e=-1)}$, and $V_s^{(e=-1)}$ equal to $-94.0$ MeV, $-11.4$ MeV, $-79.64$ MeV, $1.1$ MeV, and $-13.12$ MeV, respectively, results in a $^{10}$Li spectrum with a low-lying $2^+$ $s_{1/2}$ virtual state at 50 keV, and a $1^+/2^+$ $p_{1/2}$ doublet at 0.25 MeV and 0.54 MeV, respectively, consistent with the available experimental data. This neutron-$^9$Li interaction has a deeply bound $s_{1/2}$ state and a bound $p_{3/2}$ state at $-4.1$ MeV. These two states are Pauli forbidden and subsequently removed in the three-body calculation by use of the corresponding phase equivalent potentials [26]. In this way, the $s_{1/2}$ and the $p_{3/2}$ forbidden states are explicitly excluded from the calculation.

As shown in Ref. [26], the use of this two-body interac-

tion results in a $^{11}$Li ground state with a two-neutron separation energy of 0.30 MeV, a $p$-wave content of around 40%, and a rms radius of 3.2 fm. These results are obtained after a fine-tuning with an effective three-body interaction that is known to be necessary in three-body calculations to account for the polarizations of the particles that are beyond those described by the two-body interactions. At the same time, the $^{11}$Li wave function obtained is consistent with the experimental invariant mass spectrum, core momentum distribution, and angular distribution obtained after fragmentation of $^{11}$Li.

Furthermore, in Ref. [13] we show that the same interaction gives rise to a $1/2^+$ $^{11}$Li resonance at an energy above the threshold of about 0.6 MeV and a width of 0.5 MeV. These results are similar to the ones obtained with the calculations in the preceding section for the interaction given in Eq. (9).

Let us perform now the same kind of calculations for potential (11). We then use the $s$-wave neutron-$^9$Li interaction specified above, with a deeply bound $s_{1/2}$ state, forbidden by the Pauli principle, that is removed from the three-body calculation by use of the phase equivalent potential. For the $p$-wave interaction the good quantum numbers of the spin operators in the two-body potential are the total two-body spin $s$ and the total two-body angular momentum $j$, and therefore the eigenfunctions mix the $p_{1/2}$ and $p_{3/2}$ states [see Eqs. (8a)–(8d)]. It is then impossible to find an interaction binding pure $p_{3/2}$ states into a Pauli forbidden state, and with two pure low-lying $p_{1/2}$ resonances. This is due to the inconsistency between the good quantum numbers of interaction (11) and the mean-field description used for the core neutrons.

This inconsistency cannot be cured by an appropriate treatment of the $p$-wave states. Let us, nevertheless, describe various attempts. First, we take the same shallow $p$-wave potential as in the preceding section [the strengths of the Gaussians of interaction (11) are given in the caption of Fig. 3]. Proceeding in this way, we observe that an appropriate treatment of the Pauli principle only in the $s$ waves while keeping unchanged the $p$ interaction is not giving new results compared to the previous ones. As before, the $^{11}$Li ground state wave function can be considered to be reasonable, but the same interaction gives rise to a bound $1/2^+$ state with 1 MeV separation energy, clearly more bound than the experimental ground state.

A second option is to construct an interaction (11) such that four of the $p$-wave eigenfunctions are bound, while the other two are low-lying resonances. The bound states can be interpreted as the four neutrons occupying the $p$ shell in the $^9$Li core. These four states should be removed from the calculation, and the remaining two states would correspond to the $p$ resonances at 0.25 MeV and 0.54 MeV. As mentioned, this is in itself inconsistent, since the excluded states necessarily contain some $p_{1/2}$ contribution, and the two low-lying $p$ resonances contain part of the $p_{3/2}$ waves. In any case, this can be achieved by taking Gaussian radial potentials in Eq. (11) with a range of 2 fm and strengths for $V_c^{(e=-1)}$, $V_s^{(e=-1)}$, and $V_s^{(e=-1)}$ equal to $-77.6$ MeV, $-2.3$ MeV, and 6.8 MeV. When this two-body $p$ potential is used, and the four bound $p$
states are removed from the three-body calculation, the ground state \(^{11}\text{Li}\) wave function needs a very large three-body effective interaction to recover the experimental two-neutron separation energy of 0.3 MeV. Furthermore, the \(p\)-wave content is extremely large (80\%), and the rms radius (2.4 fm) is far below the experimental value. We see that in this case even the ground state wave function shows important deficiencies. Also, the \(1/2^-\) state does not show any low lying resonance.

A final attempt can be to use a repulsive core only for the \(p_{3/2}\) waves. For this purpose, we can employ the phase equivalent potential constructed to be used with interaction (9). However, this repulsive potential is implicitly assuming the shell model quantum numbers for the neutron state, and when used in combination with the spin operators in Eq. (11) the energies of the different two-body \(p\) states bear no resemblance to the initial \(p\) states, and some of them are even bound.

We have now accounted for the Pauli principle in various ways, i.e., using a shallow potential without bound states, using phase equivalent potentials and repulsive cores. The conclusion remains that the spin-dependent interaction must be simultaneously consistent with the treatment of both core and valence neutrons. No parameter variations alter this conclusion.

**CONCLUSIONS**

The first step towards a reliable description of few-body systems is to construct appropriate two-body interactions between the pairs of particles. We discuss the spin dependence of this effective interaction. Three different terms combining spin and orbital angular momentum are possible with the necessary rotational invariance and parity conservation. Various combinations correspond to applications in different fields of physics. We focus especially on the forms appropriate for the nucleon-nucleon interaction and the fine and hyperfine interactions for electrons in the atom.

The properties of different two-body interactions are first compared. Then the effects on computed three-body structures are investigated for \(^{11}\text{Li}\) \((n + n + ^9\text{Li})\). We show that parameters adjusted to reproduce the three-body ground state properties can lead to wrong results for the excited states, depending on the form of the spin-dependent effective interactions. We conclude that only one choice is consistent with the mean-field treatment implicitly assumed for the core nucleons. Violating this condition compromises the treatment of the Pauli forbidden states and reliable predictions are not possible.