Towards a self-consistent shell model

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In most cases shell-model calculations are not performed using Hartree-Fock self-consistency conditions. In calculations limited to the valence space, this may not lead to any problems, but when higher shell admixtures are allowed the calculated observables implicitly include Hartree-Fock terms that may be undesirable. In this work, we compare non-self-consistent and nearly self-consistent calculations of the spin-orbit splitting of the $p_{1/2}$ and $p_{3/2}$ hole states in $A=15$. We find that when higher shell admixtures ($2\hbar\omega$) are included in the model space, and when a ''standard'' interaction is used, the spin-orbit splitting increases relative to a $0\hbar\omega$ calculation. However, when the interaction and/or the kinetic energy are modified so as to achieve self-consistency the reverse is true, with the spin-orbit splitting in the $(0+2)\hbar\omega$ space becoming smaller than that in the $0\hbar\omega$ space. Furthermore, we show that self-consistency cannot be achieved by modifying the two-body spin-orbit or tensor terms, but is possible by adding a monopole-monopole term.

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I. INTRODUCTION

Two popular appoaches to nuclear structure calculations are shell-model calculations and Hartree-Fock calculations. The latter are usually not done with realistic interactions, but rather with simpler interactions like the Skyrme-type interactions [1] where the parameters are chosen so as to give the right binding energy at the right radius, and good single-particle energies [1–3]. The self-consistency condition can be stated as follows: there can be no admixing of one-particle–one-hole ($1p$-$1h$) excitations into the self-consistent intrinsic state. Indeed, it does not make much sense to use these interactions to go beyond Hartree-Fock, i.e., one should not use them to calculate $2p$-$2h$ and higher admixtures into the ground state. To quote from Vautherin and Brink ''Skyrme interactions can be considered as a kind of phenomenological *G* matrix, which already includes the effects of short-range correlations . . . .'' This is one reason why it would be meaningless to calculate second-order corrections with Skyrme's force, and a perturbation theory would actually diverge because of the *zero range*.'' Thus, any Hartree-Fock wave function calculated using a Skyrme-type interaction would consist of a single Slater determinant.

In shell-model calculations involving several shells, we will, of course, get ground state correlations, e.g., $2p$-$2h$ admixtures, but one may also get $1p$-$1h$ admixtures, which are undesirable in a Hartree-Fock sense.

The self-consistency problem in shell-model calculations have been discussed previously by several authors, e.g., Sharp and Zamick [4], Hoshino, Sagawa, and Arima [5] and by Jaqua *et al.* [6].

In the Sharp and Zamick work, a density-dependent interaction of the form $-\alpha\delta(\vec{r}_1-\vec{r}_2)+\gamma\rho^{\sigma}\delta(\vec{r}_1-\vec{r}_2)$ was considered. The first term is attractive and serves to bind the nucleus, while the second (density-dependent) term is repulsive and prevents the nucleus from collapsing to a point. It was noted that if that interaction is used for calculating binding energies then, for single-particle energies, the interaction to be used is $-\alpha\delta(\vec{r}_1-\vec{r}_2)+\gamma(1+\sigma/2)\delta(\vec{r}_1-\vec{r}_2)$. Popular choices of σ are 2/3 and 1, the latter used for Skyrme interactions. Since the factor $(1+\sigma/2)$ is greater than 1, the repulsive term is larger when calculating single-particle energies, and the overall interaction is less attractive (i.e., weaker).

In the work of Hoshino *et al.*, they use a non-density-dependent interaction V_{M3Y} to calculate the energies of giant resonances. In calculating the energy of the isoscalar giant monopole resonance, it is crucial that one is at a Hartree-Fock minimum. Rather than getting involved in complicated rearrangement-effect calculations, the authors simply add a repulsive interaction $\delta V=V_0\Sigma_i r_i^2$ in the particle-hole channel and adjust the parameters so as to get a Hartree-Fock minimum at the desired nuclear radius.

In the work of Jaqua *et al.*, the importance of treating the kinetic energy properly is emphasized, and the removal of the spurious states is crucial. They have shown that the Hartree-Fock single-particle energies and their relationship to experimental removal energies depend sensitively on whether or not the center-of-mass kinetic energy is retained in the nuclear Hamiltonian. In a very large shell-model calculation by Haxton and Johnson [7], the main motivation of which was to get the $J=0^+$ $4p$-$4h$ state in ^{16}O at the correct excitation energy, they concern themselves with the large $1p$-$1h$ admixtures that can arise. They do not give many details but say ''in the spirit of Brown and Green, the strong interaction was only allowed to operate in the $1p$-$2s$-$1d$ shells.'' It turns out that this choice also eliminates large $2\hbar\omega$ and $4\hbar\omega$ $1p-1h$ amplitudes that could mix into the low-lying states, only because the shell-model interaction does not properly respect the Hartree-Fock condition.

In the works of Hoshino *et al.* [5] and Haxton and Johnson [7], the main emphasis is on getting the correct nuclear structure—the right excitation energies for giant resonances in the former case—and to demonstrate for the first time that the $4p$-$4h$ highly deformed states could come down to a reasonable energy in a shell-model calculation

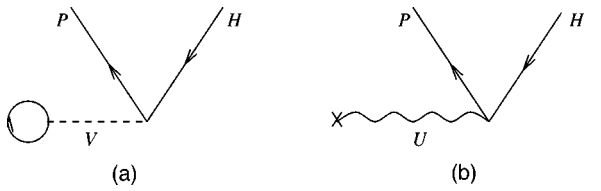

FIG. 1. The two Hartree-Fock diagrams that enter in the self-consistency condition: the two-body potential-energy term (a), and the one-body harmonic-oscillator term (b).

done in a large enough model space in the latter case. But the interactions used in these calculations are somewhat hybrid.

In this particular work, we are less concerned with fitting the experimental data, and instead, using a realistic interaction in shell-model calculations, we examine the consequences of achieving near Hartree-Fock self-consistency on the interaction itself as well as on nuclear observables of interest.

In shell-model calculations one generally uses a much more detailed interaction involving many two-body matrix elements. These can either be obtained completely phenomenologically as was done in the early days, or one can obtain G matrices from realistic two-body interactions. The most popular method at the present time is a compromise between these two extremes, e.g., one starts out with a G matrix from a realistic interaction but then one makes some phenomenological modifications to get a better fit to the data.

In either case, phenomenological or realistic, little thought is given to Hartree-Fock self-consistency. Indeed, it is not even clear that one should impose such a condition since in the shell-model one has a correlated ground state.

If one limits the particles to one major shell, then one can get away with ignoring the ''self-consistency'' problem. However, if one admixes say $2\hbar\omega$ excitations in order to improve the ground state, the problem comes back to haunt us. Part of the $2\hbar\omega$ admixtures consists of two particles being excited through one major shell. But one also gets admixtures where one particle gets excited through two major shells. In Hartree-Fock theory, the latter configuration should not admix into the uncorrelated ground state [8]. The reason for this is that the only effect of admixing $1p$-$1h$ excitations is to change the radial shapes of the wave functions of the occupied states. But if one already has the best shape, there should be no further change. In the shell-model, it is not clear what to do with such configurations.

The Hartree-Fock condition can be shown diagrammatically by the cancellation of the two diagrams shown in Figs. 1(a) and 1(b). This leads to the equation

$$\frac{1}{\sqrt{2(2j_P+1)}}\sum_{I,T}(2I+1)(2T+1)\langle[PC]^{I,T}|V|[HC]^{I,T}\rangle_U \times\delta_{j_P,j_H}\delta_{n_P,n_H+1}=\frac{1}{\sqrt{2(2j_P+1)}}\langle p|U|h\rangle\delta_{j_p,j_h}, \quad (1)$$

where the two-particle matrix element is antisymmetrized but unnormalized, and C is an occupied (or core) state. Since $U=T+U-T$, where T is the kinetic energy, and $T+U$ cannot connect to the PH state, we can replace U by $-T$ in the last matrix element. Then the problem becomes that of finding a *kinetic energy* matrix consistent with the two-particle potential energy.

It has already been shown by one of the authors [9] that ''Hartree-Fock diagrams'' can affect the spin-orbit splitting in perturbation theory. In calculating the contribution of $2\hbar\omega$ admixtures to single-particle energies, besides the $2p$-$1h$ and $3p$-$2h$ terms (Eqs. (2) and (3) in [9]), there are single Hartree-Fock and double Hartree-Fock diagrams, and both must be taken into account. The expression for the single Hartree-Fock (SHF) diagrams is

$$\delta\epsilon_j(\mathrm{SHF})=2\sum_{p,h}\frac{D(j,j,p,h)}{\epsilon_h-\epsilon_p}\left[\sum_c D(h,p,c,c)-\langle h|U|p\rangle\right],$$

where

$$D(a,b,c,d)=\delta_{j_a,j_b}\sum_{J,T}\frac{(2J+1)(2T+1)}{2(2j_a+1)}\langle ac|V|bd\rangle_{J,T}.$$

The point here is that this expression involves the difference $[\Sigma_c D(h,p,c,c)-\langle h|U|p\rangle]$. This is a difference between a term involving the two-body interaction and the one-body interaction. If these are chosen independently, then this difference can be either positive or negative, and so one can get a variety of answers.

Note that if the Hartree-Fock condition of Fig. 1 is satisfied, then $\delta\epsilon_j$ (SHF) will also vanish, i.e., the factor $[\Sigma_c D(h,p,c,c)-\langle h|U|p\rangle]$ will vanish. However, in the work of Zamick, Zheng, and Müther [9], there are also what they call double Hartree-Fock (DHF) diagrams that will *not* vanish even when the Hartree-Fock condition is satisfied. The expression for these is given by

$$\delta\epsilon_j(\mathrm{DHF})=\sum_p\frac{\left[\sum_c D(j,p,c,c)-\langle p|U|j\rangle\right]^2}{\epsilon_j-\epsilon_p} -\sum_h\frac{\left[\sum_c D(j,h,c,c)-\langle h|U|j\rangle\right]^2}{\epsilon_h-\epsilon_j}.$$

In the harmonic oscillator approximation, $U=\frac{1}{2}m\omega^2r^2$, and the matrix elements are as follows:

$$\langle p|U|j\rangle=-\frac{\hbar\omega}{2}\delta_{j,j_p}\delta_{l,l_p}\delta_{n_p,n+1}\sqrt{(n+1)(n+l+3/2)}$$

and

$$\langle h|U|j\rangle=-\frac{\hbar\omega}{2}\delta_{j,j_h}\delta_{l,l_h}\delta_{n_h,n-1}\sqrt{n(n+l+1/2)}.$$

In actual shell-model calculations, however, U is a much more complicated function of r, and one usually adopts the following phenomenological expression for $\hbar\omega$:

$$\hbar\omega = \frac{45}{A^{1/3}} - \frac{25}{A^{2/3}}. \quad (2)$$

However, one may wish to vary $\hbar\omega$ in order to achieve approximate Hartree-Fock self-consistency. In such shell-model calculations, both the single Hartree-Fock and double Hartree-Fock terms given above are implicitly present, although it is not so easy to isolate these effects as it is in perturbation theory. If such effects are present one must certainly include them, and indeed in shell-model calculations this is unavoidable. However, we may perhaps choose our interaction so that such effects are minimized. As we will show below, we try out different approaches to achieve this. One is to weaken the two-body central interaction in the spirit of the work by Sharp and Zamick [4], and one is to add a two-body monopole-monopole interaction to the existing one. This latter approach is similar in spirit to the work of Hoshino *et al.* [5], except that we have a two-body interaction instead of a one-body one.

II. RESULTS OF THE CALCULATIONS

We perform our calculations in the framework of the ''no-core shell model'' (NCSM) using harmonic-oscillator basis states. The matrix diagonalization is performed for the following shell-model Hamiltonian:

$$H_{SM} = \sum_{i=1}^{A} t_i - T_{\text{c.m.}} + \sum_{i<j}^{A} v_{ij}^{eff} + \lambda\left(H_{\text{c.m.}} - \frac{3}{2}\hbar\omega\right),$$

where $T_{\text{c.m.}}$ is the center-of-mass (c.m.) kinetic energy, and the last term (with $\lambda \gg 1$) is added to remove the spurious effects of the c.m. motion from the low-lying states in the spirit of the Gloeckner-Lawson technique [10]. We have not included the Coulomb interaction, and we should also point out that our NCSM calculations involve no phenomenological single-particle energies. These are implicitly generated from the two-body *G*-matrix elements as well as the one-body kinetic energy terms in the matrix diagonalization, which is performed for us by the *m*-scheme shell-model code OXBASH [11].

In Table I we present the results of calculations of the $p_{1/2}^{-1}$-$p_{3/2}^{-1}$ ''spin-orbit'' splitting for $A=15$ both in a valence space $(0\hbar\omega)$ and in a $(0+2)\hbar\omega$ space that allows $2\hbar\omega$ excitations. We use the (x,y) interaction that was previously outlined in Ref. [12], but multiply the central interaction term by a factor p,

$$V(r) = pV_c(r) + xV_{s.o.} + yV_t. \quad (3)$$

Here $V_c(r)$ is the (spin-dependent) central interaction, $V_{s.o.}$ stands for the two-body spin-orbit interaction, and V_t stands for the tensor interaction. These interaction terms have been adjusted so as to obtain a good fit to the nonrelativistic matrix elements of the Bonn A potential with $p=1$, $x=1$ and $y=1$ [13].

In Table I we take $x=1$, $y=0$ so that there is no tensor interaction, and we have the ''normal'' spin-orbit interaction, i.e., the one obtained with a nonrelativistic *G* matrix. In our previous papers [9,12–15], we have always set p to unity, whereas here we vary p for the first time in order to make some points about self-consistency. First, we note that in the valence space, the spin-orbit splitting is due only to the $xV_{s.o.}$ term and does not depend on the strength of the central interaction (i.e., on p), whereas in the $(0+2)\hbar\omega$ space it is a decreasing function of p.

TABLE I. Calculated values of the spin-orbit splitting ESO $\equiv E(3/2^-) - E(1/2^-)$ for $A=15$, using $x=1$, $y=0$ and multiplying the central interaction V_c by the factor p, but keeping the kinetic energy term unchanged.

	ESO($0\hbar\omega$)	ESO[$(0+2)\hbar\omega$]	%$2\hbar\omega$ admixture	
p	(MeV)	(MeV)	in $1/2^-$ (ground state)	in $3/2^-$
1.2	5.062	6.134	40.53	40.39
1.0	5.062	6.008	36.60	36.29
0.8	5.062	5.659	28.07	27.56
0.6	5.062	4.525	15.13	17.39
0.4	5.062	3.714	27.75	29.70
0.2	5.062	3.607	37.09	37.80
0	5.062	3.584	41.15	41.50

The value of the $p_{1/2}^{-1}$-$p_{3/2}^{-1}$ splitting for $A=15$ in the valence space is 5.062 MeV, whereas in the large $(0+2)\hbar\omega$ space this splitting increases to 6.008 MeV for $p=1$, with the percentage of $2\hbar\omega$ admixtures in the ground state being 36.60% for $p_{1/2}^{-1}$ and 36.29% for $p_{3/2}^{-1}$. However, we see that by reducing the strength p of the central interaction, the amount of $2\hbar\omega$ admixture in the ground state first decreases until it is 15.13% for $p=0.6$, and if one reduces the value of p further, it starts to increase again, reaching 41.15% for $p=0$. We also note from Table I that, for a given value of p, the amount of $2\hbar\omega$ admixtures in both the $1/2^-$ ground state and the $3/2^-$ first excited state are very nearly equal. Indeed, more detailed calculations which involved varying p by steps of 0.01, show a minimum $2\hbar\omega$ admixture of 15.084% in the ground state at $p=0.59$ and a minimum of 17.32% for the $3/2^-$ first excited state at $p=0.61$.

These results clearly indicate that we are closest to Hartree-Fock self-consistency at $p \approx 0.6$ since, as we will show below, the $2\hbar\omega$ admixture in the ground state is smallest when the $1p$-$1h$ admixture is smallest. Moreover, we can achieve near self-consistency for the same value of p simultaneously for both the ground state and the first excited state. We also note that the calculated values of the spin-orbit splitting for $p=0.6$ are 5.062 MeV in the $0\hbar\omega$ space and 4.525 MeV in the $(0+2)\hbar\omega$ space. Clearly, for the $p=0.6$ case, there is a *qualitative* difference from the $p=1$ case,

TABLE II. Composition of the ground state $(1/2^-)2\hbar\omega$ admixture in $A=15$ as a function of the factor p multiplying the central interaction, using $x=1$ and $y=0$ and keeping the kinetic energy term unchanged (as in Table I).

p	% $(1p\text{-}1h)$	% $(2p\text{-}2h)$	Total %$2\hbar\omega$ admixture
1.2	33.7	6.8	40.5
1.0	28.7	7.9	36.6
0.8	17.8	10.3	28.1
0.7	9.7	11.1	20.8
0.65	4.9	12.2	17.1
0.6	3.3	11.8	15.1
0.55	6.0	10.2	16.2
0.5	10.6	9.1	19.7
0.4	22.5	5.3	27.8
0.2	34.8	2.3	37.1
0.0	39.3	1.8	41.1

with the spin-orbit splitting now *decreasing* when $2\hbar\omega$ admixtures are allowed into the ground state.

It may be surprising at first that, when $p=0$ (i.e., when the central interaction is set equal to zero), the amount of $2\hbar\omega$ admixture is large ($\approx 41\%$). But we must remember that the kinetic energy part of the Hamiltonian can couple a $2\hbar\omega$ $1p\text{-}1h$ ''monopole'' state to the $0p\text{-}0h$ state. Another way of saying this is that the zero-order wave functions are of the harmonic oscillator type, whereas the eigenstates of the kinetic energy operator are of the plane wave type ($\propto e^{i\vec{k}\cdot\vec{r}}$). The large admixtures of $2\hbar\omega$ excitations in both the ground state and the first excited state correspond to an attempt to change the wave functions from a harmonic oscillator type to a plane wave type.

In Table II, we show how much of the ground state $2\hbar\omega$ admixture is of type $1p\text{-}1h$ and how much of it is of type $2p\text{-}2h$. The ground state $1p\text{-}1h$ admixture drops from 33.7% for $p=1.2\%$ to 3.3% for $p=0.6$, and then rises to 39.3% for $p=0$. More detailed calculations involving steps in p of 0.01 show a minimum ground state $1p\text{-}1h$ admixture of 2.8% at $p=0.61$, and a corresponding minimum of 2.7% for the $3/2^-$ first excited state at $p=0.63$. We also note in Table II that the percent $1p\text{-}1h$ admixture varies greatly as a function of p, whereas the percent $2p\text{-}2h$ admixture changes more moderately with p as it never exceeds 13.5%. Also, for the most part, $1p\text{-}1h$ admixtures tend to dominate over $2p\text{-}2h$ admixtures, except near $p=0.6$ where the percent ground state $2p\text{-}2h$ admixture is the largest and the $1p\text{-}1h$ contributions the smallest. This is why a minimum $1p\text{-}1h$ admixture corresponds to a minimum total $2\hbar\omega$ admixture. It is well known that the $1p\text{-}1h$ admixtures should vanish when exact Hartree-Fock self-consistency is realized in the ground state. Thus, near self-consistency, the total $2\hbar\omega$ admixture is largely $2p\text{-}2h$ in origin. However, we found that for a standard central interaction ($p=1$) close to 80% of the ground state $2\hbar\omega$ admixture is of type $1p\text{-}1h$. Clearly then, we are closest to Hartree-Fock self-consistency at $p\approx 0.6$, i.e., when the central interaction is only about 60% as strong as our ''standard'' interaction.

TABLE III. Same as Table I, but this time multiplying the kinetic energy term by the factor k, and keeping the central interaction V_c unchanged.

	ESO$(0\hbar\omega)$	ESO$[(0+2)\hbar\omega]$	%$2\hbar\omega$ admixture	
k	(MeV)	(MeV)	in $1/2^-$ (ground state)	in $3/2^-$
5.0	5.062	3.664	37.2	37.4
2.0	5.062	3.972	19.2	20.8
1.6	5.062	4.760	14.4	15.5
1.2	5.062	5.773	29.9	29.4
1.0	5.062	6.008	36.6	36.3
0.8	5.062	6.137	41.2	41.1
0.4	5.062	6.266	46.6	46.7
0	5.062	6.323	49.6	49.7

In Table III, we keep the central and spin-orbit interaction terms fixed (with the standard strengths $p=1$ and $x=1$), but vary the kinetic energy by varying $\hbar\omega$. We find that we get a minimum in the percentage of $2\hbar\omega$ admixtures when the kinetic energy is increased by a factor of about 1.6. Indeed, whereas for the usual phenomenological value of $\hbar\omega=14.136$ MeV [from Eq. (2)] the amount of $2\hbar\omega$ admixtures is 36.6%, for $\hbar\omega'=1.6\hbar\omega=22.618$ MeV it is reduced to 14.4%.

These results are completely consistent with those in Table I (note that $0.6\times 1.6\approx 1$). Indeed, by multiplying the kinetic energy by the factor of 1.6, the spin-orbit splitting is calculated to be 5.062 MeV and 4.760 MeV in the $0\hbar\omega$ and $(0+2)\hbar\omega$ model spaces, respectively. Indeed, with $p=0.6$ multiplying the central component of our interaction and the kinetic energy matrix unchanged, we obtain ESO $=4.525$ MeV and 15.1%$2\hbar\omega$ admixture.

Looking into the details of the $1p\text{-}1h$ and $2p\text{-}2h$ contributions to the $2\hbar\omega$ admixture in the ground state of $A=15$, we find that the minimum $2\hbar\omega$ admixture of 13.8% occurs for $k=1.65$–1.70, whereas the minimum for $1p\text{-}1h$ contributions of 1.5% occurs for $k=1.59$–1.65. The value $k\approx 1.65$ thus minimizes *both* the $1p\text{-}1h$ admixture and the total $2\hbar\omega$ admixture in the ground state.

TABLE IV. Same as Table I, but this time keeping the central interaction V_c as well as the kinetic energy term unchanged, and multiplying the spin-orbit component of the interaction $V_{s.o.}$ by the factor x.

	ESO($0\hbar\omega$)	ESO[$(0+2)\hbar\omega$]	%$2\hbar\omega$ admixture	
x	(MeV)	(MeV)	in $1/2^-$ (ground state)	in $3/2^-$
1.5	7.593	8.934	36.80	36.38
1.2	6.075	7.186	36.67	36.32
1.0	5.062	6.008	36.60	36.29
0.8	4.050	4.820	36.53	36.28
0.6	3.037	3.625	36.46	36.28
0.4	2.025	2.324	36.40	36.29
0.2	1.012	1.215	36.35	36.30
0.0	0	0	36.32	36.32

Thus we can get close to Hartree-Fock self-consistency either by weakening the central interaction or by increasing $\hbar\omega$ and hence the kinetic energy. The approach is equivalent to making the radius of the nucleus smaller. It is also interesting to note once more by comparing Tables I and III how close the results for a given p in Table I correspond to those for $k=1/p$ in Table III (consider, for example, $p=0.2$ in Table I and $k=5.0$ in Table III).

A. The effect of varying the strength of the spin-orbit interaction

In Table IV we examine the effect of varying the strength of the spin-orbit interaction on the ground state correlations. Here again we do *not* include a tensor interaction ($y=0$) and keep the kinetic energy term as well as the central interaction term with their standard strengths (i.e., $k=1$ and $p=1$).

We see from Table IV that, as x is reduced from 1.5 to 0, the percentage of $2\hbar\omega$ admixture into the ground state does not change much, decreasing from 36.8% to 36.3%. More detailed calculations show that as x decreases from 1.5 to 0, the contribution of $1p$-$1h$ admixtures into the ground state decreases slightly from 29.2% to 27.8%, while that of $2p$-$2h$ admixtures increases slightly from 7.6% to 8.5%. For the first excited $3/2^-$ state, the percentage of $2\hbar\omega$ admixture changes even less, ranging from 36.4% to 36.3%, the contribution of $1p$-$1h$ admixtures from 27.0% to 27.9%, and that of $2p$-$2h$ admixtures from 9.3% to 8.4%. We also see from Table IV that the strength x of the two-body spin-orbit component of the effective interaction has a decisive effect on the magnitude of the ESO (the effective spin-orbit splitting of the $3/2^-$, $1/2^-$ spin doublet) in agreement with the results in Ref. [12]. In the $0\hbar\omega$ space the ESO is exactly linear in x, and in the $(0+2)\hbar\omega$ space such is also very nearly the case.

For $A=15$, the observed value of ESO is 6.324 MeV for ^{15}N and 6.176 MeV for ^{15}O [16]. The results of Table IV suggest that including $2\hbar\omega$ excitations and taking $x=1$ lead to results in closer agreement with experiment [12].

TABLE V. Same as Table I, but this time keeping the central interaction V_c, the spin-orbit interaction as well as the kinetic energy term unchanged, and multiplying the tensor component V_t by a factor y.

	ESO($0\hbar\omega$)	ESO[$(0+2)\hbar\omega$]	%$2\hbar\omega$ admixture	
y	(MeV)	(MeV)	in $1/2^-$ (ground state)	in $3/2^-$
1.2	5.062	5.623	36.72	36.56
1.0	5.062	5.698	36.66	36.47
0.8	5.062	5.769	36.63	36.40
0.6	5.062	5.836	36.61	36.35
0.4	5.062	5.898	36.59	36.31
0.2	5.062	5.956	36.59	36.30
0	5.062	6.008	36.60	36.29

B. The effect of adding a tensor interaction

In Table V we examine the effect of varying the strength of the tensor interaction on ground state correlations, keeping the kinetic energy term unchanged, the spin-orbit interaction fixed at $x=1$ and the central interaction fixed at $p=1$. From $y=1.2$ to $y=0$ there is very little change in the ground state $2\hbar\omega$ admixture, only a slight decrease from 36.72% to 36.59%. A more detailed calculation shows that for the ground state, as we vary y from 1.2 to 0, the $1p$-$1h$ admixture increases slightly from 26.5% to 28.7%, while the $2p-2h$ admixture decreases from 10.2% to 7.9%. The two changes tend to cancel each other when the two contributions are added, resulting in a total $2\hbar\omega$ ground state admixture that varies by less than 0.15% as y decreases from 1.2 to 0.

We also see from Table V that changing y from 0 to 1.2 has no effect on the ESO in the $0\hbar\omega$ space, and that it has only a very small effect (less than 7%) on the ESO in the $(0+2)\hbar\omega$ space. This is fully consistent with the results of Ref. [12], and is in line with the more modern two-nucleon interaction having a weaker tensor component [14].

C. The effect of adding a monopole-monopole interaction

We shall here adopt a poorman's self-consistency criterion by using harmonic oscillator wave functions to determine the kinetic energy. These self-consistency conditions are for each $p-h$ pair. However, in the harmonic oscillator model, there

is only one parameter $\hbar\omega$. So, rather than demanding that each individual particle-hole pair does not get admixed into the ground state, we will only demand that a linear combination of particle-hole states (namely the isoscalar monopole states) does not get mixed into the uncorrelated ground state by the Hamiltonian.

The monopole state is defined by

$$|M\rangle = N\sum_{P,H}\left\langle [a^{\dagger P}\alpha^{H}]^{0,0}\left|\sum_i r_i^2\right|0\rangle [a^{\dagger P}\alpha^{H}]^{0,0}\right\rangle$$

and, in general,

$$|M\rangle = \sum_{P,H} D_{PH}[a^{\dagger P}\alpha^{H}]^{0,0},$$

where we use the notation $[\Psi]^{J,T}$ for a given wave function, and where $\alpha_m^j \equiv (-1)^{j-m}a_{-m}^j$. Using the formula

$$\langle n+1,l|r^2|n,l\rangle = -b^2\sqrt{(n+1)(n+l+3/2)},$$

where $b^2=\hbar/(m\omega)$, we find the following monopole wave function for ^{16}O:

$$|M\rangle = \sqrt{\frac{3}{18}}[a_{1s}^{\dagger}\alpha_{0s}]^{0,0} + \sqrt{\frac{10}{18}}[a_{1p_{3/2}}^{\dagger}\alpha_{0p_{3/2}}]^{0,0} + \sqrt{\frac{5}{18}}[a_{1p_{1/2}}^{\dagger}\alpha_{0p_{1/2}}]^{0,0}.$$

The Hartree-Fock self-consistency condition that the sum of all $1p$-$1h$ admixtures into the ground state vanish can be expressed in terms of diagrams 1(a) and 1(b) of Fig. 1 as 1(a) + 1(b) =0, as discussed in the introduction.

The kinetic energy term [Fig. 1(b)] can be evaluated in the harmonic oscillator approximation by noting that

$$K = K + \sum_i \frac{1}{2}m\omega^2 r_i^2 - \sum_i \frac{1}{2}m\omega^2 r_i^2.$$

The first two terms give the harmonic oscillator Hamiltonian, which obviously cannot connect between two major shells, and the contribution of the third term is obtained from $\langle n+1,l|r^2|n,l\rangle$ given above.

The condition we imposed then, including averaging over the monopole states, is

$$\sum_{P,H} D_{PH}\frac{1}{\sqrt{2(2j_P+1)}}\sum_{I,T,C}(2I+1)(2T+1)\times\langle [PC]^{I,T}|V|[HC]^{I,T}\rangle_U = -\sum_{P,H} D_{PH}\sqrt{2(2j_P+1)}\,\frac{\hbar\omega}{2}\sqrt{(n+1)(n+l+3/2)}. \quad (4)$$

We can use this condition to determine the value of $\hbar\omega$, which leads to self-consistency. Alternatively, we can choose the two-body interaction V so that self-consistency is satisfied for a desired value of $\hbar\omega$.

TABLE VI. Same as Table I, but this time keeping the central interaction V_c, the spin-orbit interaction as well as the kinetic energy term unchanged, and adding a monopole-monopole term multiplied by the factor q.

	ESO($0\hbar\omega$)	ESO[$(0+2)\hbar\omega$]	%$2\hbar\omega$ admixture	
q	(MeV)	(MeV)	in $1/2^-$ (gound state)	in $3/2^-$
1.0	5.062	3.651	62.430	62.40
0.50	5.062	3.644	62.411	62.349
0.10	5.062	3.539	58.393	58.168
0.045	5.062	4.558	26.975	28.653
0.01	5.062	5.900	36.02	35.654
0	5.062	6.008	36.60	36.29
−0.1	5.062	6.312	37.392	37.241
−0.5	5.062	6.399	37.292	37.241
−1.0	5.062	6.409	37.235	37.208

The values of $\hbar\omega$ we obtain for ^{16}O are as follows (in MeV):

Using the Hartree-Fock criterion	Using $\hbar\omega = 45/A^{1/3} - 25/A^{2/3}$	Ratio k
22.143	13.920	1.591

The ratio k obtained above is remarkably consistent with that obtained in the $A=15$ calculation for which the kinetic energy parameter $\hbar\omega$ gives the least amount of $2\hbar\omega$ admixture into the ground state of the ^{15}O nucleus (see Table III).

In Table VI we examine the effect of adding a monopole-monopole term to the interaction on the $2\hbar\omega$ admixture in the ground state of ^{15}O. This is similar in spirit to what Hoshino *et al.* [5] do, except that we add a two-body interaction and they add a one-body term $\Sigma_i r_i^2$. In both cases, the motivation is to reduce the overall $1p$-$1h$ coupling term. Hence, the Hamiltonian used is

$$V(r) = pV_c(r) + xV_{s.o.} + qV_{monopole} \quad (5)$$

and where $V_{monopole}$ is defined by its two-body matrix element

TABLE VII. Excitation energies of dominantly $2p$-$2h$ states calculated with various interactions in a $(0+2)\hbar\omega$ model space. The intreactions are denoted by the following coupling coefficients: k for the kinetic energy term, p for the central interaction, x for the spin-orbit interaction, y for the tensor interaction, and q for the monopole-monopole interaction. The percentages of the $2p$-$2h$ admixture in the wave functions of the excited states are shown in parentheses.

Interaction	$J=1/2^-$ $2p$-$2h$ state	$J=3/2^-$ $2p$-$2h$ state
$k=1,\ p=1,\ x=1,\ y=1,\ q=0$	$E_x=43.260$ MeV (89%)	$E_x=43.594$ MeV (95%)
$k=1,\ p=1,\ x=1,\ y=0,\ q=0$	$E_x=41.829$ MeV (90%)	$E_x=42.250$ MeV (100%)
$k=1,\ p=0.6,\ x=1,\ y=0,\ q=0$	$E_x=19.914$ MeV (95%)	$E_x=20.055$ MeV (97%)
$k=1.6,\ p=1,\ x=1,\ y=0,\ q=0$	$E_x=34.823$ MeV (93%)	$E_x=34.569$ MeV (95%)
$k=1,\ p=1,\ x=1,\ y=0,\ q=0.045$	$E_x=21.671$ MeV (92%)	$E_x=21.203$ MeV (95%)

$$\langle j_1 j_2|V_{monopole}|j_3 j_4\rangle = \frac{1}{\sqrt{1+\delta_{1,2}}}\frac{1}{\sqrt{1+\delta_{3,4}}}\delta_{j_3,j_1}\delta_{l_3,l_1}\langle R_3|r^2|R_1\rangle \times \delta_{j_4,j_2}\delta_{l_4,l_2}\langle R_4|r^2|R_2\rangle$$

with R_i being the radial wave function of a Harmonic oscillator shell $|i\rangle\equiv|n_i,l_i,j_i\rangle$.

Note that we do not include a tensor component, and that we keep the strengths of the central, spin-orbit, and kinetic terms fixed at $p=x=k=1$. We find that, by varying the strength q of the monopole-monopole term, it is possible once again to minimize the total percentage of $2\hbar\omega$ admixture in the ground state. The minimum percentages of $1p$-$1h$ admixtures occur at $q=0.045$ and are equal to 3.76% for the $1/2^-$ state and 1.09% for the $3/2^-$ state. Interestingly, the minima occur for a very small but nonzero value of q. Furthermore, the minimum percentage of $2\hbar\omega$ admixture ($\approx$27%, corresponding to $q=0.045$) is about twice that obtained by varying the strength of the central interaction V_c or by increasing the kinetic energy term.

III. ADDITIONAL REMARKS AND SUMMARY

In this paper we studied the effects of changing the strengths of various parts of a typical nuclear Hamiltonian on the correlations in the wave functions of the two lowest states in the $A=15$ system. We found that the amount of $2\hbar\omega$ admixtures in the nuclear wave functions is quite insensitive to varying the strengths of the two-body spin-orbit and tensor components of the effective interaction. It is, however, very sensitive to changing the strength of the central two-body interaction, to the magnitude of $\hbar\omega$ (i.e., the magnitude of the kinetic energy term), and to the strength of a monopole-monopole interaction term that we add to the Hamiltonian.

The $2\hbar\omega$ admixtures in the nuclear wave functions have both $1p$-$1h$ and $2p$-$2h$ contributions. We find that usually the minima of the $2\hbar\omega$ admixtures occur when $1p$-$1h$ contributions are the smallest. We show that, by carefully decreasing the strength of the central component of the two-body nuclear interaction by a factor of about 0.6 (or, alternatively, by increasing the value of $\hbar\omega$ by a factor of about 1.6), we can minimize the $1p$-$1h$ admixtures, making them very small (less than 4%). We have found that, typically, the $1p$-$1h$ admixtures are minimized under the same conditions for the ground state and for the first excited state.

We have shown that the results we have just stated are closely related to the Hartree-Fock self-consistency condition, which states that the Hartree-Fock Hamiltonian does not allow one-particle-one-hole admixtures into the ground state. Indeed, by making some judicious and reasonable adjustments to a realistic effective N-N interaction, we have shown that it is possible to do no-core shell-model calculations in a harmonic-oscillator basis and still come fairly close to Hartree-Fock self-consistency.

The main result of this work, however, is to show that one gets *qualitative* differences in the relative values of the ''spin-orbit splitting'' when one includes higher shells, depending upon whether our interaction is close to Hartree-Fock self-consistency or not. As shown for example, in Table III, when we use the value of $\hbar\omega=45/A^{1/3}-25/A^{2/3}$ (MeV) in the kinetic energy term (a choice that gives a good radius for most nuclei), we find that the splitting $E(3/2^-)-E(1/2^-)$ in $A=15$ as calculated in a $(0+2)\hbar\omega$ model space differs from that calculated in a $0\hbar\omega$ model space by $+0.946$ MeV. However, when we vary the value of $\hbar\omega$ in order to achieve Hartree-Fock self-consistency, the difference in the splitting is now -0.302 MeV. This shows that one has to take care in how one interprets the results of higher-shell admixtures.

A. Hartree-Fock self-consistency and the $2p$-$2h$ states

In Table VII, and for the various interactions considered so far, we list the calculated energies of the lowest excited $J=1/2^-$ and $J=3/2^-$ states that are dominantly $2p$-$2h$ (or $2p$-$3h$ relative to the ^{16}O core). Recalling that our model space consists of $(0+2)\hbar\omega$ excitations, we expect the states to be too high in energy. However, one gratifying result is that the excitation energies come down by a large amount when the self-consistency criteria are applied.

With the original realistic interaction ($k=1,\ p=1,\ x=1,\ y=1,\ q=0$), the excitation energies are very high: 43.260 MeV and 43.594 MeV, respectively. Turning off the tensor interaction does not make much of a change (41.829 MeV and 42.250 MeV). However, if we weaken the central interaction ($p=0.6$) to achieve self-consistency, the excitation energies of these states come down by more

than a factor of 2 (to 19.914 MeV and 20.055 MeV, respectively). Similar results are obtained by keeping the full central interaction ($p=1$), but introducing the monopole-monopole term ($q=0.045$). In this case, the excitation energies also come down to 21.671 MeV and 21.203 MeV.

Obviously, the beneficial effects come from the reduction of the $1p-2h$ coupling to the $1h$ state relative to the ^{16}O core, where in the latter it would be the $1p$-$1h$ coupling to the $0p$-$0h$ state. There is much less level repulsion when the Hartree-Fock self-consistency criteria are applied, and we expect that these excited states will come down even lower in energy when $4\hbar\omega$ excitations are allowed.

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