Evolution of the N=20 and 28 Shell Gaps and 2-particle-2-hole states in the FSU Interaction.

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Abstract

The connection between fundamental nucleon-nucleon forces and the observed many-body structure of nuclei is a main question of modern nuclear physics. Evolution of the mean field, inversion of traditional shell structures and structure of high spin states in nuclei with extreme proton to neutron ratios is at the center of numerous recent experimental investigations targeting the matrix elements of the effective nuclear Hamiltonian that is responsible for these phenomena. The FSU spsdp cross-shell interaction for the shell model was successfully fitted to a wide range of mostly intruder negative parity states of the sd shell nuclei. This paper reports the application of the FSU interaction to systematically trace out the relative positions of the effective single-particle energies (ESPE) of the 0f7/2 and 1p3/2 orbitals forming the N = 20 and 28 shell gaps, we explore the evolution from normally ordered low-lying states to the Island of Inversion (IoI). We find that above a proton number of about 13 the 0f7/2 orbital lies below that of 1p3/2, which is considered normal ordering, but systematically at Z = 10 to 12 the orbitals cross. Our Hamiltonian reproduces remarkably well the absolute binding energies for a broad range of nuclei, and the 2p2h - 0p0h inversion in the configurations of nuclei inside the IoI. The important role of 1p3/2 neutron pairs in the IoI is also demonstrated. Our results account well for the energies of the fully aligned states with 0, 1, or 2 individual sd nucleons aligned in spin with the aligned π0f7/2 - ν0f7/2 pair and reproduce well their systematic variation with A and number of aligned sd nucleons. As a result, this paper presents a successful empirically determined effective Hamiltonian as an important tool for further experimental work. The results presented in this paper give hope for the predictive power of the FSU interaction for more exotic nuclei to be explored in the near future.

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I. INTRODUCTION

Recent experimental works in the $1s0d$ shell with large $\gamma$ detector arrays and heavy-ion fusion reactions have substantially extended knowledge of relatively high spin states. However, these do not form well-behaved rotational bands amenable to study by collective models because rotational energies are comparable to single-particle energies. On the other hand microscopic configuration-interaction model calculations are feasible in these lighter nuclei. The USD family of effective interactions $^{1,2}$ have been very successful in describing most lower-lying positive-parity states of nuclei with $8 \leq (N, Z) \leq 20$. However, higher spin states involve excitations into the $fp$ shell where orbitals contributing larger values of angular momentum are occupied, which is beyond the scope of the USD interaction. Also, neutron-rich isotopes quickly move beyond the $sd$ shell boundaries $^{3-8}$.

Several configuration interaction models over the years have made significant contribution in explaining cross-shell excitations $^{9-13}$. A case in point is the “Island of Inversion” (IoI). Perhaps in an inverse way the first contribution came from the failure of the otherwise very successful pure $sd$ interactions $^{1,2}$ to reproduce the stronger binding energy measured for $^{31}$Na $^{14}$, pointing to the importance of effects outside the $sd$ shell. Pioneering shell model calculations using interactions like SDPF-NR $^{9}$, SDPF-M $^{12}$, SDPF-U-MIX $^{13}$ have shown that the IoI phenomenon can be accounted for a reduction of the $N = 20$ shell gap. Recently a significant theoretical result was reported, see Ref. $^{15}$, showing the emergence of IoI effect from nucleon-nucleon forces stemming from the fundamental principles of QCD. This highlights the importance of certain cross $sd$ - $fp$ interaction terms that we assess in this work using experimental systematics.

In search for a single cross-shell interaction which works well over a wide range of nuclei, we have developed a new interaction $^{16}$ with parallel treatment of protons and neutrons by fitting the energies of 270 states in nuclei from $^{13}$C through $^{51}$Ti and $^{49}$V originated from the WBP interaction $^{17}$ using well-established techniques. As already described in Ref. $^{16}$ the USDB Hamiltonians were used for the $sd$ shell and were kept fixed whereas 40 linear combinations of 70 single-particle and two-body matrix elements were varied. The resulting root-mean-square (RMS) difference was 190 keV for all 270 states. For comparison, an RMS deviation of 130 keV was achieved with the USDB interaction $^{2}$ over 608 pure $sd$ states in 77 nuclei where 56 linear combinations of the total 66 elements of the Hamiltonian were varied.
Fewer states, mostly cross-shell excited, were included in the FSU fit as few are known with firm spin assignments. This also limits the number of interaction parameters which can be determined reliably. All the shell model calculations in this paper were performed with the shell model code CoSMo [18]. A graph of the differences between experiment and theory is shown in Figure 1. No $0p0h$ $sd$ states are included in this figure or the fit because the USDB interaction which was previously fitted to them was used unchanged. Predictions from the FSU interaction have compared well with the experimental data presented in Refs. [16] and [19]. In the present report we are applying the model to understand a few interesting features of the $sd$-shell nuclei.

II. EFFECTIVE SINGLE PARTICLE ENERGY (ESPE)

A key question in any shell model is the single particle energies of the orbitals and how their positions change with the changing number of protons and neutrons. This is a particularly interesting and non-trivial question in the strongly-interacting two-component many-body system of atomic nuclei because the ideal single-particle strength is distributed over many states. Systematic studies have been performed before with other shell model interactions [10, 12, 20] to understand the evolution of the ESPE. An experimental approach of determining the ESPEs has been to measure and sum up the energies of appropriate states (such as $7/2^-$) weighted by the reaction spectroscopic factors. This process is limited by decreasing cross sections for higher lying states, difficulties of making spin assignments and of determining what fraction of the cross sections come from direct reaction components. Theoretical approaches do not suffer from most of these experimental limitations, but have their own uncertainties. Perhaps chief among them being the reliability of the determination of the interaction. The FSU interaction was fitted to a wide range of mostly negative-parity states in $sd$ nuclei involving one particle in the $fp$ shell. As such, it samples a broad spectrum of configurations not limited by those experimentally reachable with single-nucleon transfer reactions. The bare single-particle energies in this or any other such interaction tell only part of the story of the effective shell positions. The two-body matrix elements (TBME) between $sd$ and $fp$ nucleons have a major influence on the positions of the orbitals. In fact, the TBMEs shift the orbitals based on the number of particles in shells and are the major reason that one interaction could fit such a wide range of nuclei.
In order to determine the ESPE of the $0f_{7/2}$ and $1p_{3/2}$ orbitals, we have followed a procedure similar to the experimental approach, but using the theoretical state energies and calculated neutron spectroscopic factors using the following formula:

$$\text{ESPE} = \frac{\sum_{i=1}^{30} SF_i \times E_i^*}{\sum_{i=1}^{30} SF_i}$$

(1)

where, $SF_i$ is the spectroscopic factor and $E_i^*$ is the excitation energy of the $i$-th state for a given spin calculated with the FSU interaction. It has been observed from the calculations that the SF reach a saturation within first 30 states. From the formal theoretical perspective, Eq. 1 represents single particle energies of the mean field determined by the exact diagonalization of the shell model Hamiltonian.

The ESPEs obtained from the above formula across the $sd$ shell are plotted in Figure 2 as a function of proton number $Z$. The points represent the ESPEs of the $0f_{7/2}$ and $1p_{3/2}$ orbitals above the ground state for one neutron added to the even-even nuclei indicated in the Figure. The systematic crossing of the ESPEs of the $0f_{7/2}$ and $1p_{3/2}$ orbitals with increasing neutron number is evident in the Figure. The cross occurs between $Z = 10$ and 12, suggesting that the $N = 28$ shell gap shifts to $N = 24$ with lower $Z$, which points to the inversion of $0f_{7/2}$ and $1p_{3/2}$ neutron orbitals. The ground state of $^{31}\text{Ne}$ is tentatively assigned $3/2^-$ as is the first excited state in $^{27}\text{Ne}$ [21]. In $^{27}\text{Mg}$ the lowest $3/2^-$ and $7/2^-$ states are essentially degenerate [21].

This inversion of the $1p_{3/2}$ and $0f_{7/2}$ ESPE is related to the 2-body interactions between nucleons in the $sd$ and $fp$ shells; the effect of this interaction is density dependent and varies as a function of shell filling. In the FSU interaction these TBME emerge as a consequence of fitting the energies of the states in a wide range of nuclei. Over half a century ago Talmi and Unna [22] attributed the inversion of the $1s_{1/2}$ and $0p_{1/2}$ orbitals to the same principle. Alternate explanations, especially for the $1s_{1/2}$ and $0p_{1/2}$ case, have been given in terms of the effects of weak binding on the mean field of low $\ell$ orbitals. Hoffman et al. [23] have explored the weak binding effect for pure single-particle shells in a Woods-Saxon potential and have shown that it is large near the threshold for neutron $s$ states. While much smaller for $p$ states, there is still a crossing between the $0p_{1/2}$ and $0d_{5/2}$ orbitals at the threshold. A similar effect for the $1p_{3/2}$ and $0f_{7/2}$ orbitals could be a contributing factor to the inversion shown in Figure 2. If so, then it was incorporated through the fitting of
the effective interaction, but this can be a challenge for theoretical methods that do not take continuum of reaction states into account. This inversion of the $1p_{3/2}$ and $0f_{7/2}$ ESPE at high neutron excess also has implications for the IoI phenomenon discussed in the next section.

Another way of examining the systematics of shell evolution and migration which is closer to experiment is from the positions of the states carrying the largest part of the single-particle strength. Such a comparison is shown in Table I which lists the experimental and theoretical excitation energies of the lowest $3/2^+$, $7/2^-$, and $3/2^-$ states, of the even $Z$ odd mass nuclei, along with the predicted and measured ($d$, $p$) reaction spectroscopic factors (SF). As mentioned before, there is more uncertainty in measuring the values of SF than excitation energies and in some cases the SF cannot (lack for appropriate targets) or have not been measured. With this in mind, the agreement is generally good between experiment and predictions using the FSU interaction for both excitation energies and SF. Also the relatively large values of the SF show that these represent the dominant single-particle states.

Figure 3(a) provides a pictorial summary of the relative positions between the $7/2^-$ and $3/2^-$ states as a function of the proton number $Z$. The black circles and red lines show the average values from Table I for experiment and theory, respectively, while the black error bars represent the variation of the experimental differences. The observed trends are reproduced by theory, see Figure 3(a). This graph agrees qualitatively with those in Figure 2. It demonstrates that the evolution of the separation between the $7/2^-$ and $3/2^-$ states is largely a function of the proton number $Z$ and that the $3/2^-$ energies drop below the $7/2^-$ ones between $Z = 14$ and 12. By comparison and contrast the ESPEs which represent the center of gravity of many such states and approximate the positions of the $0f_{7/2}$ and $1p_{3/2}$ orbitals also show $1p_{3/2}$ falling below $0f_{7/2}$ with decreasing $Z$, but the crossing lies a little lower between $Z = 10$ and 12. Together these show that the trend is robust, but that what seems like such a simple question of the relative position of the orbitals is more complex and nuanced than was expected earlier.
III. EVOLUTION OF THE N=20 SHELL GAP AND THE ISLAND OF INVERSION (IOI)

One of the first indications that the pure sd shell model could not represent low-lying states in all sd nuclei came from the experimentally measured mass of $^{31}\text{Na}$ [14]. The experimental mass was $\approx 1.6$ MeV lower than that predicted from the USD interaction [1] which did account for the other ground state masses. This was further clarified when many more sd states, but not those for the highest $N - Z$ nuclei were fitted. A consistent over-prediction of 1 to 2 MeV of the ground state energies of these nuclei can be seen in Figure 9 of Ref. [2]. This region of nuclei is now known as the “Island of Inversion” (IoI) and its origin has been discussed a lot. Most explanations center around the filled or almost filled neutron sd shell and fp intruder configurations leading, counter-intuitively, to lowering the energy of the 2p2h state below that of the “normal” 0p0h one through increased correlation energy or higher deformation, lowering Nilsson orbitals. However the effect fades away with filling of the proton sd shell, and this should also be accounted for in complete theoretical calculations.

While a number of shell model calculations in the past have reproduced many aspects of the IoI, as discussed in the Introduction, here we study what the FSU interaction, which was not fitted to any 2p2h states, would predict for this basically 2p2h effect. We first discuss the case of $^{31}\text{Na}$ ($N = 20$) [14]. As shown in Figure 4 the total binding energies for the first four 2p2h states were found to be below that of the lowest 0p0h state. The first three 2p2h states agree well with what is so far known experimentally, whereas the spin sequence of the first two 0p0h states is opposite to experiment. Within the limited experimental information available, the FSU interaction has depicted the correct picture of $^{31}\text{Na}$ as one with the inverted configuration. As mentioned above, only the low $Z$ and $N \approx 20$ nuclei exhibit the IoI or inverted 2p2h - 0p0h behavior. To explore the transition from IoI to “normal” behavior, Figure 5 compares experimentally measured energies and calculations with the FSU cross-shell interaction for the lowest levels in a sequence of $N = 20$ even $A$ sd nuclei. For $Z = 10$ and 12, not only do the lowest states have 2p2h character, but the whole 0$^+, 2^+, 4^+$ 2p2h sequence agrees well with experiment. In addition to starting much higher in energy, the spacing between 0p0h states differs significantly from experiment. The story changes for $Z = 14$ where the 0p0h 0$^+$ state is substantially lower than the 2p2h
one. Above this the second experimental $0^+$ and first $2^+$ states are much closer to the $2p2h$ ones while the second experimental $2^+$ level corresponds well with the $0p0h$ one in a clear illustration of shape coexistence, as discussed in Ref. [24] also. For $Z = 16$ and $18$ both the first experimental $0^+$ and $2^+$ states correspond with the $0p0h$ calculations. The second $0^+$ states in both the nuclei were discussed to have $2p2h$ dominant configurations [25–27] and are in very good agreement with the FSU predictions. The $4^+$ states of $^{36}S$ and $^{38}Ar$ lie much closer to the calculated $2p2h$ ones. Note that the FSU cross-shell interaction describes the transition from inverted $0p0h$-$2p2h$ order to normal as a function of $Z$ despite not having been fitted to any of these states.

This interpretation of the IoI does not involve any $fp$ orbitals dropping below the $sd$ shell, at least not for spherical shape. The lowering in energy of the $2p2h$ configurations does not extend so much to $1p1h$ ones, as shown for $^{31}Na$ in Figure 4. The lowest $1p1h$ state (3579 keV, $3/2^-$) lies over an MeV above the lowest $0p0h$ state. So it is the promotion of a neutron pair to the $fp$ shell which lowers the $2p2h$ configuration so much. The promotion of a neutron pair to the $fp$ orbital appears to lower its energy because of correlation energy in the shell model. In a geometrical picture this corresponds to increased prolate deformation due to promotion of the pair into a down-sloping Nilsson orbital whose excitation energy decreases rapidly with increasing deformation. An indication of this difference in deformation is shown in the lower panel of Figure 6. For $^{30}Ne$ and $^{32}Mg$ the calculated $B(E2)$ transition strengths from the lowest $2^+$ to ground states (both of which have $2p2h$ configurations) are relatively large at over 400 $e^2fm^4$, consistent with relatively high deformation, and agree relatively well with experiment. In contrast those for $^{36}S$ and $^{38}Ar$ are rather low, consistent with near spherical shape, although slightly higher than experiment.

The calculated total binding energies are compared with the measured ground state masses from the 2016 mass evaluation in Table Ⅲ. Looking at the $N = 20$ isotonic chain, the agreement is quite good with an RMS deviation of 257 keV comparing the $2p2h$ results below $A = 33$ and with $0p0h$ for higher $Z$. Note that the definition used here where the number of particle-hole excitations (npnh) is relative to the dominant g.s. configuration. For nuclei up to $N = 20$ npnh means $n$ nucleons in the $fp$ shell. For $N = 21$ $0p0h$ ($2p2h$) configurations have $1(3)$ nucleons in $fp$ and for $N = 22$ $2p2h$ actually have $4$ $fp$ nucleons. Figure 7 gives a wider view of the differences between experiment and theory of the binding energies around the IoI. For $10 \leq Z \leq 12$ and $19 \leq N \leq 21$ the $2p2h$ inverted
configuration is lower in energy and agrees better with experiment. Outside this range the 0p0h configuration is lower and agrees better with experiment. For \( N = 22 \) it appears that promoting a second neutron pair to \( fp \) does not increase binding enough to compensate for the extra cost of promoting that pair.

Since the IoI involves excitations into the \( fp \) shell, the question arises how the inversion of the \( 0f_{7/2} \) and \( 1p_{3/2} \) single particle energies at low \( Z \) discussed above affects our understanding of the IoI. The answer, within the context of the FSU interaction which predicts the IoI well without having been fitted to these nuclei, is shown in Table III. This table shows some of the \( fp \) shell occupancies calculated for the lowest 2p2h states in Figures 4 and 5 along with some 1p1h calculations for negative-parity states in \( ^{31}\text{Na} \). There is almost no proton \( fp \) occupancy calculated for these nuclei and there is a relatively constant \( \nu 1p_{1/2} \) occupancy of about 0.1 neutron. For \( Z = 10 \ ^{30}\text{Ne} \), which is the most strongly inverted, the \( \nu 1p_{3/2} \) occupancy is about twice that of \( \nu 0f_{7/2} \). With increasing \( Z \), the ratio of \( \nu 1p_{3/2} \) to \( \nu 0f_{7/2} \) decreases steadily from about 2 to about 0.2 across this region. Of course, the energies of the 2p2h configurations rise above that of the 0p0h ones around \( Z = 14 \). This is perhaps illustrated more clearly in Figure 3(b) which shows the \( \nu 1p_{3/2} \) and \( \nu 0f_{7/2} \) occupancies of the lowest 2p2h states in the \( N = 20 \) nuclei as a function of proton number \( Z \). Note that for \( ^{34}\text{Si} \) the 2p2h \( 0^+ \) state lies 2432 keV above the 0p0h ground state but the 2p2h \( 2^+ \) level lies close in energy with the lowest experimental \( 2^+ \) state. Together these calculations imply that the \( \nu 1p_{3/2} \) orbital plays a larger role in the IoI phenomenon than does the \( \nu 0f_{7/2} \) one.

IV. FULLY ALIGNED STATES

In describing the states used in the fit of the FSU interaction, we included only 0p0h(1p1h) configurations for natural(unnatural) parity sectors. In particular, no 2p2h configurations were used to adjust the interaction parameters. After the fitting, two early tests were performed to explore the predictive properties of the FSU interaction for 2p2h configurations. One was a calculation of the lowest 2p2h \( 7^+ \) states in \( ^{34}\text{Cl} \) and \( ^{36}\text{Cl} \) [16]. These agreed within 200 keV with the experimental states. The other test was performed on \( ^{38}\text{Ar} \) [19], since experimental states up to \( 8^+ \) and \( (10^+) \) are known. Calculations using the USD family of interactions agree within 200 keV with the excitation energy of the lowest \( 2^+ \) state of \( ^{38}\text{Ar} \), but over-predict the lowest experimental \( 4^+ \) level by over 3 MeV. With only two holes in
the $sd$ shell, the maximum spin from coupling two $0d_{3/2}$ protons is $2\hbar$. The very high $4^+$ energy represents the cost of promoting a $0d_{5/2}$ proton to $0d_{3/2}$, but nature finds another less energetic way of achieving $4^+$. This must be by promoting an $sd$ nucleon pair to the $fp$ shell. A 2p2h calculation with the FSU interaction predicts the lowest $4^+$ level only 300 keV above the experimental one, and it predicts the $6^+$ state 200 keV below experiment, while the predicted $8^+$ state is 100 keV above experiment as shown in Ref. [19].

With this success we have searched for other states with confirmed 2p2h structure to compare with theory. One such group of excited states across the $sd$ shell are often called the “fully aligned” states. One subgroup of fully-aligned states is the lowest $J^\pi = 7^+$ states. These states have been suggested to have both odd nucleons in the highest spin orbital around $0f_{7/2}$ and with their spins fully aligned, which, from the Pauli principle, is only possible for non-identical nucleons. For these calculations it is critical that the FSU interaction treats protons and neutrons on an equivalent basis. These fully-aligned $\pi f_{7/2} \otimes \nu f_{7/2}$ are yrast and strongly populated in high-spin $\gamma$-decay sequences. Stronger evidence of their unique nature comes from $(\alpha,d)$ reactions [29–35] where they are the most strongly populated states with an orbital angular momentum transfer of $\ell = 6$. In most cases such states involve two nucleons beyond those in the dominant ground state configuration outside the $sd$ shell. The energies of these $7^+$ states (including those in $^{34}$Cl and $^{36}$Cl mentioned above) are graphed in Figure 8 along with calculated results using the FSU interaction. The agreement is quite good both in value and in the trend which extends from 10 MeV for the lightest nuclei down to 2 MeV for the heaviest and from 2p2h to 1p1h excitations relative to the ground state. The calculations also indirectly confirm the spin alignment with approximately equal proton and neutron occupancies in the $0f_{7/2}$ orbitals, even though most 2p2h states in these neutron-rich nuclei as discussed in the IoI section involve predominantly two neutron configurations.

Fully aligned states are also known for some odd-A nuclei where an $sd$ nucleon is also aligned in spin with the aligned $0f_{7/2}$ nucleons. Five such cases in Figure 8 are known experimentally as the strongest states populated in $(\alpha,d)$ reactions. They have an unpaired nucleon in the $0d_{3/2}$ orbital which contributes an extra spin of $3/2\hbar$. Again the 2p2h and 1p1h calculations with the FSU interaction agree well. In lighter odd-A nuclei the aligned $sd$ nucleon could be in the $1s_{1/2}$ or $0d_{5/2}$ orbitals, leading to total spins of $15/2$ or $19/2$ and higher excitation energies. Their calculated energies are also shown in Figure 8 but none
have been seen in \((\alpha, d)\) reactions. An \((11/2^+, 15/2^+)\) state which decays only to the lowest \(13/2^+\) state and is very likely the \(15/2^+\) fully aligned state has been reported \([21]\) in \(^{31}\text{P}\), as shown in the figure would agree well with the predictions.

The last category of aligned states in the \(sd\) shell is those in even-even nuclei. Their excitations involve the breaking of a proton and a neutron pair and promotion of one of each nucleon to the \(0f_{7/2}\) orbital, with, for example, all 4 unpaired nucleons coupled to maximum spin of \(10^+\) if both unpaired \(sd\) nucleons are in the \(0d_{3/2}\) orbital. No \((\alpha, d)\) reactions to the fully aligned state in even-even nuclei are known because of the absence of stable odd-\(Z\) odd-\(N\) targets in the \(sd\) shell. However, the lowest experimentally known \(10^+\) state in \(^{38}\text{Ar}\) observed by other reactions does compare well with a \(2p2h\) calculation using the FSU interaction, as shown in Figure \(8\). In the case of \(^{42}\text{Ca}\) the analogous state would involve breaking a \(\pi d_{3/2}\) pair, promoting one proton to \(0f_{7/2}\), breaking the \(\nu f_{7/2}\) pair and coupling them to maximum spin for a total of \(11^-\). This state has been seen in \(\gamma\) decay following fusion-evaporation and its energy agrees well with the FSU calculation. We hope that future experiments in the FRIB age will be able to test these predictions.

V. SUMMARY

This report has focused on a comprehensive study of \(2p2h\) excitations outside the \(sd\) shell using the cross shell FSU interaction. In the FSU interaction, mostly the \(sd - fp\) two-body matrix elements had been adjusted to best describe experimental energy states as listed in Ref. \([16]\). This paper demonstrates that the effective cross shell matrix elements determined in \(1p1h\) excitations are consistent in describing evolution of the effective single-particle energies (ESPE) as well as the \(2p2h\) states and the Island of Inversion (IoI) phenomena. As such it is well positioned to predict how the positions of the lowest \(fp\) orbitals shift with the filling of the \(sd\) shells. The resulting ESPEs of the \(0f_{7/2}\) and \(1p_{3/2}\) (the ones best determined by the fitting process) show the expected normal ordering of \(0f_{7/2}\) below \(1p_{3/2}\) for \(Z > 12\) and a consistent trend of a decreasing separation with decreasing \(Z\) until the energy order reverses around \(Z = 10\) to 12. While there have been many indications of inverted shell ordering in the past, these results present a more systematic picture from a model very firmly rooted in data. Perhaps somewhat surprisingly, over the range explored here, the inversion appears to depend more on the proton number than the neutron excess. For comparison, the
lowest $3/2^+$, $7/2^-$, and $3/2^-$ experimental states were surveyed for a complementary view of shell evolution. These energies were compared with predictions of the FSU interaction in excitation energies and spectroscopic factors. They present a similar picture of the $0f_{7/2} - 1p_{3/2}$ shell evolution as a function of proton number $Z$ although the inversion occurs at a slightly higher proton number of $12 \leq Z \leq 14$.

Ideally if an interaction is well determined from states involving just one nucleon promoted from the ground state configuration leaving an $sd$ hole behind ($1p_1h$), it should also describe $2p_2h$ excitations. The FSU interaction was applied to the IoI region, where nuclei are more tightly bound than predicted by the USD family of interactions in the pure $sd$ model space ($0p_0h$), by calculating the absolute binding energies of the lowest few states in a range of $N = 20$ nuclei from Ne ($Z = 10$) to Ar ($Z = 18$). The $2p_2h$ configurations have lower binding energies and agree well with the measured ground state masses in the range $10 \leq Z \leq 12$ and $19 \leq N \leq 21$, while the $0p_0h$ configurations are lower in energy and agree better with the measured masses elsewhere. The lowest $2^+$ states agree well with the $2p_2h$ calculations in the region $Z = 14$ and with $0p_0h$ for $Z = 16 - 18$. The results of the FSU interaction which was not fitted to these states reproduce well both the IoI and the transition to normal behavior. $^{34}$Si with $Z = 14$ emerges as transitional with a $0p_0h$ ground state and a $2p_2h$ lowest $2^+$ state. It would be interesting to locate experimentally the $4^+_1$ state which is predicted as $2p_2h$ at 5523 keV. Another implication of the FSU shell model calculations is that $\nu 1p_{3/2}$ pairs dominate over $\nu 0f_{7/2}$ ones in the IoI, but $\nu 0f_{7/2}$ pairs dominate the lowest $2p_2h$ states beyond the IoI. Interestingly the IoI coincides relatively well with the region where the $\nu 1p_{3/2}$ orbital falls below the $\nu 0f_{7/2}$ one.

Another success of the FSU interaction has been the calculation of the energies and occupancies of the fully aligned states, first identified in the early 1960's in ($\alpha, d$) reactions and frequently observed in high-spin $\gamma$-decay cascades. Most involve $2p_2h$ excitations relative to the ground state. Their energies are reproduced very well across the mass range, and their occupancies prove the excitation of both protons and neutrons, even though pure neutron excitations are more common in other states.

Additionally, this work brings forward an interesting comparison between traditional shell model interactions, with those arising from first principles methods. While the former are obtained from simply fitting SPEs and TBMEs to experimental data, the latter require renormalizations, many-body forces and explicit inclusion of the reaction continuum
to achieve agreement with experiment. This dichotomy, presents a modern challenge to
uclear theory and deserves a full investigation.

The capability of the FSU interaction to explain the exotic phenomena of the nuclei
carries the prospect that the interaction will be successful for more exotic nuclei or states.
It is hoped that the interaction will prove valuable in the coming FRIB age.

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TABLE I: Comparison of the experimentally observed $7/2^-$, $3/2^-$ and $3/2^+$ states of even $Z$ odd mass $sd$-shell nuclei to the predictions by the FSU interaction. The measured spectroscopic factors were taken from NNDC [21]. All the experimental spectroscopic factors were compiled from the $(d, p)$ reactions.

| Nucleus | $J^\pi$ | Energy (2J+1)SF | EXP | Th | EXP | Th |
|---------|--------|----------------|-----|----|-----|----|
| $^{25}$Ne | $7/2^-$ | 4030 | 3957 | 5.8 | 4.5 |
|         | $3/2^-$ | 3330 | 3471 | 3.0 | 1.9 |
|         | $3/2^+$ | 2030 | 2044 | 1.6 | 1.8 |
| $^{27}$Ne | $7/2^-$ | 1740 | 1634 | 2.8 | 3.9 |
|         | $3/2^-$ | 765  | 858  | 2.6 | 2.4 |
|         | $3/2^+$ | 0    | 0    | 1.7 | 2.8 |
| $^{25}$Mg | $7/2^-$ | 3971 | 3902 | 2.2-3.3 | 3.9 |
|         | $3/2^-$ | 3413 | 3525 | 0.9-1.2 | 1.5 |
|         | $3/2^+$ | 974  | 1098 | 0.8  | 0.9 |
| $^{27}$Mg | $7/2^-$ | 3761 | 3827 | 4.6  | 3.5 |
|         | $3/2^-$ | 3559 | 3644 | 1.6  | 2.2 |
|         | $3/2^+$ | 984  | 994  | 2.4  | 1.56 |
Table I continued

| Nucleus | J°       | Energy    | (2J+1)SF |
|---------|----------|-----------|----------|
|         | EXP Th   | EXP Th    |          |
| 29 Mg   |          |           |          |
| 7/2⁻    | 1430 1719| 3.0 4.4   |          |
| 3/2⁻    | 1094 1396| 0.4 2.0   |          |
| 3/2⁺    | 0 0      | 1.2 1.8   |          |
| 29 Si   |          |           |          |
| 7/2⁻    | 3623 3684| 7.0 4.5   |          |
| 3/2⁻    | 4934 4373| 2.2 2.3   |          |
| 3/2⁺    | 1273 1285| 3.0 2.7   |          |
| 31 Si   |          |           |          |
| 7/2⁻    | 3134 2855| 4.8 5.6   |          |
| 3/2⁻    | 3533 3435| 1.6 2.8   |          |
| 3/2⁺    | 0 0      | 2.8 2.4   |          |
| 33 Si   |          |           |          |
| 7/2⁻    | 1435 1452| 6.0       |          |
| 3/2⁻    | 1981 1944| 2.9       |          |
| 3/2⁺    | 0 0      | 1.4       |          |
| 35 Si   |          |           |          |
| 7/2⁻    | 0 0      | 4.5 7.4   |          |
| 3/2⁻    | 910 909  | 2.8 3.7   |          |
| 3/2⁺    | 974 936  |           |          |
| 33 S    |          |           |          |
| 7/2⁻    | 2935 2942| 4.2 5.8   |          |
| 3/2⁻    | 3221 3386| 3.5 2.3   |          |
| 3/2⁺    | 0 0      | 3.5 2.6   |          |
| 35 S    |          |           |          |
| 7/2⁻    | 1991 2042| 5.4 6.4   |          |
| 3/2⁻    | 2348 2409| 2.1 2.7   |          |
| 3/2⁺    | 0 0      | 1.7 1.5   |          |
| 37 S    |          |           |          |
| 7/2⁻    | 0 0      | 5.5 7.3   |          |
| 3/2⁻    | 646 573  | 1.8 3.5   |          |
| 3/2⁺    | 1398 1303|           |          |
| 37 Ar   |          |           |          |
| 7/2⁻    | 1611 1543| 6.1 6.3   |          |
| 3/2⁻    | 2491 2679| 1.8 2.6   |          |
| 3/2⁺    | 0 0      | 2.2 1.5   |          |
### Table I continued

| Nucleus | J^± | Energy | (2J+1)SF |
|---------|-----|--------|----------|
|         |     | EXP    | Th EXP   | Th       |
| ^39Ar   | 7/2^-| 0      | 0        | 5.0      | 6.7      |
|         | 3/2^-| 1267   | 1186     | 2.0      | 2.8      |
|         | 3/2^+| 1517   | 1457     |          |          |

### Table II: A comparison of the measured absolute binding energies \[28\] of the ground states of around \(N = 20\) nuclei with the energies calculated using the FSU cross-shell \(spsdfp\) interaction with 0p0h (pure \(sd\)) and 2p2h configurations. For \(N = 20\), the calculated binding energies with 2p2h configurations (inverted) for \(Z \leq 12\) and those with 0p0h configurations (normal order) for \(Z \geq 16\) agree well with experiment. In-between, the ground state of \(^{34}\)Si (\(Z = 14\)) agrees with the normal 0p0h calculation while the lowest experimental \(2^+\) energy is best represented by the 2p2h (inverted) configuration.

| Nucleus | \(B_{E_{\text{exp}}}\) (MeV) | Order | \(B_{E_{\text{FSU}}}\) (MeV) | \(B_{E_{\text{FSU}}} - B_{E_{\text{exp}}}\) (keV) |
|---------|--------------------------|-------|--------------------------|-----------------------------------------------|
| ^29F    | 186.877                  | 0p0h  | 185.622                  | 1255                                          |
|         |                          | 2p2h  | 187.863                  |                                               |
| ^28Ne   | 206.864                  | 0p0h  | 206.733                  | 131                                           |
|         |                          | 2p2h  | 206.014                  | 850                                           |
| ^29Ne   | 207.843                  | 0p0h  | 206.392                  | 1451                                          |
|         |                          | 2p2h  | 207.635                  | 208                                           |
| ^30Ne   | 211.036                  | 0p0h  | 208.374                  | 2662                                          |
|         |                          | 2p2h  | 211.197                  | -161                                          |
| ^31Ne   | 211.203                  | 0p0h  | 208.091                  | 3112                                          |
|         |                          | 2p2h  | 210.248                  | 955                                           |
| ^32Ne   | 213.472                  | 0p0h  | 211.824                  | 1648                                          |
| Nucleus | $BE_{\text{exp}}$ (MeV) | Order | $BE_{FSU}$ (MeV) | $BE_{FSU} - BE_{\text{exp}}$ (keV) |
|---------|-----------------|-------|-----------------|-----------------|
| $^{29}$Na | 222.782 | 0p0h | 222.904 | -121 |
|         |       | 2p2h | 221.818 | 965 |
| $^{30}$Na | 225.059 | 0p0h | 224.262 | 798 |
|         |       | 2p2h | 224.939 | 121 |
| $^{31}$Na | 229.359 | 0p0h | 226.975 | 2384 |
|         |       | 2p2h | 229.422 | -63 |
| $^{32}$Na | 231.037 | 0p0h | 227.718 | 3319 |
|         |       | 2p2h | 230.007 | 1030 |
| $^{33}$Na | 233.970 | 0p0h | 232.119 | 1851 |
|         |       | 2p2h | 231.665 | 2305 |
| $^{30}$Mg | 241.635 | 0p0h | 241.648 | -12 |
|         |       | 2p2h | 239.660 | 1976 |
| $^{31}$Mg | 243.994 | 0p0h | 241.007 | 2938 |
|         |       | 2p2h | 243.268 | 677 |
| $^{32}$Mg | 249.723 | 0p0h | 247.491 | 2232 |
|         |       | 2p2h | 249.157 | 566 |
| $^{33}$Mg | 252.003 | 0p0h | 248.607 | 3396 |
|         |       | 2p2h | 250.285 | 1718 |
| $^{34}$Mg | 256.714 | 0p0h | 253.901 | 2814 |
|         |       | 2p2h | 253.566 | 3148 |
| $^{31}$Al | 254.991 | 0p0h | 255.173 | -181 |
|         |       | 2p2h | 251.336 | 3656 |
| $^{32}$Al | 259.211 | 0p0h | 259.124 | 87 |
|         |       | 2p2h | 256.643 | 2896 |
| $^{33}$Al | 264.680 | 0p0h | 264.584 | 97 |
|         |       | 2p2h | 263.662 | 1019 |
| $^{34}$Al | 267.255 | 0p0h | 266.543 | 712 |
| Nucleus | $B_{E_{exp}}$ (MeV) | Order | $B_{E_{FSU}}$ (MeV) | $B_{E_{FSU}} - B_{E_{exp}}$ (keV) |
|---------|---------------------|-------|---------------------|---------------------------------|
| $^{32}$Si | 271.407             | 0p0h  | 271.387             | 20                              |
|         |                     | 2p2h  | 266.254             | 5153                            |
| $^{33}$Si | 275.915             | 0p0h  | 275.840             | 75                              |
|         |                     | 2p2h  | 272.355             | 3560                            |
| $^{34}$Si | 283.439             | 0p0h  | 283.578             | -149                            |
|         |                     | 2p2h  | 281.146             | 2283                            |
| $^{35}$Si | 285.935             | 0p0h  | 285.991             | -56                             |
|         |                     | 2p2h  | 283.500             | 2435                            |
| $^{36}$S | 308.714             | 0p0h  | 308.652             | 62                              |
|         |                     | 2p2h  | 305.279             | 3435                            |
| $^{38}$Ar | 327.343             | 0p0h  | 327.202             | 141                             |
|         |                     | 2p2h  | 324.069             | 3274                            |
TABLE III. 2p2h energies and occupancies of the $\nu 0f_{7/2}$ and $\nu 1p_{3/2}$ orbitals for the first $0^+$, $2^+$ and $4^+$ calculated states using the FSU interaction for nuclei with $N = 20$ and $Z$ between 10 and 18.

| Nucleus | $E^*$ (keV) | $J^\pi$ | $\nu f_{7/2}$ | $\nu p_{3/2}$ |
|---------|-------------|---------|---------------|---------------|
| $^{30}$Ne | 0           | $0^+$   | 0.62          | 1.22          |
|         | 819         | $2^+$   | 0.69          | 1.15          |
|         | 2406        | $4^+$   | 0.76          | 1.07          |
| $^{31}$Na | 0           | $3/2^+$ | 0.70          | 1.16          |
|         | 417         | $5/2^+$ | 0.71          | 1.14          |
|         | 3579        | $3/2^-$ | a             | 0.33          | 0.62          |
|         | 3622        | $7/2^-$ | a             | 0.26          | 0.65          |
| $^{32}$Mg | 0           | $0^+$   | 0.78          | 1.1           |
|         | 816         | $2^+$   | 0.80          | 1.07          |
|         | 2535        | $4^+$   | 0.88          | 0.98          |
| $^{33}$Al | 922         | $5/2^+$ | 1.01          | 0.88          |
|         | 1561        | $1/2^+$ | 0.91          | 0.98          |
| $^{34}$Si | 2432        | $0^+$   | 1.35          | 0.56          |
|         | 3666        | $2^+$   | 1.26          | 0.66          |
|         | 5523        | $4^+$   | 1.52          | 0.41          |
| $^{36}$S | 5303        | $0^+$   | 1.31          | 0.61          |
|         | 4507        | $2^+$   | 1.17          | 0.76          |
|         | 6285        | $4^+$   | 1.45          | 0.49          |
| $^{38}$Ar | 3140        | $0^+$   | 1.60          | 0.32          |
|         | 4300        | $2^+$   | 1.68          | 0.27          |
|         | 5646        | $4^+$   | 1.88          | 0.05          |

* 1p1h configuration
FIG. 1. Histogram of the differences in excitation energy between experiment and the FSU interaction fit. The root-mean-square deviation is 190 keV.
FIG. 2. Neutron Effective Single Particle Energies (ESPEs) of $0f_{7/2}$ and $1p_{3/2}$ orbitals calculated with the FSU interaction. They represent the theoretical centroids of the energies of the $0f_{7/2}$ and $1p_{3/2}$ orbitals above the ground state in the nuclei with one more neutron than the indicated even-even ones. In the “normal” ordering the red diamonds ($1p_{3/2}$) lie above the black circles ($0f_{7/2}$).
FIG. 3. (a) Average energy differences between the lowest $7/2^-$ and $3/2^-$ experimental levels in Table I. The error bars give an indication of the range of values for different neutron numbers. Positive (negative) values of the ordinate correspond to the $3/2^-$ state above (below) the $7/2^-$ one. (b) Occupancies of the neutron $0f_{7/2}$ and $1p_{3/2}$ orbitals in neutron number $N = 20$ nuclei as a function of proton number $Z$ for the lowest 2p2h states. The values are shown as filled circles for the cases where the lowest 2p2h state is the ground state (IoI) and as open circles where the lowest 2p2h state is excited above the ground state.
FIG. 4. The experimentally known levels of $^{31}\text{Na}$ compared to the lowest ones predicted using the FSU interaction for 0p0h, 1p1h, and 2p2h configurations. The experimental levels agree well with the 2p2h results while the 0p0h states start almost 2.5 MeV higher in excitation energy. Only the two lowest calculated 1p1h states are labeled because of the high level density above this.
FIG. 5. The lowest experimental energy levels of $N = 20$ $sd$ nuclei compared to those calculated using the FSU shell model interaction for 0p0h and 2p2h configurations. The levels of the known IoI nuclei $^{30}$Ne and $^{32}$Mg agree well with the 2p2h results while the lowest states in the higher Z nuclei agree much better with the 0p0h results.
FIG. 6. Experimental $E(2^+_1)$ and $B(E2: 0^+_1 \rightarrow 2^+_1)$ values for the $N = 20$ isotones are compared to those calculated by using the FSU interaction. The $B(E2: 0^+_1 \rightarrow 2^+_1)$ value of $^{34}\text{Si}$ has not been calculated because of the different configurations associated with the $0^+_1$ and $2^+_1$ states.
FIG. 7. Comparison of the differences in binding energy between experiment and shell model predictions using the FSU interaction with 0 or 2 particle-hole configurations. Green squares have the best agreement and red, the worst. We call the states over-bound where the calculated states are more bound than that of the experimental ones and under-bound when it is otherwise.
FIG. 8. Comparisons of the energies of fully aligned states in sd-shell nuclei with those predicted employing the FSU interaction. Many of the experimental points are confirmed by both selective population in $\alpha, d$ reactions and in high-spin gamma decay sequences and are displayed with solid black circles, while dotted black circles are used to represent states observed by only one of the two signatures. The structure of many of these aligned states involve the promotion of two (extra) nucleons to the $0f_{7/2}$ orbital and are shown with solid red diamonds. Those with at least one nucleon in the $0f_{7/2}$ orbital may require only one more promotion (1p1h excitation) and are shown with dotted red diamond symbols.