A Comparison of Shell Model Results for Some properties of the Even-Even Ge Isotopes

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In this work we examine two recent effective shell model interactions, JUN45 and JJ4B, that have been proposed for use in the $f_{5/2},p_{3/2},p_{1/2},g_{9/2}$ model space for both protons and neutrons. We calculate a number of quantities that did not enter into the fits undertaken to fix the parameters of both interactions. In particular we consider static quadrupole moments (Q's) of excited states of the even-even 70–76 Ge isotopes, as well as the B(E2) values in these nuclei. (We have previously studied 70Zn isotopes using JJ4B.) Some striking disagreements between the JUN45 prediction and the experimental results had already been noted for the quadrupole moments of the $2_1^+$ states of these nuclei. We investigate whether these discrepancies also occur for the JJ4B interaction. Subsequently, we also apply both interactions to calculate the Q's of some more highly excited states and compare the two sets of predictions regarding the nature of the nuclear states under consideration. In order to gain insight into these more complex large-scale shell-model calculations, we examine the corresponding and much simpler single-j shell model calculations in the $g_{9/2}$ neutron shell.

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I. INTRODUCTION

To make shell model calculations tractable one must limit the number of allowed shell model orbitals that are included. One must then find a suitable effective interaction in the resulting truncated model space. One would prefer to construct such an interaction from first principles. In practice however, one sets the final parameters of a given interaction by optimizing simultaneously, for many nuclei, fits to the experimental data for selected nuclear properties (usually the level excitation energies and the binding energies). This is now normally done by a process due to Chung and Wildenthal known as the Linear Combination Method (LCM). An example using this procedure can be seen in [2]. When the resulting interaction is utilized it leads to calculated results for these selected nuclear properties that are often in very good agreement with the corresponding measured values. However, such agreement is not always obtained for nuclear properties whose data were not utilized in the fitting of the interaction parameters.

In the present work on the medium mass Germanium isotopes we show that two such interactions constructed for this region, although very promising, do not always yield sufficiently accurate results for some of the nuclear properties. Indeed, developing a good phenomenological interaction is not a trivial matter. This is especially true for the T=0 parts of the two-body interactions, parts which are not present for systems of identical particles. This challenge has been addressed in [3,4].

Previously the current authors showed the importance of including the $g_{9/2}$ shell in explaining the properties of 70Zn[5]. In that work only one effective interaction, JJ4B, was used. Here we continue on to the Ge isotopes using two proposed effective interactions, JJ4B [6–9] and the newer JUN45 [10], which were constructed for the $p_{3/2},p_{1/2},f_{5/2}$ and $g_{9/2}$ orbitals for both protons and neutrons. The model space consists of a closed $^{56}$Ni core plus many valence nucleons.

Our testing ground will be the 70,72,74,76 Ge isotopes, where we investigate the B(E2)'s and the static quadrupole moment values. These properties were not considered in fitting the parameters for either interaction. We also study, to provide contrast, the excitation energies which were involved in the fitting procedures.

One of the motivations for the present work are the results presented for the Ge isotopes in Figure 8 of a recent paper by Honma et al [11]. It is seen that for N ≥ 38, with the JUN45 interaction, the E(2$_1^+$) values are well described, the B(E2; 2$_1^+ → 0_1^+$) values fairly well described, while the Q(2$^+_1$) values were not in good agreement with the experimental values. We were therefore motivated to use the previously-employed JJ4B interaction of Lisetskiy and Brown [6] to calculate in the same space these same nuclear properties. Subsequently we continue using both interactions to study the excitation energies, B(E2) values, and Q moments of some more highly excited states in the Ge isotopes to compare with each other, and whenever possible, with experimental data.

Finally, to gain insights into the above complex large-scale shell model calculations, we compute the static quadrupole moments of the $2_1^+$ states of these Ge isotopes with the simpler single-j shell model, using only $g_{9/2}$ neutron configurations.
II. RESULTS

A. Energies

Since the excitation energies were used in the fits for the interaction parameters, we expect that the calculations for them with the two interactions will yield results in reasonable agreement with the experimental data. This is indeed the case. For the $E(2_1^+)$’s we see excellent agreement with the JUN45 interaction in the upper-most right hand part of Figure 8 of Reference [11]. In Table I we present the energies for the $J^e = 2_1^+, 0_2^+, 2_2^+$, and $4_1^+$ states of the Ge isotopes calculated with both the JJ4B and JUN45 interactions. The fits are pretty good except for the JJ4B fits for the $0_2^+$ states.

With JUN45, the average absolute deviation between experimental and calculated excitation energies is 0.133 MeV. With JJ4B that average deviation is 0.234 MeV leaving out the $0_2^+$ states and 0.349 MeV if they are included. The best fit with JUN45 is for $^{72}$Ge with an average deviation of 0.068 MeV; with JJ4B the the smallest average deviation is 0.226 MeV for $^{76}$Ge. If we ignore the possible intruder $0^+_5$ state, it would be in $^{72}$Ge, at 0.089 MeV.

B. B(E2) Values

Next we examine the B(E2) values. The calculated values for B(E2)'s will depend on the effective charges used. We use the standard $e_p = 1.5$ and $e_n = 0.5$ values and present our results in Table II for both the JUN45 and JJ4B interactions. However, these are not always the preferred values. In [11] the values of $e_p = 1.5e$ and $e_n = 1.1e$ were used with JUN45 resulting in larger B(E2) values closer to the experimental values. Values of $e_p = 1.76e$ and $e_n = 0.97e$ were used with JJ4B in [5] also putting calculated values closer to experimental measurements. The experimental values in Table II are derived from the NNDC database. In Federman and Zamick [14] the calculated neutron effective charge was larger than 0.5.

Excluding the $2_2^+ \rightarrow 0_1^+$ transition which has very small B(E2) values both experimentally and theoretically, the JJ4B values are almost always bigger by 10 to 30 percent than the JUN45 values.

The experimental value of the B(E2: $2_2^+ \rightarrow 2_1^+$) for $^{70}$Ge is exceptionally large. Excluding the very small $2_2^+ \rightarrow 0_1^+$ transition, the experimental B(E2) values are larger than the JUN45 calculated values for every case and larger than the JJ4B results in 10 of the 12 cases. These experimental values are always larger than 17 W.u., indicating some collectivity.

Overall, the calculated values with either interaction are clearly smaller than the experimentally measured values for $^{74,76}$Ge (which are very similar experimentally) by an average of about 40 percent indicating an underestimate of the collectivity. This can be remedied by the use of larger effective charges, a choice which may be justified because our shell-model space is too small, especially for the neutrons.

In the calculated B(E2) results with either interaction there is little change across the Ge isotopes, ranging from about an 8 to 22 percent change for any specific transition. Experimentally more change is seen.

The experimental value of $BE(4_1^+ \rightarrow 2_1^+)/BE(2_1^+ \rightarrow 0_1^+)$ ratios in these nuclei are for $^{70}$Ge 1.14, for $^{72}$Ge 2.08, for $^{74}$Ge 1.24 and for $^{76}$Ge 1.31. In a simple vibrational picture the value of this ratio would be 2.

As is common in LC fit interactions, the B(E2) values were not included in fitting either interaction’s parameters. The experimental B(E2) values are indeed not fit nearly as well as the energies. With the standard effective charges, the calculated results with the JJ4B interaction are closer to the experimental results than the JUN45 interaction. The use of larger effective charges would be a sensible decision as excitations from the $f_{7/2}$ orbit are not included in the model space and bring the calculated B(E2) values closer to the experimental ones.

C. Static Quadrapole Moments

We now look at the static quadrapole moments of the $2_1^+, 2_2^+$, and $4_1^+$ states of the $^{70,72,74,76}$Ge isotopes. The measured and calculated results are presented in Table III. For the quadrupole moments, experimental results are available only for the $2_1^+$ states. For the $2_2^+$ and $4_1^+$ states we can only compare the different calculated predictions of the two effective interactions. Again the proton and neutron effective charges play an important role. We continue to use in all of our calculations $e_p = 1.5$ e and $e_n = 0.5$ e.

We begin by comparing the experimental and calculated results for the $Q(2_1^+)$’s. The JUN45 predictions, while in agreement with the measured results for $^{70}$Ge, are in disagreement for the other three isotopes. Indeed, for the other three isotopes the experimental $Q(2_1^+)$ values are larger and negative, indicating a prolate intrinsic shape, while the JUN45 results are positive suggesting an oblate intrinsic shape. The JJ4B interaction does a little better than JUN45. The JJ4B values agree with experiment in the case of $^{70}$Ge and $^{76}$Ge but have the opposite sign for $^{72}$Ge and while of the correct sign are much smaller in magnitude in the case of $^{74}$Ge. The use of larger effective charges does not resolve the above discrepancies.

We also calculated quadrapole moments for the $2_2^+$ state and $4_1^+$ state even though there are no available experimental data. Here, we can only compare the results obtained with the two interactions. For $^{70}$Ge and $^{72}$Ge there is some agreement, the signs are the same with roughly similar magnitudes. However, the results are quite different for $^{74}$Ge and $^{76}$Ge. There the signs are almost half of the two interactions except for the $Q(4_1)$ of $^{76}$Ge where the signs agree but there is
a large difference in magnitude.

We cannot assess on the basis of Table III which interaction is better. The disagreement with experiment for the $Q(2^+_2)$ are too large for both interactions. But our results indicate that more theoretical work must be done to improve the calculated values of the quadrupole moments of these excited states of the even Germanium isotopes. Of course, any experimental measurement of the $Q(2^+_2)$ and $Q(4^+_1)$ would be of great value in clarifying this picture.

It is not clear why there is such a large discrepancy between the theoretical and experimental $Q(2^+_2)$ values, but the results point out the importance of including data on static quadrupole moments when fitting the parameters of effective interactions. We note that in the simple harmonic vibrational model the static quadrupole moments would be zero. The results seem to be very sensitive to specific details. We would guess that the problem is not so much with the two specific interactions that are used but rather with the specific truncated shell-model space which is used by both interactions.

From the collective perspective, we note that the ratio of excitation energies $E(4^+_1)/E(2^+_2)$ for the 4 isotopes under consideration has the respective values of 2.07, 2.07, 2.46 and 2.80 in $^{70}$Ge, $^{72}$Ge, $^{74}$Ge, and $^{76}$Ge. In the simple vibrational model the value of this ratio would be two. Thus the two lighter isotopes appear to be more vibrational than the two heavier ones. Such a trend is also present in the experimental $Q(2^+_2)$ values where the $Q(2^+_2)$ of $^{74}$Ge and $^{76}$Ge are larger. The B(E2) ratios data also appeared vibrational in the case of $^{72}$Ge.

To gain a further perspective for trying to understand the behavior of the static quadrupole moments of the even Ge isotopes, we consider in the next section the static quadrupole moments of the Ge isotopes in a single-j shell model. More specifically we consider the $g_{9/2}$ neutron subshell. This is not a totally realistic picture. The wavefunctions that we obtain for the even Ge nuclei in our large-scale shell model calculations with either JUN45 or JJ4B are very fractionated, fragmented over many shell model configurations. This indicates a more collective, rather than a single particle, picture. For example with the JUN45 interaction, the “closed shell” configuration in $^{72}$Ge with J=0 is only 7 percent. However our work does shed light on what happens to the static quadrupole moments as neutrons gradually fill a single j shell.

III. QUADRUPOLE MOMENTS IN THE $g_{9/2}$ SHELL

By definition the quadrupole moment is proportional to the expectation value of the $(2z^2 - x^2 - y^2)$ operator in the state where the m projection is equal to j.

In a corresponding semiclassical picture for a single nucleon in a j shell orbiting outside a closed spherical core, if the orbital angular momentum vector points along the z axis then the particle is orbiting in the xy plane. Thus for the ground state of a nucleus with a single valence nucleon the shape is oblate and the quadrupole moment is negative for this pancake-like situation.

The formula for the quadrupole moment $Q_{sp}$ of a single nucleon is a single j shell is

$$Q_{sp} = \frac{-2j - 1}{2(j + 1)} < r^2 > \frac{e_{eff}}{\epsilon}$$

(1)

where $sp$ denotes single-particle values, $e_{eff}$ is the effective charge, and $<r^2>$ is the expectation value of $r^2$ in the single-particle state.

Aside from the case of $j=\frac{1}{2}$, where the quadrupole moment is zero, the expression is negative for all half-integer values assuming a positive nucleon charge $\epsilon$. The expectation value with harmonic oscillator wave functions is given by

$$< r^2 > = (2N + 3/2)b^2.$$  

(2)

Here N is the principle quantum number (N=2n+1 where n is the number of nodes in the radial wave function, not counting r= infinity, and l is the orbital angular momentum) and $b^2 = \hbar/\omega m$, where m is the nucleon mass and $\omega$ the harmonic oscillator frequency. The $\hbar\omega$ is usually evaluated as $\hbar\omega = 45/A^{1/3} - 25/A^{2/3}$ or sometimes more simply $\hbar\omega = 41/A^{1/3}$.

The $Q_{sp}$ formula can be generalized to the case of N identical particles in a single j shell, with n odd. It becomes, for the ground state of an odd nucleus with $J=j$ and seniority 1, $Q = \frac{-2j-1-2n}{2(j+1)} < r^2 > \frac{e_{eff}}{\epsilon}$ which for n=1 reduces to Eqn. (1).

In this simple model, Q is linear in n. As the single j shell fills up n goes from 1 to (2j+1). As n increases, the quadrupole moment is negative and of decreasing magnitude till midshell, where Q=0. As n increases past the midshell, the quadrupole moment becomes increasingly positive. It thus follows that at midshell Q vanishes and due to the odd symmetry about the midshell the quadrupole moment of a hole is minus that of a particle.

Evaluating Eq. 1 for $Q_{sp}$ for a neutron in the $g_{9/2}$ shell with $e_{n,eff}=1$, j=9/2 we find $Q_{sp} = -4b^2$. With $\Lambda=72$, $b^2 = 4.424 \text{ fm}^2$ and $Q_{sp} = -17.696 \text{ (fm)}^2$, a negative value as expected.

We can next use Racah coefficients to evaluate the values of the quadrupole moments of the $(g_{9/2})^2$ and $(g_{9/2})^4$ neutron configurations when these configurations are coupled to a total angular momentum I of 2 or 4. The results, using in the calculations the same parameters as for $Q_{sp}$, are tabulated in Table IV both in terms of their values and in terms of $Q_{sp}$. We see there that the states for $(g_{9/2})^2$ all have seniority $v=2$ while for $(g_{9/2})^4$ the states can have $v=2$ or $v=4$.

For the $(g_{9/2})^4$ configuration there is one special $I=4$ $v=4$ state that is denoted by $v_4 = 4$ in Table IV. That state is an eigenstate of any interaction and it does not
mix with either the $I=4$ $v=2$ state or the other $I=4$ $v=4$ state \[10\].

We see from Table IV that $Q$ is positive for both the $I=2$ and $I=4$ states of the $n=2$ case and for both $I=2$ $v=2$ and $I=4$ $v=2$ states of the $n=4$ case. We can associate as a simplistic approximation $^{74}\text{Ge}$ with $n=2$ and $^{76}\text{Ge}$ with $n=4$ (all while acknowledging the fragmented/collective nature of the $^{74}\text{Ge}$ and $^{76}\text{Ge}$ calculated shell-model wavefunctions.) Then the single-$j$ shell model signs for the $Q$'s disagree with the experimental results but agree with the signs of the JUN45 results better than with the signs of the JJ4B results. For the $(g_{9/2})^2$ configuration for $I=2$, $Q = -\frac{2}{3}Q_{sp}$ and for $I=4$, $Q = -0.424Q_{sp}$.

It is interesting to investigate, for various values of $j$, the relationship to $Q_{sp}$ of the quadrupole moment $Q(2_1^+)$ of the $(j)^2$ $I=2$ $v=2$ state. These results are given in Table V. Aside from the case of $j = \frac{7}{2}$ [where $Q = 0$ as the $(3/2)^2$ configuration corresponds to the midshell], the ratio of the $Q(2_1^+)/Q_{sp}$ varies very little, always being negative and ranging from -0.57 to -0.67.

One might note that the neutron $(g_{9/2})^2$ $I=2$ $v=2$ result in Table IV, $Q(2_1^+) = 11.797 (fm)^2$ is very close to the values in Table III for $^{72}\text{Ge}$ in the large shell model calculations. This is true regardless of which of the two interactions one considers. This cannot however be taken seriously. The calculated wavefunctions are highly fractionated and, furthermore, in the $g_{9/2}^2$ neutron configuration the magnetic moment would be negative (-0.425) but from \[13\] it is known that in $^{72}\text{Ge}$ the measured magnetic moment is positive. One possible explanation is that a $p_{1/2}$ particle has no quadrupole moment. So if the low-lying configurations are dominated by $p_{1/2}$ and $g_{9/2}$ neutrons, then only the $g_{9/2}$ would contribute.

In the simplest shell model picture $^{72}\text{Ge}$ consists of a closed proton shell and a closed neutron shell. The last occupied orbits are for the protons $p_{3/2}$ and for the neutrons $p_{1/2}$. One simple configuration for the $2^+$ state would be to promote 2 neutrons from $p_{1/2}$ to $g_{9/2}$. In this approximation the results of Table IV would apply.

### IV. SUMMARY

In this paper, using the even Ge isotopes, we have called attention to the importance of trying to include as many nuclear properties as possible when fitting the residual effective interaction parameters. The excitation energies, which were included in such fits, can be calculated well. On the other hand, the $(E2)$ values and the $Q(2_1^+)$ values were not included in the fits for the interaction parameters. Their calculated values, especially for the quadrupole moments, are shown to differ substantially from their measured values.

The single-$j$ shell model provides some physical insights into how the static quadrupole moments behave in a simple model as the $j$ shell occupation increases.

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### TABLE I: Excitation Energies in MeV for the even-even Germanium isotopes. Experimental values taken from the NND database.

| Isotopes | $^{70}\text{Ge}$ | $^{72}\text{Ge}$ | $^{74}\text{Ge}$ | $^{76}\text{Ge}$ |
|----------|------------------|------------------|------------------|------------------|
| Experiment | 16.39 | 0.834 | 0.596 | 0.563 |
| JJ4B | 0.737 | 0.710 | 0.737 | 0.718 |
| JUN45 | 0.907 | 0.814 | 0.717 | 0.745 |

| $E(1^+)$ | $E(0^+)$ | $E(2^+)$ | $E(4^+)$ |
|----------|----------|----------|----------|
| Experiment | 1.216 | 0.691 | 1.483 | 1.911 |
| JJ4B | 1.952 | 2.025 | 1.937 | 2.162 |
| JUN45 | 1.084 | 0.761 | 1.461 | 1.995 |

### TABLE II: $(E2)$ reduced transition strength in W.u. Effective charges $e_p = 1.5$ $e_n = 0.5$ were used. Experimental values were taken from the NND database.

| States | $^{70}\text{Ge}$ | $^{72}\text{Ge}$ | $^{74}\text{Ge}$ | $^{76}\text{Ge}$ |
|--------|------------------|------------------|------------------|------------------|
| $E(2^+ \rightarrow 0^+)$ | Experiment | 20.9(4) | 17.8(3) | 33.0(4) | 29(1) |
| | JJ4B | 19.68 | 19.88 | 19.90 | 18.24 |
| | JUN45 | 14.47 | 14.55 | 16.59 | 16.36 |

| States | $^{70}\text{Ge}$ | $^{72}\text{Ge}$ | $^{74}\text{Ge}$ | $^{76}\text{Ge}$ |
|--------|------------------|------------------|------------------|------------------|
| $E(2^+ \rightarrow 2^+)$ | Experiment | 114(5) | 62(9 -11) | 43(6) | 42(9) |
| | JJ4B | 26.55 | 29.34 | 29.17 | 22.94 |
| | JUN45 | 23.48 | 24.70 | 24.88 | 25.38 |

| States | $^{70}\text{Ge}$ | $^{72}\text{Ge}$ | $^{74}\text{Ge}$ | $^{76}\text{Ge}$ |
|--------|------------------|------------------|------------------|------------------|
| $E(4^+ \rightarrow 2^+)$ | Experiment | 24(7) | 37(5) | 41(3) | 38(9) |
| | JJ4B | 28.22 | 27.62 | 27.04 | 24.15 |
| | JUN45 | 23.65 | 25.08 | 23.46 | 22.04 |

| States | $^{70}\text{Ge}$ | $^{72}\text{Ge}$ | $^{74}\text{Ge}$ | $^{76}\text{Ge}$ |
|--------|------------------|------------------|------------------|------------------|
| $E(2^+ \rightarrow 0^+)$ | Experiment | 0.9(+4 -8) | 0.130 (+18 -24) | 0.71 (11) | 0.90(22) |
| | JJ4B | 1.67 | 1.37 | 0.12 | 0.01 |
| | JUN45 | 0.71 | 1.21 | 1.35 | 0.42 |
TABLE III: Static quadrupole moments in (fm)$^2$. Effective charges of $e_p = 1.5$ and $e_n = 0.5$ were used. N/A indicates unavailable data. The experimental data is from [13].

|          | $^{70}$Ge | $^{72}$Ge | $^{74}$Ge | $^{76}$Ge |
|----------|-----------|-----------|-----------|-----------|
| Experiment | 3(6) or 9(6) | -13(6) | -26(6) | -19(6) |
| JJ4B     | 15.13     | 10.97    | -5.89    | -14.50   |
| JUN45   | 9.94      | 12.85    | 12.02    | 1.77     |
| Q(2$^+$) |           |          |          |          |
| Experiment | N/A      | N/A      | N/A      | N/A      |
| JJ4B     | -15.42    | -11.31   | 5.37     | 15.49    |
| JUN45   | -13.27    | -13.48   | -11.53   | -0.06    |
| Q(4$^+$) |           |          |          |          |
| Experiment | N/A      | N/A      | N/A      | N/A      |
| JJ4B     | 3.16      | 3.15     | -8.30    | -14.03   |
| JUN45   | 1.36      | 8.50     | 11.29    | -1.32    |

TABLE IV: Calculated static quadrupole moments in the single-$j$ shell model space for the $g_{9/2}$ neutrons. Here $n$ is the number of particles, $I$ the total angular momentum, and $v$ the seniority. For $n=1$ $Q_{sp} = -4b^2 = -17.7 fm^2$ (see text)

|          |          |          |          |          |
|----------|-----------|-----------|-----------|-----------|
| $n=1$     | $Q_{sp}$  | $Q_{sp}$  | $Q_{sp}$  | $Q_{sp}$  |
| $Q_{sp}$  | $-4b^2$   | $-4b^2$   | $-4b^2$   | $-4b^2$   |
| $I=2$     | $v=2$    | $v=2$    | $v=2$    | $v=2$    |
|          | -2/3      | 11.79i   |          |          |
|          | -4/3      | 7.686    |          |          |
| $I=4$     | $v=2$    | $v=2$    | $v=2$    | $v=2$    |
|          | 0.129     | -2.279   |          |          |
|          | -0.141    | 2.502    |          |          |
|          | -0.751    | 13.28i   |          |          |
|          | 0.499     | -8.76i   |          |          |

TABLE V: For various $(j^2)^I=2,v=2$ configurations, the relationship of $Q/Q_{sp}$ for that $j$ value.

|          |          |          |          |
|----------|-----------|-----------|-----------|
| $n=2$     | $j$       | $Q/Q_{sp}$ |          |
| $I=2$     | $v=2$    | -0.5714   | 0         |
|          | $v=2$    | -0.6531   | -0.0667   |
|          | $v=2$    | -0.6549   | 0.6505    |
|          | $v=2$    | 0.6530    |          |

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