Comparison of shell model results for some properties of even-even Ge isotopes

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(Received 14 July 2010; revised manuscript received 23 August 2010; published 25 February 2011)

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 the 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 previously studied ^{70}Zn isotopes using JJ4B.) Some striking disagreements between the JUN45 predictions and the experimental results had already been noted for the quadrupole moments of the 2_1^+ states, $Q(2_1^+)$'s, 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. We seek to understand the measured signs of the $Q(2_1^+)$'s in the isotopic Ge chain by looking at a simple single-j shell model and also at the collective vibrational and rotational pictures.

DOI: 10.1103/PhysRevC.83.027302 PACS number(s): 21.60.Cs, 21.30.Fe, 27.50.+e

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 devised by Chung and Wildenthal known as the linear combination (LC) method [1]. In the LC method, certain linear combinations of the matrix elements and single-particle energies of an effective interaction are found to be well determined by the data used in the fit, while other linear combinations are not. An example using this procedure with some level of detail can be seen in Ref. [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. 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 Ref. [3].

Previously the current authors showed the importance of including the $g_{9/2}$ orbit in explaining the properties of ^{70}Zn [4]. In that work, only one effective interaction, JJ4B, was used. Here we continue on to the Ge isotopes, using two proposed effective interactions, JJ4B [4–9] 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 is the results presented for the Ge isotopes in Fig. 8 of a recent paper by Honma *et al.* [10]. It is seen that for $N \geqslant 38$, with the JUN45 interaction, the $E(2_1^+)$ values are well described, and the $B(E2; 2_1^+ \to 0_1^+)$ values fairly well described, while the $Q(2_1^+)$ values are not in good agreement with the experimental values. We were therefore motivated to use the previously employed JJ4B interaction of Lisetskiy and Brown [5] 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 the results with each other, and, whenever possible, with experimental data.

We also compute the static quadrupole moments of the 2_1^+ states of these Ge isotopes with the unrealistic but simpler single-j shell model, using only $g_{9/2}$ neutron configurations. In addition we consider the collective rotational and vibrational perspectives.

Excitation energies. Since the excitation energies are used in the fits for the interaction parameters, we expect the calculated results with the two interactions will be 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 Fig. 8 of Ref. [10]. In Table I, we present the energies for the $J^\pi = 2_1^+, 0_2^+, 2_2^+$, 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.

TABLE I. Excitation energies in MeV for the even germanium isotopes. Experimental values are from the NNDC database.

	^{70}Ge	^{72}Ge	^{74}Ge	^{76}Ge
$E(2_1^+)$				
Expt.	1.039	0.834	0.596	0.563
JJ4B	0.737	0.710	0.737	0.718
JUN45	0.907	0.814	0.717	0.745
$E(0_2^+)$				
Expt.	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
$E(2_2^+)$				
Expt.	1.708	1.464	1.204	1.108
JJ4B	1.347	1.351	1.371	1.368
JUN45	1.404	1.375	1.351	1.364
$E(4_1^+)$				
Expt.	2.153	1.728	1.464	1.410
JJ4B	1.870	1.698	1.735	1.653
JUN45	2.027	1.820	1.613	1.637

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.

As seen in Table I, the JUN45 interaction accounts much better than the JJ4B interaction for the excitation energies of the 0_2^+ states in the even Ge isotopes. This is especially evident for the anomalously low 0_2^+ state in ^{72}Ge, with an excitation energy of 0.691 MeV. In Ref. [10], the 0_2^+ states are discussed explicitly, and possible explanations for their behavior are noted. A study of the detailed ^{72}Ge 0_2^+ wave functions suggests that with JUN45 the occupation numbers for neutrons in the $f_{5/2}$ orbit are higher, and in the $g_{9/2}$ they are lower, than they are with JJ4B. In the JUN45 0_2^+ wave functions, proton excitations from the $p_{3/2}$ orbit are also less common. This arises in part due to the difference in the input single-particle energies. Normalizing in MeV all the single-particle energies with respect to the lowest $p_{3/2}$ orbital, we obtain in JJ4B:

$$p_{3/2} = 0.0, \quad f_{5/2} = 0.3707,$$
$$p_{1/2} = 1.3871, \quad g_{9/2} = 3.7622;$$

in JUN45:

$$p_{3/2} = 0.0, \quad f_{5/2} = 1.1193,$$
$$p_{1/2} = 1.9892, \quad g_{9/2} = 3.5663.$$

All of the above combine to lower the 0_2^+ state in the JUN45 interaction. In Ref. [11] the low excitation energy of the 0_2^+ in ^{72}Ge is ascribed to the excitation of both protons and neutrons into the $g_{9/2}$ orbit.

$B(E2)$ values. The calculated $B(E2)$'s will depend on the effective charges used. The commonly used $e_p = 1.5$ and $e_n = 0.5$ values, in units of e, appear to be too small for our present model space. In Refs. [9,10] the modified values of $e_p = 1.5$ and $e_n = 1.1$ were used, corresponding to greater collectivity. In both these cases, larger calculated $B(E2)$ values, closer to the experimental results, were obtained. The use of larger effective charges is also sensible, since in our model space excitations from the $f_{7/2}$ orbit are excluded. In Table II, we present our calculated $B(E2)$ results using both the common values of $e_p = 1.5$ and $e_n = 0.5$ and the modified values of $e_p = 1.5$ and $e_n = 1.1$. In Federman and Zamick [12] the calculated neutron effective charge was larger than 0.5.

Excluding the $2_2^+ \rightarrow 0_1^+$ transitions which have very small $B(E2)$ values both experimentally and theoretically, the JJ4B

TABLE II. $B(E2)$ reduced transition strength in W.u. Two sets of effective charges are used, first $e_p = 1.5$ and $e_n = 0.5$ and then $e_p = 1.5$ and $e_n = 1.1$, shown after the /. Experimental values are from the NNDC database.

	^{70}Ge	^{72}Ge	^{74}Ge	^{76}Ge
$BE(2_1^+ \rightarrow 0_1^+)$				
Expt.	20.9(4)	23.5(4)	33.0(4)	29(1)
JJ4B	19.68/39.53	19.88/40.01	19.90/38.24	18.24/33.47
JUN45	14.47/27.66	14.55/28.27	16.59/32.01	16.36/29.77
$BE(2_2^+ \rightarrow 2_1^+)$				
Expt.	114(5)	62(+9 −11)	43(6)	42(9)
JJ4B	26.55/47.79	29.34/54.78	29.17/55.63	22.94/41.80
JUN45	23.48/41.01	24.70/42.73	24.88/43.29	25.38/44.21
$BE(4_1^+ \rightarrow 2_1^+)$				
Expt.	24(7)	37(5)	41(3)	38(9)
JJ4B	28.22/56.34	27.62/56.44	27.04/53.09	24.15/45.15
JUN45	23.65/45.47	25.08/49.57	23.46/46.48	22.04/40.93
$BE(2_2^+ \rightarrow 0_1^+)$				
Expt.	0.9(+4 − 8)	0.130(+18 − 24)	0.71(11)	0.90(22)
JJ4B	1.67/1.71	1.37/1.48	0.12/0.09	0.01/0.004
JUN45	0.71/0.60	1.21/1.11	1.35/1.35	0.42/0.41

values are almost always bigger by 10–40% than the JUN45 values.

The experimental value of the $B(E2; 2_2^+ \to 2_1^+)$ for ^{70}Ge is exceptionally large. Excluding the very small $2_2^+ \to 0_1^+$ transition, with $e_p = 1.5$ and $e_n = 0.5$, the experimental $B(E2)$ values are larger than the JUN45 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. This underestimation of the experimental data is mostly removed by the use of the larger effective charges.

With $e_p = 1.5$ and $e_n = 0.5$, the calculated $B(E2)$ results with either interaction, there is usually little change across the Ge isotopes, ranging from about 8% to 20% change for any specific transition. Experimentally, more change is seen.

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 smaller effective charges, the calculated results with the JJ4B interaction are closer to the experimental results than the JUN45 interaction. With the larger effective charges, JUN45 results are usually closer to the experimental values.

As seen in Table II, the calculated $B(E2)$'s with the first set of effective charges gives a good fit to ^{70}Ge and ^{72}Ge, while the second larger set fits ^{74}Ge and ^{76}Ge better. So the situation is fairly complicated.

Quadrupole moments. We now look at the static quadrupole 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 for the $J = 2$ states. Again the proton and neutron effective charges play an important role; we continue to use in all of our calculations $e_p = 1.5$ and $e_n = 0.5$ as well as $e_p = 1.5$ and $e_n = 1.1$.

We begin by comparing the experimental and calculated results for the $Q(2_1^+)$'s. The JUN45 predictions, while in agreement with the measured result for ^{70}Ge, are in disagreement for the other three isotopes. Indeed, for the other three isotopes, the experimental $Q(2_1^+)$ values are 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 experimental values for ^{76}Ge and is of the correct sign in ^{70}Ge and ^{74}Ge. However in the latter two cases the magnitude is too large in one case and in the other too small while in ^{72}Ge the sign is incorrect. The use of larger effective charges does not resolve the above discrepancies. These systematic disagreements are repeated in the 2_2^+ states.

We also calculated quadrupole moments for the 4_1^+ states. Here, we compare the results obtained with the JUN45 and JJ4B 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, as for the $J = 2$ states, the signs are always different between the two interactions except for the $Q(4_1^+)$ of ^{76}Ge where the signs agree but there is a large difference in magnitude. Neither interaction agrees with the limited experimental data for $Q(4_1^+)$.

We cannot assess on the basis of Table III which interaction is better. The disagreements with experiment for the $Q(J^\pi = 2^+)$'s are too large for both interactions. 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 $Q(4_1^+)$ values would be of help in this effort.

It is not clear why there is such a large discrepancy between the theoretical and experimental $Q(J^\pi = 2^+)$ values. We would guess that the problem is not so much with the two specific interactions that are employed as with the specific truncated shell model space which is used by both interactions. For example, the possibility of excitations from the $f_{7/2}$ orbit is excluded. Using the larger effective charges adds collectivity and increases the magnitude of the $B(E2)$ and Q values, but does not resolve the problems with the $Q(J^\pi = 2^+)$ signs. The $Q(J^\pi = 2^+)$ results seem to be very sensitive to specific wave function details. It will be interesting to investigate the possibility of also including the data of the quadrupole moments in fitting the parameters of the effective interaction. Such a procedure, if it leads to stable results, may offer better agreement between theory and experiment for the quadrupole moment results. In carrying out such a procedure, one would face considerable technical difficulties. The small number of available data points, and the uncertainties on those points, would have to be carefully considered in determining how to do the fit.

We note that in the simple collective harmonic vibrational model, the static quadrupole moments would be zero. The measured ratio of excitation energies $E(4_1^+)/E(2_1^+)$ for the four 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 2 and in the collective rotational model it would be $\frac{10}{3}$. Thus the two lighter isotopes appear to be more vibrational than the two heavier ones. Such a trend is also present in the experimental $Q(2_1^+)$ values, where the $Q(2_1^+)$'s of ^{74}Ge and ^{76}Ge are larger.

TABLE III. Static quadrupole moments in e fm^2. Two sets of effective charges are used $e_p = 1.5$ and $e_n = 0.5$(displayed first) and $e_p = 1.5$ and $e_n = 1.1$. N/A indicates unavailable data; references are given for available experimental data.

	^{70}Ge	^{72}Ge	^{74}Ge	^{76}Ge
$Q(2_1^+)$				
Expt.	+4(3) [13]	−12(8) [14]	−19(2) [15]	−14(4) [16]
	+3(6) or 9(6) [17]	−13(6) [17]	−25(6) [17]	−19(6) [17]
JJ4B	+15/+25	+11/+19	−6/−6	−15/−19
JUN45	+10/+17	+13/+22	+12/+20	+2/+5
$Q(2_2^+)$				
Expt.	−7(4) [13]	+23(8) [14]	+26(6) [15]	+28(6) [16]
JJ4B	−15/−25	−11/−19	+5/+6	+15/+20
JUN45	−13/−21	−13/−22	−12/−19	−0.1/−2
$Q(4_1^+)$				
Expt.	+22(5) [13]	N/A	N/A	−1 (5) [16]
JJ4B	+3/+11	+3/+10	−8/−9	−14/−17
JUN45	+1/+8	+8/+8	+11/+19	−1/+1

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.

n	I	v	Q (e fm^2)
2	2	2	11.797
	4	2	7.686
4	2	2	3.913
	2	4	−2.279
	4	2	2.502
	4	4	13.287
	4	4	−8.767

The $B(E2)$ ratio also supports a more vibrational picture for ^{72}Ge and a more rotational picture for ^{74,76}Ge. The experimental values of the $\frac{B(E2;4_1^+\to 2_1^+)}{B(E2;2_1^+\to 0_1^+)}$ are 2.08 for ^{72}Ge, 1.24 for ^{74}Ge, and 1.31 for ^{76}Ge. In simple vibrational and rotational models, the ratio would be 2 and $\frac{10}{7}$, respectively.

In contrast to the collective models, we also sought an intuitive understanding of the trends in the experimental data for the $Q(2_1^+)$ values in the Ge isotopes (all with $Z = 32$) as the neutron number increased. We therefore investigated how the quadrupole moments would behave as neutrons are gradually added into the single-j $g_{9/2}$ shell. This simplistic picture is not intended to be, and is not, a realistic description of the Ge nuclei. The larger scale shell model calculations with either interaction lead to very fractionated wave functions, indicating collectivity. Yet in the Ge isotopic chain, the average proton occupation numbers in these fractionated wave functions display little change from nucleus to nucleus as the neutron number increases. This provides some justification for trying out such a neutron-only analysis.

For n identical particles in a single-j shell, with n odd, one obtains [18] for the ground state of an odd nucleus with $J = j$ and seniority 1,

$$Q = -\frac{2j+1-2n}{2(j+1)}\langle r^2\rangle e_{\mathrm{eff}}. \qquad (1)$$

Here e_{eff} is the effective charge, and $\langle r^2\rangle$ the expectation value of r^2 in the single-particle state which is usually found using harmonic oscillator wave functions.

In this simple model, Q is linear in n. As n increases, the quadrupole moment is negative and of decreasing magnitude till midshell, where Q =0. Past the midshell, the quadrupole moment becomes increasingly positive.

Using Racah coefficients, we can 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 [19]. The results are tabulated in Table IV.

The trends within the single-j shell model signs [positive $Q(2_1^+)$ for the low-lying $v = 2$ state] disagree with the experimental results [negative $Q(2_1^+)$]. In a collective rotational picture $Q(2_1^+) = -\frac{2}{7}Q_{\mathrm{intrinsic}}$. If $Q_{\mathrm{intrinsic}}$ is positive (prolate shape), then $Q(2_1^+)$ would be negative, in agreement with the measured values beyond ^{70}Ge.

We are not saying that the neutron-only picture is correct, but it does offer an explanation to the preponderance of calculated positive quadrupole moments in our large space calculations.

In this paper, using the even Ge isotopes, we have called attention to the possible value of including 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 $B(E2)$ values and the $Q(2_1^+)$ values are not included in LC method fits for the parameters of the effective interaction. Their calculated values, especially for the quadrupole moments, are shown to differ substantially from their measured values. It is possible these values could be sensitive to poorly determined parameters in the original LC method fit. This is an idea that we believe is worth pursuing despite the technical difficulties mentioned earlier.

The single-j shell model fails to account for the trends of the experimental quadrupole moment results for the Ge isotopes. To a limited extent, the collective rotational model does better on this point. In the pure vibrational model, the static quadrupole moments would vanish.

S.J.Q.R. thanks Millsaps College for travel support. L.Z. thanks the Weizmann Institute for support by the Morris Belkin visiting professor program. Y.Y.S. thanks Richard Stockton College for a sabbatical grant. The authors thank Dr. N. Benczer-Koller for her interest in this work.

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