Shell model calculations of $B(E2)$ values, static quadrupole moments, and g factors for a number of $N = Z$ nuclei

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In this work we look at the low-lying nuclear structure properties of several $N = Z$ nuclei residing between the doubly magic nuclei ^{40}Ca and ^{100}Sn. Using large shell model codes, we calculate and discuss the systematics of energies. We show energy levels, $B(E2)$'s, static quadrupole moments, and g factors of these $N = Z$ nuclei. In all cases, we compare the results of two different interactions which yield significantly different occupation numbers. We compare our shell model results with those of the rotational and vibrational models. By examining $B(E2)$'s and static quadrupole moments, we make associations with collective models and find that in the model space considered here, ^{88}Ru is oblate. The quadrupole moment of the lowest 2^+ state of ^{92}Pd is calculated to be very small. This would appear to support a vibrational picture and indeed recent measurements give equally spaced levels up to $J = 6^+$ but the authors also point out that the $B(E2)$'s do not steadily increase as is required by such a model.

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I. INTRODUCTION

In this work we use large-scale shell model calculations to study the properties of $N = Z$ even-even nuclei. We consider energy levels, $B(E2)$'s, static quadrupole moments, and magnetic g factors. Many of the quantities that we calculate have not been measured, especially static quadrupole moments of high spin states. However, they are useful for seeing how the shell model stacks out in comparison with collective models.

Large-space shell model calculations of energy levels and $B(E2)$'s in the $f_{7/2}$ shell were performed in the past by Robinson, Escuderos, and Zamick [1]. They calculated in part $B(E2)$'s to high spin states in ^{44}Ti and ^{48}Cr. Such calculations will be also done here, but instead of calculating transitions from J to $J + 2$, we will reverse and go from $J + 2$ to J. This makes comparisons with the vibrational model easier. We will also include the heavier $N = Z$ nuclei ^{96}Cd, ^{92}Pd, and ^{88}Sr. Indeed this study is in part motivated by the recent work of Cederwall and collaborators on ^{92}Pd [2]. They note that the energy levels of ^{92}Pd are equally spaced, as predicted by the vibrational model, but that $B(E2)$'s are closer to the rotational model.

In the f-p region, two interactions are used, GXFP1 and FPD6; in the heavier mass nuclei, which will require the inclusion of the $g_{9/2}$ orbital, we used JUN45 and JJ4B. One of the purposes of this work is to compare the occupancy numbers with these different interactions, as well as the consequences of these differences.

It was noted in Ref. [1] that the $B(E2)$'s dropped as one went to the highest spins allowed by the f-p model space. As we will see in the next section, this is quite different from what happens in the simplest versions of collective models.

II. COLLECTIVE MODELS

In the rotational model, the formulas for $B(E2, J \to J - 2)$ and $Q(J)$ are related to the intrinsic quadrupole moment Q_0 as follows:

$$B(E2, J \to J-2) = \frac{5}{16\pi}[J2K0|(J-2)K]^2 Q_0^2, \quad (1)$$

$$Q(J) = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0. \quad (2)$$

For a $K = 0$ band, we also have

$$B(E2, J \to J-2) = B(E2, 2 \to 0)\frac{15J(J-1)^2}{(2J-2)(2J-1)(2J+1)}. \quad (3)$$

In this model the relation between the static quadrupole moment and $B(E2)$ for $J = 2^+$ is

$$Q(2^+) = -2.0256607\sqrt{B(E2, 2 \to 0)} \quad (4)$$

in the prolate case. For higher values of J, we have

$$Q(J) = 3.5\frac{J}{2J+3}Q(2^+). \quad (5)$$

As J becomes very large, the ratio $B(E2, J \to J - 2)/B(E2, 2 \to 0)$ reaches an asymptotic limit of $15/8 = 1.875$, while $Q(J)/Q(2)$ reaches a limit of $7/4$.

In the vibrational model the $B(E2)$ for the yrast sequence $J = 0, 2, 4, 6, 8$, etc. is given by

$$B(E2, J+2 \to J) = \frac{J+2}{2}B(E2, 2 \to 0), \quad (6)$$

i.e., the $B(E2)$ is proportional to the number of quanta and increases with J. The static quadrupole moment vanishes.

As far as energy levels are concerned, in the simple rotational model one has a $J(J + 1)$ spectrum. For the yrast sequence $J = 0, 2, 4, 6$, etc., one gets equally spaced levels in the harmonic vibrational model.

In either collective model, the g factors for all the states are given by Z/A, which in this work is equal to 0.5 as we are considering $N = Z$ nuclei.

TABLE I. Excitation energies, $B(E2)$'s, g factors, and quadrupole moments of ^{44}Ti using the GXFP1 (FPD6) interaction.

Yrast state	Theor. energy	Expt. energy	$B(E2)\downarrow$	g factor	Quadrupole moment
2_1^+	1.408 (1.300)	1.083	103 (139.8)	0.546 (0.514)	−5.1 (−21.7)
4_1^+	2.552 (2.498)	2.454	133.1 (190.4)	0.538 (0.515)	−16.4 (−29.0)
6_1^+	3.295 (3.775)	4.015	103.2 (160.9)	0.528 (0.519)	−30.7 (−33.4)
8_1^+	5.521 (6.248)	6.508	70.5 (111.9)	0.551 (0.540)	−19.5 (−27.1)
10_1^+	6.678 (7.613)	7.671	92.3 (109.4)	0.549 (0.546)	−22.7 (−25.7)
12_1^+	7.085 (8.312)	8.039	53.8 (63.3)	0.549 (0.549)	−28.3 (−28.5)

III. EXCITATION ENERGIES

The calculated excitation energies (MeV), $B(E2)$'s (e^2 fm^4), g factors, and static quadrupole moments (e fm^2) are shown in Tables I–VI for ^{44}Ti, ^{48}Cr, ^{52}Fe, ^{88}Ru, ^{92}Pd, and ^{96}Cd. In all cases the energy levels are neither pure rotational or pure vibrational. One can say, however, that they are overall closer to vibrational with deviations towards the rotational.

For high spins one can get crossovers which lead to long-lived isomeric states. Experimentally, in ^{52}Fe the 12^+ state comes below the 10^+ state. The 12^+ cannot decay via an $E2$ transition and has a half-life of over 15 min. In the rotational model, one would not get a crossover if both the 10 and 12 were members of a $K = 0$ band. In the large-scale shell model, we fail to get the crossover with the FPD6 interaction, whereas with GXFP1 the two states are almost degenerate.

IV. $B(E2)$ VALUES

The $B(E2)$ values are shown in Tables I–VI. To make the comparison easy, we note that for the rotational model the $B(E2, J+2 \rightarrow J)/B(E2, J \rightarrow J-2)$ ratios for $J = 0, 2, 4,$ 6, 8, and 10 are, respectively, 1, 1.428, 1.105, 1.044, 1.027, and 1.018. The corresponding values in the vibrational model are 1, 2, 3, 4, 5, and 6. A rough common feature of all the nuclei here considered is that in the shell model (with both sets of interactions) the ratio $B(E2,4 \rightarrow 2)/B(E2,2 \rightarrow 0)$ is greater than unity. This is in qualitative, if not quantitative, agreement with the two collective models. However, with the exception of ^{88}Ru, there is a slight decrease in $B(E2,6 \rightarrow 4)$ relative to $4 \rightarrow 2$. This is in quantitative disagreement with the collective models, although the disagreement with the rotational model is less severe. In the f-p shell, we then found a rapid drop-off in $B(E2)$ with increasing J, in disagreement with the collective models. This is probably true for the heavier nuclei as well, but is somewhat obscured by the fact that we have a $J = 10$ cutoff for these nuclei. The nucleus ^{88}Ru is unusual in that the $B(E2)$ values increase as the angular momentum increases, more in line with a collective model picture than any other nucleus considered here.

For the calculated $B(E2)$'s shown in Tables I–VI, we find that in the lighter $f_{7/2}$ nuclei the trends are reproduced using either interaction. In ^{44}Ti, the value of the $B(E2)$ increases with $4 \rightarrow 2$, being larger than $2 \rightarrow 0$, in line with the expectations of either collective model but then decreases. In ^{48}Cr, the value increases again in $4 \rightarrow 2$ compared to $2 \rightarrow 0$, but then remains relatively constant in the $6 \rightarrow 4$ and $8 \rightarrow 6$ cases before decreasing. In the case of ^{52}Fe, the two interactions start to show different behaviors, the $B(E2,8 \rightarrow 6)$ behaving very differently depending on which interaction we consider. The experimental values of $B(E2,2 \rightarrow 0)$ in ^{44}Ti, ^{48}Cr, and ^{52}Fe are, respectively, 130, 272, and 164 e^2 fm^4.

The ^{92}Pd calculations for the $B(E2)$'s show a relatively flat value while the ones for ^{96}Cd are more like the $f_{7/2}$ results, where the $4 \rightarrow 2$ value represents an increase over the $2 \rightarrow 0$ value, but then it immediately decreases when we look at the $6 \rightarrow 4$ value and others as we increase in angular momentum and energy. The ^{92}Pd results agree with those in Refs. [2,3].

Another point of interest is how the values of $B(E2)$ vary with the number of valence particles (holes). With the first interaction in each list, the values of $B(E2,2 \rightarrow 0)$ for 4, 8, and 12 valence particles in the f-p shell (^{44}Ti, ^{48}Cr, and ^{52}Fe) are, respectively, 103, 244, and 218 e^2 fm^4. The ^{48}Cr value

TABLE II. Excitation energies, $B(E2)$'s, g factors, and quadrupole moments of ^{48}Cr using the GXFP1 (FPD6) interaction.

Yrast state	Theor. energy	Expt. energy	$B(E2)\downarrow$	g factor	Quadrupole moment
2_1^+	0.8837 (0.789)	0.752	243.9 (312.4)	0.522 (0.518)	−30.2 (−35.4)
4_1^+	1.8626 (1.940)	1.858	329.2 (436.0)	0.524 (0.520)	−40.4 (−45.5)
6_1^+	3.441 (3.657)	3.445	325.9 (452.2)	0.531 (0.524)	−39.1 (−48.0)
8_1^+	5.017 (5.569)	5.188	300.6 (426.5)	0.533 (0.528)	−40.6 (−48.9)
10_1^+	6.719 (7.664)	7.063	204.9 (341.1)	0.542 (0.536)	−20.4 (−41.5)
12_1^+	7.9704 (9.219)	8.411	160.6 (152.1)	0.549 (0.549)	−2.7 (−8.0)
14_1^+	9.994 (11.360)	10.280	125.8 (137.9)	0.546 (0.546)	−5.3 (−9.4)
16_1^+	13.226 (14.620)	13.309	62.4 (68.9)	0.547 (0.548)	−8.6 (−8.7)
18_1^+	17.731 (19.431)		0.7 (2.0)	0.530 (0.532)	−31.4 (−34.0)
20_1^+	22.478 (24.262)		3.1 (7.8)	0.521 (0.523)	−44.7 (−46.7)

TABLE III. Excitation energies, $B(E2)$'s, g factors, and quadrupole moments of ^{52}Fe using the GXFP1 (FPD6) interaction.

Yrast state	Theor. energy	Expt. energy	$B(E2)\downarrow$	g factor	Quadrupole moment
2_1^+	0.976 (1.003)	0.849	218.5 (291.2)	0.515 (0.515)	−30.5 (−33.7)
4_1^+	2.604 (2.749)	2.385	286.0 (424.3)	0.523 (0.520)	−37.5 (−38.5)
6_1^+	4.361 (4.662)	4.326	166.0 (344.5)	0.538 (0.520)	−0.6 (−14.8)
8_1^+	6.205 (6.488)	6.361	4.7 (425.3)	0.522 (0.514)	−18.3 (−24.7)
10_1^+	7.073 (7.715)	7.382	42.2 (8.7)	0.549 (0.553)	20.0 (21.3)
12_1^+	7.089 (8.202)	6.958	57.4 (52.4)	0.554 (0.556)	54.1 (62.2)
14_1^+	10.920 (11.482)		29.1 (34.4)	0.550 (0.550)	62.2 (64.8)
16_1^+	14.960 (15.777)		10.7 (3.6)	0.536 (0.538)	22.7 (27.4)
18_1^+	19.150 (20.553)		8.3 (27.8)	0.550 (0.536)	16.7 (24.4)
20_1^+	22.951 (23.692)		2.5 (22.7)	0.524 (0.527)	−8.7 (−5.4)

is somewhat more than a factor of 2 greater than the one for ^{44}Ti. The drop-off for Fe can be explained by the fact that it can be regarded as 4 holes relative to a closed $f_{7/2}$ shell, $Z = 28$, $N = 28$. Indeed in the single-j-shell model the values of $B(E2)$ would be identical for ^{52}Fe and ^{44}Ti.

The corresponding values for ^{96}Cd, ^{92}Pd, and ^{88}Ru are, respectively, 152, 304, and 492 e^2 fm^4. Somewhat loosely speaking the $B(E2)$ is proportional to the number of valence holes relative to $Z = 50$, $N = 50$. There are no experimental values at present for the $B(E2)$'s in these nuclei.

V. QUADRUPOLE MOMENTS

By looking only at $B(E2)$'s, one cannot tell if a ground state band is prolate or oblate. For this reason we have extended the calculations to static quadruple moments. Perhaps the most interesting result is that for ^{88}Ru we get a robust oblate deformation. This has already been reported in Ref. [4]. We can compare this "8-particle system" (beyond $Z = 40, N = 40$) with a corresponding one in the f-p shell, ^{48}Cr. The value of $Q(2^+)$ for ^{88}Ru is $+36.7\, e$ fm^2, whereas it is $-30.2\, e$ fm^2 for ^{48}Cr, i.e., similar magnitudes but opposite signs. One word of caution, the calculation for ^{88}Ru is in a less complete model space with only the $g_{9/2}$ orbital from the s-d-g shell included. Also it is better stated that ^{88}Ru is a 12-hole system relative to ^{100}Sn.

The values of $Q(2^+)$ for the 8-hole system ^{92}Pd are almost equal and opposite for the two interactions used, −3.5 and +4.6 for june45 and jj4b, respectively. But the key point is that both are very small. Recall that in the harmonic vibrational model $Q(2^+)$ is equal to zero. This supports the statements in Refs. [2,3] about the equally spaced levels. They find the excitation energies of the $J = 2+, 4+$, and $6+$ states in ^{92}Pd to be 874,1786 and 2535 keV, respectively. However, the ratio of $B(E2)$'s $6 \to 4/4 \to 2$ would be 1.5 in the vibrational model, whereas we calculate, in agreement with experiment, that this ratio is slightly less than unity with both interactions. So the entire situation is more complicated.

Note that in ^{48}Cr there is a dramatic drop in the magnitude of the static quadrupole moment Q when one goes from 10^+ to 12^+, from -41.5 to $-8.0\, e$ fm^2. Similar behavior was reported in the context of ^{50}Cr by Zamick, Fayache, and Zheng [5]. They asserted that in the rotational model the $J = 10^+$ state of ^{50}Cr does not belong to the $K = 0$ ground state band. Indeed it could belong to a $K = 10^+$ band. They used static quadrupole calculations to support their claim. This was also discussed by a dominantly experimental group, Brandolini *et al.* [8].

Calculations of quadrupole moments of 2^+ states have previously been performed for the Ge isotopes by Honma *et al.* [6] and by Robinson *et al.* [7]. There are no experimental values for the static quadrupole moments of any of the nuclei here considered.

VI. g FACTORS

We note that there is very little variation in the values of the g factors. A typical value is 0.54 with small fluctuations around this value. This result is not unexpected. In the single-j-shell model the g factor of any $N = Z$ even-even nucleus is given by $g = (g_{j\pi} + g_{j\nu})/2$ for all nuclei and is independent of the details of the wave function. In the $f_{7/2}$ shell we get $g = 0.554$; in the $g_{9/2}$ shell we get 0.542. Additionally, this is very close to the collective Z/A value of 0.5. Either extreme picture, be it pure collectivity or pure single j shell, yields values close to this value. This has previously been commented upon by Yeager *et al.* [9]. The experimental value of the g factor of ^{44}Ti is 0.50(15). No other g factors referred to in this work have been measured.

TABLE IV. Excitation energies, $B(E2)$'s, g factors, and quadrupole moments of ^{88}Ru using the JUN45 (JJ4B) interaction.

Yrast state	Theor. energy	Expt. energy	$B(E2)\downarrow$	g factor	Quadrupole moment
2_1^+	0.576 (0.566)	0.616	492.0 (578.3)	0.529 (0.528)	36.7 (29.0)
4_1^+	1.314 (1.281)	1.416	764.1 (842.6)	0.531 (0.530)	43.2 (37.1)
6_1^+	2.115 (2.030)	2.380	890.9 (972.0)	0.533 (0.533)	47.5 (45.5)
8_1^+	2.881 (2.803)	3.480	979.9 (1056.1)	0.535 (0.534)	52.3 (49.5)
10_1^+	3.674 (3.648)		1061.1 (1102.4)	0.537(0.535)	52.4 (51.1)

TABLE V. Excitation energies, $B(E2)$'s, g factors, and quadrupole moments of ^{92}Pd using the JUN45 (JJ4B) interaction.

Yrast state	Theor. energy	Expt. energy	$B(E2)\downarrow$	g factor	Quadrupole moment
2_1^+	0.840 (0.785)	0.874	304.5 (366.2)	0.537 (0.529)	−3.5 (4.6)
4_1^+	1.720 (1.750)	1.786	382.6 (497.6)	0.539 (0.530)	−8.0 (11.1)
6_1^+	2.515 (2.719)	2.536	364.1 (465.2)	0.541 (0.534)	−1.9 (23.9)
8_1^+	3.217 (3.570)		315.1 (283.4)	0.541 (0.539)	8.3 (33.8)
10_1^+	4.070 (4.525)		334.6 (344.6)	0.542 (0.539)	7.9 (40.0)

VII. COMPARISON OF SHELL MODEL OCCUPANCIES WITH DIFFERENT INTERACTIONS

In this section we point out that there are surprising differences in the calculated occupation percentages that result when different "standard" interactions are used. The importance of getting correct occupancies via transfer reactions, e.g., (d,p) and (p,d), has been emphasized over the years by John Schiffer and collaborators. We here cite only the most recent relevant reference, Ref. [10]. In this work the authors acknowledge that there is a quenching problem when one tries to extract spectroscopic factors—they give a quenching factor of about 0.55 due to many-body correlations. But they feel that they can handle this in a global analysis. We quote from their paper, "Correcting for this quenching makes the measured spectroscopic factors directly comparable to spectroscopic factors from shell model calculations of nuclear structure."

In Table VII we give the percent occupancy of the lowest configuration of the $J = 0^+$ ground state and first 2^+ state. By this we mean the percent occupancy of the state (4,6,2,4) for neutrons (and the same for protons) in ^{88}Ru and (4,6,2,6) in ^{92}Pd. Here we refer to $p_{3/2}$,$f_{5/2}$, $p_{1/2}$, and $g_{9/2}$, respectively. We also give $B(E2,2 \to 0)$ and $Q(2^+)$ for the two interactions. We see that interactions which have lower occupancies of the lowest states (i.e., more fragmentation) have larger $B(E2)$'s. The situation with the static quadrupole moments is more complicated. As mentioned before, the $Q(2^+)$ values for ^{92}Pd are small and of opposite sign. And most surprising, with both interactions the values of $Q(2^+)$ are large and positive for ^{88}Ru, an indication of an oblate deformation. Whether this result persists when larger model spaces become feasible remains to be seen.

Also of interest is the fact that the $B(E2)$'s increase with the number of valence particles almost in a linear fashion, e.g., 155, 366, and 579 e^2 fm^4 for $A = 96$, 92, and 88 (4, 8, and 12 holes relative to the doubly closed shell ^{100}Sn). We also have here noted dramatic changes in static quadrupole moments $Q(J)$ beyond certain spin values, an indication perhaps of changing from $K = 0$ bands to high-K bands. This is certainly worthy of future study.

In closing we note that, although the collective models can supply valuable insights concerning the behaviors of electromagnetic properties of nuclei, the simplest versions of these models are clearly inadequate. For example they fail to predict the decrease in $B(E2)$'s after a certain point with increasing spin. Undoubtedly more sophisticated collective models can be constructed which might be more successful, but then the simplicity is lost and the insights obscured.

The large-scale shell models are not off the hook either. One must remember that they depend on what interactions are used and the current state of affairs is such that different widely used interactions can and do yield quite different results, and these can be most easily traced to the differences in the occupation numbers for various basis states. Also the model spaces may be too restricted. For the heavier nuclei the orbits included are $p_{3/2}$, $f_{5/2}$, $p_{1/2}$, and $g_{9/2}$. It would be good to have more positive-parity orbits.

We conclude by noting that the region below ^{100}Sn has been very active of late. Besides the references already mentioned, we add Refs. [11–17]. Also, to a large extent, one can regard earlier studies of properties in the $f_{7/2}$ shell as precursors to analogous studies in the $g_{9/2}$ shell. This has been made especially clear by Neergaard [18]. For example, in a single-j-shell calculation ($g_{9/2}$) of the $J = 0^+$ ground state of ^{96} Cd there is a substantial probability that the 2-proton holes couple to angular momentum $J_p = 2$, and likewise the 2-neutron holes to $J_n = 2$. The same point was made many years ago in a single-j-shell calculation ($f_{7/2}$) of the ground state of ^{44}Ti [19,20]. In both cases the neutron-proton interaction destroys

TABLE VI. Excitation energies, $B(E2)$'s, g factors, and quadrupole moments of ^{96}Cd using the JUN45 (JJ4B) interaction. There are no known experimental energies.

Yrast state	Theor. energy	$B(E2)\downarrow$	g factor	Quadrupole moment
2_1^+	0.901 (0.901)	151.9 (154.7)	0.541 (0.539)	−19.3 (−16.4)
4_1^+	1.987 (1.964)	206.0 (205.7)	0.542 (0.540)	−21.5 (−15.2)
6_1^+	3.021 (2.957)	191.0 (187.1)	0.542 (0.541)	−10.5 (−2.4)
8_1^+	3.483 (3.404)	46.7 (71.4)	0.541 (0.540)	40.2 (37.2)
10_1^+	4.801 (4.789)	52.3 (80.9)	0.544 (0.537)	14.9 (24.0)

TABLE VII. Occupation percentages for different interactions.

Nucleus	Interaction	$J = 0^+$	$J = 2^+$	$B(E2)$	$Q(2^+)$
^{44}Ti	GXFP1	72.1	66.1	103	– 5.1
	FPD6	42.9	26.8	140	– 21.6
^{48}Cr	GXFP1	43.2	34.7	244	– 30.1
	FPD6	21.2	16.2	312	– 35.4
^{96}Cd	JJ4B	49.6	61.0	155	– 16.4
	JUN45	58.8	76.4	152	– 19.3
^{92}Pd	JJ4B	9.7	9.0	366	4.6
	JUN45	28.8	32.6	304	– 3.5
^{88}Ru	JJ4B	1.65	1.24	578	29.0
	JUN45	7.14	5.29	492	36.7

the pairing. In a final reference, Girod [21] presents a cluster model of ^{88}Ru consisting of four ^{16}O and two ^{12}C nuclei. It would be of interest to make a connection of this with our oblate ^{88}Ru.

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