Shell-model test of the rotational-model relation between static quadrupole moments $Q(2_1^+)$, $B(E2)$'s, and orbital $M1$ transitions

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In this work, we examine critically the relation between orbital magnetic dipole (scissors mode) strength and quadrupole deformation properties. Assuming a simple $K = 0$ ground-state band in an even-even nucleus, the quantities $Q(2_1^+)$ (i.e., the static quadrupole moment) and $B(E2)_{0_1\to 2_1}$ both are described by a single parameter—the intrinsic quadrupole moment Q_0. In the shell model, we can operationally define Q_0(static) and $Q_0(BE2)$ and see if they are the same. Following a brief excursion to the *sd* shell, we perform calculations in the *fp* shell. The nuclei we consider (^{44,46,48}Ti and ^{48,50}Cr) are far from being perfect rotors, but we find that the calculated ratios $Q_0(\text{static})/Q_0(BE2)$ with an FPD6 interaction are often very large (very close to unity) and far from the simple vibrational limit of zero. The experimental ratios for ^{46}Ti and ^{48}Ti are somewhat smaller ($\sim$0.75), but the ^{50}Cr value is larger, exceeding unity. We also discuss the quadrupole collectivity of orbital magnetic dipole transitions. We find that the large orbital $B(M1)$ strength in ^{44}Ti relative to ^{46}Ti and ^{48}Ti cannot be explained by simple deformation arguments.

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In this work we make a comparison of the shell model and the collective model for several quantities that are sensitive to nuclear deformation. These include $B(E2)$'s, static quadrupole moments, and orbital magnetic dipole transitions. This will be a theory versus theory work. Some experimental results are quoted and serve as anchors for our results, but we will not be inhibited by the lack of experimental data in doing these calculations. We plan in the near future to make a more extensive theory/experiment comparison. But there are holes in the experimental data that must be filled.

The main thrust of our work is to understand the relationship of orbital magnetic dipole transitions to quadrupole deformations in the nucleus. For example, after the experimental discovery in heavy deformed nuclei of the relation between the orbital magnetic dipole strength and nuclear deformation [1], there have been many works that relate the orbital $M1$ (scissors mode) strength to electric quadrupole transition rates [$B(E2)_{0_1\to 2_1}$], often assuming that they are proportional to each other [2–7].

First, though, we do survey calculations of $B(E2)$'s and static quadrupole moments in the *fp* shell to see how well the shell model relates to the simple rotational model of Bohr and Mottelson [8]. In this rotational model, the formulas for $B(E2)$'s and static quadrupole moments involve a single parameter—the intrinsic quadrupole moment. These formulas are, respectively,

$$B(E2) = \frac{5}{16\pi} Q_0^2(B)\,|\langle I_1 K 20 | I_2 K\rangle|^2 \tag{1a}$$

$$Q(I) = \frac{3K^2 - I(I+1)}{(I+1)(2I+3)} Q_0(S), \tag{1b}$$

where B and S stand for $B(E2)$ and "static," respectively. Here Q_0 is the intrinsic quadrupole moment—what we would see in the rotational frame. However, $Q(I)$ is what we measure in the laboratory. In the simple rotational model, $Q_0(B)$ is equal to $Q_0(S)$.

For the case $I_1 = 0$, $I_2 = 2$, the Clebsch-Gordan coefficient above is 1. For a simple $K = 0$ band in an even-even nucleus, we obtain

$$B(E2)_{0\to 2} = \frac{5}{16\pi} Q_0^2(B) \tag{2a}$$

$$Q(2^+) = -\frac{2}{7} Q_0(S). \tag{2b}$$

Note that the laboratory quadrupole moment has the opposite sign of the intrinsic quadrupole moment—a well-known result. It can be understood physically by imagining rotating a cigar (which has a positive quadrupole moment; i.e., prolate) about an axis perpendicular to the line of the cigar. This will trace out a flat pancake shape that is oblate.

TABLE I. Experimental data on $Q(2_1^+)$ and $B(E2)$ in the *sd* shell and the ratio $|Q_0(S)/Q_0(B)|$; we also give the experimental values of $E(4)/E(2)$.

	$Q(2_1^+)$ [e fm^2]	$B(E2)$ [e^2 fm^4]	$\lvert Q_0(S)/Q_0(B)\rvert$	$E(4_1^+)/E(2_1^+)$
^{20}Ne	−23 (3)	340 (30)	1.38 (19)	2.600
^{22}Ne	−19 (4)	230 (10)	1.38 (28)	2.634
^{24}Mg	−16.0 (8)	432 (12)	0.85 (4)	3.012
^{28}Si	+16 (3)	326 (12)	0.98 (18)	2.596
^{32}S	−15 (2)	300 (13)	0.96 (13)	2.000
^{36}Ar	+11 (6)	340 (40)	0.66 (36)	2.240
^{40}Ar	+1 (4)	330 (39)	0.06 (24)	1.980

We then find that the ratio

$$\frac{Q_0(S)}{Q_0(B)} = -\frac{7}{2}\sqrt{\frac{5}{16\pi}}\frac{Q(2^+)}{\sqrt{B(E2)}} = -1.1038705\frac{Q(2^+)}{\sqrt{B(E2)}}. \quad (3)$$

Although we will be performing calculations in the *fp* shell, we shall here briefly look over the experimental situation in the *sd* shell. In Table I we show experimental values of $Q(2_1^+)$ [9], $B(E2)$ [10], and the ratio $|Q_0(S)/Q_0(B)|$ as given by Eq. (3). We also show the experimental values of $E(4_1^+)/E(2_1^+)$ as a measure of how close we are to the rotational limit of 10/3, or the vibrational limit of 2/1.

Note that the static quadrupole moments of ^{20}Ne, ^{22}Ne, ^{24}Mg, and ^{32}S are negative, whereas those of ^{28}Si and ^{36}Ar are positive. If we limit ourselves to axial symmetry, this indicates that the first group has prolate ground-state bands and the second group has oblate ones. Skyrme II Hartree-Fock results by Jaqaman and Zamick [11] correctly give the signs of all the static quadrupole moments. The small static quadrupole moment of ^{40}Ar is consistent with magnetic moment results of the 2_1^+ state by Stefanova *et al*. [12].

The ratio $|Q_0(S)/Q_0(B)|$ for ^{20}Ne is *larger* than the rotational limit, 1.38 versus 1; likewise ^{22}Ne. In the case of ^{24}Mg, $|Q_0(S)/Q_0(B)|$ is smaller than for ^{20}Ne or ^{22}Ne, despite the fact that the spectrum is closer to rotational for ^{24}Mg. Also surprisingly for ^{32}S, the ratio $E(4)/E(2)$ is 2.000, the vibrational limit, for which one might expect a near-zero static quadrupole moment. But the ratio $|Q_0(S)/Q_0(B)|$ is 0.96, close to the simple rotational prediction of unity. In general, it is difficult to correlate $|Q_0(S)/Q_0(B)|$ with $E(4)/E(2)$ assuming a simple axially symmetric rotor.

We should mention that an analysis of the relationship of $Q_0(S)$ and $Q_0(B)$ has already been performed by Bender, Flocard, and Heenen [13] and Bender *et al*. [14], albeit not for the *fp*-shell nuclei considered here and using a different method. They perform angular momentum projections on BCS-Hartree-Fock states obtained with the Skyrme interaction SLy6 for the particle-hole channel and a density-dependent contact force in the pairing channel [13]. Their calculations are mainly in the *sd* shell [13] and neutron-deficient lead region [14]. For one nucleus in common, ^{40}Ca, their results for $0p$-$0h$, $2p$-$2h$, $4p$-$4h$, $6p$-$6h$, $8p$-$8h$, and $12p$-$12h$ do not differ so much from previous calculations of Zheng, Berdichevsky, and Zamick [15] as far as the intrinsic properties are concerned, but their calculation has the added feature of providing an energy spectrum and expectation values in the laboratory frame.

In Ref. [11], the authors predict that ^{36}Ar is oblate. This is confirmed by the fact that the static quadrupole moment of the 2_1^+ state is positive: $+11e$ fm^2 [9]. The experimental $B(E2)$ is 340 e^2 fm^4 and $|\beta_2| = 0.273$ [10]. Using Eq. (3), we find

$$\frac{Q_0(S)}{Q_0(B)} = 0.6585236. \quad (4)$$

The energy ratio is

$$\frac{E(4_1^+)}{E(2_1^+)} = \frac{4414.36}{1970.35} = 2.240. \quad (5)$$

These results are consistent with a nucleus not being too rotational.

The corresponding numbers in the calculation of Bender *et al*. [13] are

$$Q(2_1^+)_{\rm lab} = 13\,e\,{\rm fm}^2, \quad B(E2)\uparrow = 220\,e^2\,{\rm fm}^4, \quad \beta = -0.21. \quad (6)$$

The calculated ratios are

$$\frac{Q_0(S)}{Q_0(B)} = 0.9675, \qquad \frac{E(4_1^+)}{E(2_1^+)} = 2.6545. \quad (7)$$

These calculations [13] give a more rotational picture than experiment. There is a consistency, however, in that a larger ratio $E(4)/E(2)$ yields a larger ratio $Q_0(S)/Q_0(B)$.

It should be noted that there have been random interaction studies of $Q(2^+)$ by Velázquez *et al*. [16] and Zelevinsky and Volya [17] for nuclei in the region that we are considering; these works were based on that of Johnson, Bertsch, and Dean [18]. However, we do not discuss them in this work.

We now put the above relation ((3)) to the test in a shell-model approach for the following nuclei: ^{44}Ti, ^{46}Ti, ^{48}Ti, ^{48}Cr, and ^{50}Cr. We use the OXBASH [19] and ANTOINE [20] codes with the FPD6 [21] and KB3 [22] interactions.

The nuclei that we have chosen are far from being perfect rotors. Their description falls somewhere between vibrational and rotational. The ratios $E(4)/E(2)$, which would all be 10/3 in the simple rotational case are as follows with FPD6: 1.922, 2.010, 2.118, 2.459, 2.342 for ^{44}Ti, ^{46}Ti, ^{48}Ti, ^{48}Cr, and ^{50}Cr, respectively.

We perform shell-model calculations in a complete *fp* space. We assign effective charges of 1.5 for the protons and 0.5 for the neutrons. We calculate $B(E2)_{0_1\to 2_1}$ and $Q(2^+)$ (the laboratory Q, of course) and put them into Eq. (3) to get operational values of $Q_0(S)/Q_0(B)$. The results are given in Table II.

Except for ^{48}Ti, the FPD6 results for the ratios are all greater than 0.9, reaching a maximum of 0.9892 for ^{48}Cr. It is somewhat surprising that these ratios are so close to 1, given that the ratios $E(4)/E(2)$ are much further away from the rotational limit 10/3.

We can also obtain some of the above ratios from experiment. We refer to the compilation of nuclear moments of Stone [9] and of $B(E2)$'s by Raman *et al*. [10]. Taking these experiments at face value, we see that the ratio $Q_0(S)/Q_0(B)$

TABLE II. Calculated and experimental values for $Q(2_1^+)$ and $B(E2)$, as well as the ratios $Q_0(S)/Q_0(B)$ and $E(4_1^+)/E(2_1^+)$.

	$Q(2_1^+)$ [e fm^2]	$B(E2)$ [e^2 fm^4]	$Q_0(S)/Q_0(B)$	$E(4_1^+)/E(2_1^+)$
FPD6				
^{44}Ti	−20.156	607.24	0.9029	1.922
^{46}Ti	−22.071	682.06	0.9329	2.010
^{48}Ti	−17.714	560.78	0.8257	2.118
^{48}Cr	−33.271	1378.4	0.9892	2.459
^{50}Cr	−30.955	1219.0	0.9787	2.342
KB3				
^{44}Ti	−12.437	530.47	0.5958	1.887
^{46}Ti	−16.154	571.35	0.7458	1.904
^{48}Ti	−14.298	455.65	0.7394	2.189
^{48}Cr	−29.388	1124.8	0.9672	2.263
^{50}Cr	−26.815	951.08	0.9598	2.345
Experiment				
^{44}Ti		610 (15)		2.266
^{46}Ti	−21 (6)	950 (5)	0.75 (22)	2.260
^{48}Ti	− 17.7 (8)	720 (40)	0.728 (39)	2.334
^{48}Cr		1330 (20)		2.471
^{50}Cr	−36 (7)	1080 (6)	1.21 (23)	2.402

reduces to about 0.75 for ^{46}Ti and ^{48}Ti, but is bigger than 1 for ^{50}Cr.

It should be noted that in the simplest version of the vibrational mode, $Q_0(S)$ is zero. We can imagine a nucleus vibrating between a prolate shape and an oblate shape and causing the quadrupole moment to average to zero. However, the $B(E2)_{0_1\to 2_1}$ is quite large in this vibrational limit, causing the ratio $Q_0(S)/Q_0(B)$ to be zero or, in more sophisticated vibrational models, quite small.

To test the sensitivity of our results to the effective interaction, we also show results with KB3 in Table II. The ratio $Q_0(S)/Q_0(B)$ is now smaller for ^{44}Ti (0.60 vs 0.90) and for ^{46}Ti (0.74 vs 0.93), but about the same for the ^{48,50}Cr.

We also plot the ratios $E(4_1^+)/E(2_1^+)$ to get a feeling as to where we are relative to the rotational limit of 10/3 and the vibrational limit of 2/1. One might expect *a priori* that, if the ratio $E(4_1^+)/E(2_1^+)$ is close to 10/3, the ratio $Q_0(S)/Q_0(B)$ would be close to 1, and for an energy ratio of 2/1, $Q_0(S)/Q_0(B)$ would be close to zero. But this is clearly not the case, and it is difficult to find a precise correlation between the two ratios.

The orbital magnetic isovector dipole transitions, i.e., scissors mode excitations, also display collective behavior [1]. There are systematics that suggest that $B(M1)_{\rm orbital}$ is roughly proportional to $B(E2)$. There are more detailed, sophisticated relationships as well. If one uses a simple quadrupole-quadrupole interaction, the energy-weighted $B(M1)_{\rm orbital}$ is proportional to the difference $[B(E2)_{\rm isoscalar} - B(E2)_{\rm isovector}]$ [3].

The bare orbital $M1$ operator is

$$\sqrt{\frac{3}{4\pi}}\sum l(i)g_l(i), \tag{8}$$

where g_l is 1 for a proton and 0 for a neutron. This is the operator that we use in the calculations.

TABLE III. The calculated orbital $M1$ strengths (μ_N^2). Unless indicated, the calculations are made with the FPD6 interaction.

	^{44}Ti	^{46}Ti	^{48}Ti	^{48}Ti/^{46}Ti	^{48}Cr
$T \to T$					
Lowest state	0.0017	0.305	0.105	0.3443	
Lowest 10 states	0.0320	0.5979	0.3056	0.5111	
Lowest 100 states		0.79	0.504	0.6380	
All states	0.0355	0.9195	0.7191	0.7820	
$T \to T+1$					
Lowest state	0.862	0.0991	0.0041	0.4450	0.784
Lowest 10 states	1.4317	0.368	0.1951	0.5302	1.3855
Lowest 100 states	2.12				1.994
All states	2.127	0.5616	0.3099	0.5518	2.271[a]

[a]Lowest 300 states.

How to extract the scissors mode strength is not completely unambiguous. The mode is associated with low-lying 1^+ excitations at around 3 MeV. But the strength can be fragmented even at this lowest energy. In addition to this, there is orbital strength at higher energies, a somewhat grassy behavior where individual states are very weakly excited but, because there are so many of them, the total orbital strength can be significant.

Therefore, we give three sets of values (see Table III). First, we give the strength to the lowest state, then to the lowest 10 states, and finally to the lowest 1,000 states (except for ^{48}Cr, where we include only 300 states). The 10-states strength should encompass what we usually call the scissors mode, whereas the 1,000-states strength is close to the total strength including the grassy, noncollective part. It would appear that the highest excitation energies reached in the experiments [1,23] are not sufficient to reach the $T+1$ part of the spectrum.

We first discuss the nuclei ^{46}Ti and ^{48}Ti, for which there are some data on $B(M1)$. We see consistently that the orbital $B(M1)$ strength is larger in ^{46}Ti than in ^{48}Ti. This is consistent with the fact that ^{46}Ti has a greater $B(E2)$ and static 2^+ quadrupole moment than ^{48}Ti.

We next consider the $N=Z$ nucleus ^{44}Ti, for which there are no data because this nucleus is unstable. The isoscalar orbital $B(M1)$ strength is very weak. This is also true for the spin $B(M1)$, but for a different reason. The isoscalar spin coupling is much smaller than the isovector one. For the orbital case, the couplings are equal because the operator is $\sum_{\rm protons}\vec{\ell}$. So the reason why the $B(M1)$ isoscalar is very weak is that the correlations because of the nuclear interaction move the ground state toward the SU(4) limit, in which LS coupling holds and for which the ground state is a pure $L=0$ state. For this extreme case, the $B(M1)$ orbital isoscalar will vanish.

The transitions of interest for ^{44}Ti are, therefore, the isovector orbital dipole ones. The $(T \to T+1)$ $B(M1)_{\rm orbital}$ summed strength is larger in ^{44}Ti than the $(T \to T+1)$ and $[(T \to T) + (T \to T+1)]$ strengths in ^{46}Ti and ^{48}Ti, which are 0.5615 (1.4811) and 0.3099 (1.0290) μ_N^2, respectively. However, ^{44}Ti is not more deformed than ^{46}Ti. According to Raman *et al.* [10], the values of the quadrupole deformation parameters β for ^{44,46,48}Ti and ^{48,50}Cr are, respectively, 0.27, 0.317, 0.269, 0.335, and 0.293. Thus, we have here in *fp*-shell nuclei a counterexample to the experimentally established

proportionality between the orbital $B(M1)$ and the $B(E2)$ in heavy deformed nuclei. Perhaps there are correlations that cause an enhancement for $N = Z$ nuclei.

An analysis by Retamosa *et al*. [24] in the *sd* shell comparing ^{20}Ne, ^{22}Ne, and ^{24}Mg was performed (somewhat analogous to ^{44}Ti and ^{46}Ti for the first two cases), but no anomaly was reported there. In the SU(3) model, they found consistency in the relation of $B(M1)_{\text{orbital}}$ to deformation. In this limit, the summed $M1$ strengths (all orbital) for ^{20}Ne, ^{22}Ne, and ^{24}Mg were 1.1, 1.17, and 1.6 μ_N^2, respectively. Looking at the Raman tables [10] for these nuclei, there is some complication—the deformation parameters β_2 are not in one-to-one correspondence with the $B(E2)$'s. The values of $[B(E2), \beta]$ for these three nuclei from the Raman tables [10] are, respectively, (0.034, 0.728), (0.0236, 0.562), and (0.0432, 0.606), where the units for $B(E2)$ are b^2. The authors also do calculations with a more realistic interaction, but not enough strengths are listed to make a comparison for the point we are trying to make. Retamosa *et al*. [24] also give strengths to the first 10^+ states in ^{44}Ti; our numbers are consistent with theirs. Earlier works on the shell model for light nuclei include L. Zamick [25] and A. Poves [26].

Cases where the simple picture of a scissors mode breaks down have been discussed by Guliyev *et al*. [27], Georgii *et al*. [28], and Schwengner *et al*. [29]. These occur near shell closures. In these references, the tellurium isotopes ^{122,124,126,130}Te are considered. They interpret the lowest 1^+ state as a member of a two-phonon state $2_1^+ \otimes 2_2^+$, where the 2_2^+ state is a mixed-symmetry state. Another example is ^{94}Mo [30], which has been discussed by A. F. Lisetskiy *et al*. [31], and Lo Iudice and Stoyanov [32].

In this work we have examined what predictions the shell model makes for collective properties that are after dealt with in the rotational model. Although the nuclei are far from perfect rotors, the calculated ratio $Q_0(S)/Q_0(B)$ is fairly close to 1 (the rotational limit) in many cases. When the FPD6 interaction is used, the orbital magnetic dipole transitions for ^{46,48}Ti also fit into this picture, although there is the added complication of separating the collective from the noncollective part in this case. Also there is a substantial enhancement for the $N = Z$ nucleus ^{44}Ti, which cannot be explained as purely a deformation effect. We hope our work will stimulate more experimental investigations. There is information of $B(M1)$ rates in ^{46}Ti and ^{48}Ti, but thus far the orbital $B(M1)$ has been extracted only in ^{48}Ti. However, in a short time, we will be able to make a more extensive theory/experiment study of these magnetic dipole transitions.

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