Study of $^{44}$Ti in a Mixed–Symmetry Basis

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(March 30, 2022)

The structure of $^{44}$Ti is studied in an oblique-basis that includes spherical and SU(3) shell-model basis states. The results show that the oblique-basis concept is applicable, even though the strong spin-orbit interaction, which breaks the SU(3) symmetry, generates significant splitting of the single-particle levels. Specifically, a model space that includes a few SU(3) irreducible representations (irreps), namely, the leading (12,0) and next to the leading (10,1) irreps – including spin $S = 0$ and $1$ configurations of the latter, plus spherical shell-model configurations (SSMC) that have at least two valence nucleons confined to the $f_{7/2}$ orbit – the SM(2) case, yield results that are comparable to SSMC with at least one valence nucleon confined to the $f_{7/2}$ orbit – the SM(3) case.

PACS numbers: 21.60.Cs, 21.60.Ev, 21.60.Fw, 27.40.+z

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Keywords: mixed-mode, symmetry-mixing, non-orthogonal basis, generalized eigenvalue problem, Elliott’s SU(3) model, spherical shell model.

Introduction – In a previous paper we introduced the mixed-symmetry, oblique-basis concept and demonstrated its applicability in the sd-shell using $^{24}\text{Mg}$ as an example [1]. The successful description of $^{24}\text{Mg}$ can be understood in terms of the comparable importance of single-particle excitations that are described most naturally in terms of spherical shell-model configurations (SSMC), and collective quadrupole excitations that are best described by the SU(3) shell model. An important element to the success of the theory for lower sd-shell nuclei is the fact that SU(3) is a reasonably good symmetry [2]; that is, for lower sd-shell nuclei SU(3) is the dominant symmetry while the spherical shell-model (SSM) scheme plays an important but clearly more recessive role.

In contrast with the sd-shell situation, for lower pf-shell nuclei the strong spin-orbit splitting dominates the landscape and SU(3) symmetry is badly broken [3]. Therefore, one might anticipated that adding the leading and next to the leading SU(3) irreps to the dominate SSM configurations for lower pf-shell nuclei might not add much value to the analysis. Nevertheless, our calculations for $^{44}\text{Ti}$ show that the addition of leading SU(3) irreps speeds the convergence; that is, whereas in this case the spherical shell-model (SSM) is clearly dominant and SU(3) is recessive, the latter remains important and signals that the oblique-basis remains an important concept even in situations where one of the symmetries is rather badly broken.

Here we consider oblique-basis calculations for $^{44}\text{Ti}$ using the KB3 interaction [4]. We confirm that the spherical shell model (SSM) provides a significant part of the low-energy wave functions within a relatively small number of SSMC while an SU(3) shell-model scheme with only few SU(3) irreps is unsatisfactory. This is the opposite of the situation in the sd-shell. Since the SSM yields relatively good results with SM(2), which includes SSMC of up to two valence nucleons free to move in any of pf-shell orbitals, combining the two basis sets yields even better results with only a very small increase in the overall size of the model.
space. In particular, results in a SM(2)+SU(3) model space (47.7% + 2.1% of the full pf-shell space) are comparable with SM(3) results (84% of the full pf-shell space). Therefore, as for the sd-shell, combining a few SU(3) irreps with SM(2) configurations yields excellent results, such as correct spectral structure, good ground-state energy, and an overall improved structure of the wave functions.

**Model Space** – ⁴⁴Ti consists of 2 valence protons and 2 valence neutrons in the pf-shell. The SU(3) basis includes the leading irrep (12,0) with \( M_J = 0 \) dimensionality 7, and the next to the leading irrep (10,1). The (10,1) occurs three times, once with \( S = 0 \) (dimensionality 11) and twice with \( S = 1 \) (dimensionality \( 2 \times 33 = 66 \)). All three (10,1) irreps have a total dimensionality of 77. The total \( M_J = 0 \) dimensionality of (12,0) and (10,1) is therefore 84. In Table I we summarize the dimensionalities involved in our calculation.

Within oblique bases type calculations one expects some linearly dependent vectors \[1\]. In our example, there is one redundant vector in the SM(2)+(12,0) space, two in SM(3)+(12,0) and SM(1)+(12,0)&(10,1) spaces, twelve in SM(2)+(12,0)&(10,1) space, and thirty-three in the SM(3)+(12,0)&(10,1) space. Each linearly dependent vector is handled as discussed previously \[1\]. The structure of the oblique-basis model space is shown in Fig. 1.

| Model space | (12,0) | &(10,1) | SM(0) | SM(1) | SM(2) | SM(3) | FULL |
|-------------|--------|---------|-------|-------|-------|-------|------|
| dimension   | 7      | 84      | 72    | 580   | 1908  | 3360  | 4000 |
| dimension % | 0.18   | 2.1     | 1.8   | 14.5  | 47.7  | 84    | 100  |

**TABLE I.** Labels and \( M_J=0 \) dimensions of various model spaces for ⁴⁴Ti. The leading SU(3) irrep is (12,0); &(10,1) implies that the three (10,1) irreps (one with \( S = 0 \) and \( M_J=0 \) dimensionality 11 and two with \( S = 1 \) and \( M_J=0 \) dimensionality 33 each) are included along with the leading irrep (12,0). SM(n) is a spherical shell-model basis with n valence particles anywhere within the full pf-shell when the remaining valence particles are being confined to the \( f_{7/2} \) orbit.
FIG. 1. Orthogonality of the basis vectors in the oblique geometry. The SU(3) space consists of (12,0) & (10,1) basis vectors. The shell-model spaces (SM(n) with n = 1 and 2) is indicated by a horizontal line. (a) SM(1) and the leading SU(3) basis vectors; there are two SU(3) vectors that lie in the SM(1) space. (b) SM(2) and the leading SU(3) basis vectors; there are twelve SU(3) vectors that lie in the SM(2) space.

Ground-State Energy – The convergence of the ground-state energy as a function of the model space dimension is shown in Fig. 2. The oblique-basis calculation of the ground-state energy for \(^{44}\)Ti does not appear to be as impressive as for \(^{24}\)Mg [1], especially when we compare SM(2) with SM(1) plus SU(3). The calculated ground-state energy for the SM(1)+(12,0) & (10,1) space is 0.85 MeV below the calculated energy for the SM(1) space. In contrast, the ground-state energy for SM(2) is 2.2 MeV below the SM(1) result. Adding the two SU(3) irreps to the SM(1) basis increases the size of the space from 14.5% to 16.6% of the full space. This is a 2.1% increase, while going from the SM(1) to SM(2) involves an increase of 33.2%. However, adding the SU(3) irreps to the SM(2) basis gives ground-state
energy of $-13.76$ MeV which is compatible to the SM(3) result of $-13.74$ MeV. Therefore, adding the SU(3) to the SM(2) increases the model space from 47.7% to 49.8% and gives results that are slightly better than the results for SM(3) model space that is 84% of the full space.

FIG. 2. Ground-state energy for $^{44}$Ti as a function of the various model spaces. The SU(3) irreps used in the calculations are (12,0) and (10,1).

Low-Lying Energy Spectrum – For $^{24}$Mg the position of the K=2 band head is correct for SU(3)-type calculations but not for the low-dimensional SM(n) calculations [1]. For $^{44}$Ti we find the opposite scenario which is shown in Fig. 3. In this case the SM(n)-type calculations reproduce the position of the K=2 band head while SU(3)-type calculations put the K=2 band head too high. Furthermore, the low-energy levels for the SU(3) case are higher than the SM(n) case, which is a scenario that may not produce the necessary mixing of the levels that would lead to a better spectral structure. It is important to note that basis states with spin other than zero are essential to achieve a proper description of the low energy spectrum.
This can be seen very clearly for $^{44}$Ti in Fig. 3 where the addition of the $S = 1$ (10,1) irreps to the (12,0) and (10,1) $S = 0$ pair increases the binding energy by 2 MeV.

FIG. 3. Structure of the energy levels for $^{44}$Ti for different calculations. Pure $m$-scheme spherical-basis calculations are on the left-hand side while pure SU(3)-basis calculations are on the right-hand side. The spectrum from the FULL space calculation is in the center.

Overall, the spectral structure in the oblique-basis calculation is good with the SM(2)+(12,0)&(10,1) spectrum ($\approx$50% of the full space) delivering results that are comparable to the SM(3) case (84%). Additional details are shown in Fig. 4.
FIG. 4. Structure of energy levels for $^{44}$Ti for different oblique-basis calculations using leading and next to the leading irreps with spin $S = 0$ and 1. Pure $m$-scheme spherical-basis calculations are included for comparison.

Overlaps with Exact States – The overlap of the SU(3)-type eigenstates with the exact (full $pf$-shell model space) results are not as large as in the $sd$-shell, often running less than 40%. This result was also reported in a comparative study of SU(3) and projected Hartree-Fock [5] calculations. The SM(n) results are considerably better with SM(2)-type calculations yielding on average more than an 85% overlap with the exact states while the results for SM(3) show overlaps greater than 97%, which is consistent with the fact that SM(3) covers 84% of the full space. This situation is shown in Fig. 5.
FIG. 5. Wave function overlaps of the FULL $pf$-shell states of $^{44}$Ti with pure spherical shell model and SU(3) type calculations. The first four bars represent the SM(0), SM(1), SM(2), and SM(3) calculations, the next two bars represent the SU(3) calculations.

On the other hand, as shown in Fig. 6, SM(2) plus (12,0)\&(10,1)-type calculations yield results in about 50% of the full-space that are as good as those for SM(3) which is 84% of the full $pf$-shell model space. Notice that the SM(1)+(12,0)\&(10,1) overlaps are often bigger than the SM(2) overlaps as shown in Fig. 6.
### Eigenvectors

|        | SU(3)^+ | SM(1) | SM(1)^+SU(3)^+ | SM(2) | SM(2)^+SU(3)^+ | SM(3) |
|--------|---------|-------|----------------|-------|----------------|-------|
| 1      | 29.11   | 65.47 | 84.11          | 92.16 | 98.31          | 97.36 |
| 2      | 35.97   | 56.71 | 87.78          | 83.46 | 97.32          | 97.39 |
| 3      | 41.95   | 55.55 | 89.14          | 84.95 | 97.81          | 98.67 |
| 4      | 33.78   | 78.08 | 91.82          | 94.56 | 98.48          | 99.79 |
| 5      | 17.88   | 49.22 | 90.80          | 77.20 | 97.06          | 97.22 |
| 6      | 11.41   | 46.96 | 89.34          | 81.10 | 97.69          | 98.93 |

**FIG. 6.** Selected overlaps of SM(n), SU(3), and oblique-basis results with the exact full pf-shell eigenstates for $^{44}$Ti. Here SU(3)^+ denotes the (12,0)&(10,1) SU(3) irreps.

**Conclusion** – For $^{44}$Ti, combining a few SU(3) irreps with SM(2) configurations increases the model space only by a small ($\approx 2.3\%$) amount but results in better overall results: a lower ground-state energy, the correct spectral structure (particularly the position of the K=2^+ band head), and wave functions with a larger overlap with the exact results. The oblique-bases SM(2)+(12,0)&(10,1) for $^{44}$Ti ($\approx 50\%$ of the full space) yields results that are comparable with SM(3) results ($\approx 84\%$ of the full space). In short, the oblique-basis scheme works well for $^{44}$Ti but in contrast with $^{24}$Mg, the SSM configurations are dominant when SU(3) is recessive.

**ACKNOWLEDGMENTS**

We acknowledge support provided by the U.S. Department of Energy under Grant No.
DE-FG02-96ER40985, and the U.S. National Science Foundation under Grant Nos. PHY-9970769 and PHY-0140300.

[1] V. G. Gueorguiev, W. E. Ormand, C. W. Johnson, and J. P. Draayer, Phys. Rev. C65, 024314 (2002).

[2] J. P. Elliott and H. Harvey, Proc. Roy. Soc. London A272, 557 (1963).

[3] V. G. Gueorguiev, J. P. Draayer, and C. W. Johnson, Phys. Rev. C63, 014318 (2001).

[4] T. Kuo and G. E. Brown, Nucl. Phys. A114, 241 (1968); A. Poves and A. P. Zuker, Phys. Rep. 70, 235 (1981).

[5] C. W. Johnson, I. Stetcu, and J. P. Draayer, “SU(3) versus deformed Hartree-Fock”, Phys. Rev. C 66, 034312 (2002).