Oblique-Basis Calculations for $^{44}$Ti *

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Abstract

The spectrum and wave functions of $^{44}$Ti are studied in oblique-basis calculations using spherical and SU(3) shell-model states. Although the results for $^{44}$Ti are not as good as those previously reported for $^{24}$Mg, due primarily to the strong spin-orbit interaction that generates significant splitting of the single-particle energies that breaks the SU(3) symmetry, a more careful quantitative analysis shows that the oblique-basis concept is still effective. In particular, a model space that includes a few SU(3) irreducible representations, namely, the leading irrep $(1,2,0)$ and next to the leading irrep $(10,1)$ including its spin $S=0$ and $1$ states, plus spherical shell-model configurations (SSMC) that have at least two valence nucleons confined to the $f_{7/2}$ orbit – the SM(2) states, provide results that are compatible with SSMC with at least one valence nucleon confined to the $f_{7/2}$ orbit – the SM(3) states.

Introduction. In a previous study we demonstrated the feasibility of the oblique-basis calculations. The successful description of $^{24}$Mg followed from the comparable importance of single-particle excitations, described by spherical shell-model configurations (SSMC), and collective excitations, described by the SU(3) shell model. An important element of the success is that SU(3) is a good symmetry in $sd$-shell nuclei. For the lower $pf$-shell nuclei, there is strong breaking of the SU(3) symmetry induced by the spin-orbit interaction. Therefore, it is anticipated that adding the leading and next to the leading SU(3) irreps may not be sufficient in lower $pf$-shell.

Here we discuss oblique-basis type calculations for $^{44}$Ti using the KB3 interaction. 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 a pure SU(3) shell-model with only few SU(3) irreps is unsatisfactory. This is the opposite of the situation in the lower $sd$-shell. Since the SSM yields relatively good results for SM(2), combining the two basis sets yields even better

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Table 1: Labels and $M_J=0$ dimensions for various $^{44}$Ti calculations. The leading SU(3) irrep is $(12,0)$; $(10,1)$ implies that the $(10,1)$ irreps are included along with the leading irrep. SM(n) is a spherical shell-model basis with n valence particles anywhere within the full $pf$-shell; the remaining particles being confined to the $f_{7/2}$.

| 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  |

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%). Therefore, as for the $sd$-shell, combining a few SU(3) irreps with SM(2) configurations yields excellent results, such as correct spectral structure, lower ground-state energy, and improved structure of the wave functions. However, in the lower $sd$-shell SU(3) is dominant and SSM is recessive (but important) and in the lower $pf$-shell one finds the opposite, that is, SSM is dominant and SU(3) is recessive (but important).

Model Space. $^{44}$Ti consists of 2 valence protons and 2 valence neutrons in the $pf$-shell. The SU(3) basis includes the leading irrep $(12,0)$ with 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 $(12,0)\&(10,1)$ case has a total dimensionality of 84 and is denoted by $(12,0)\&(10,1)$. In Table 1 we summarize the dimensionalities. As in the case of $^{24}$Mg, there are linearly dependent vectors within the oblique bases sets. For 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 in the previous case.

Ground-state Energy. The oblique-basis calculation of the ground-state energy for $^{44}$Ti does not look as impressive as for $^{24}$Mg. 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. 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%. For SM(2), the ground-state energy is 2.2 MeV lower than the SM(1) result. However, adding the SU(3) irreps to the SM(2) basis gives ground-state energy of $-13.76$ MeV which is compatible to the pure 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 SM(3) which is 84% of the full space.

Low-lying Energy Spectrum. In $^{24}$Mg the position of the K=2 band head is correct for the SU(3)-type calculations but not for the low-dimensional SM(n)
calculations. In $^{44}$Ti it is the opposite, that is, the SM(n)-type calculations reproduce the position of the K=2 band head while SU(3)-type calculations cannot. Furthermore, the low-energy levels for the SU(3) case are higher than for the SM(n) case. Nonetheless, the spectral structure in the oblique-basis calculation is good and the SM(2)+(12,0)&(10,1) spectrum ($\approx$50% of the full space) is comparable with the SM(3) result (84%).

Overlaps with Exact States. The overlap of SU(3)-type calculated eigenstates with the exact (full shell-model) results are not as large as in the $sd$-shell, often less than 40%, but the SM(n) results are considerably better with SM(2)-type calculations yielding an 80% 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. On the other hand, SM(2)+(12,0)&(10,1)-type calculations yield results that are as good as those for SM(3) in only about 50% of the full-space and SM(1)+(12,0)&(10,1) overlaps are often bigger than the SM(2) overlaps.

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

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