Mixed-Symmetry Shell-Model Calculations

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Abstract. The one-dimensional harmonic oscillator in a box problem is used to introduce the concept of an oblique-basis shell-model theory. The method is applied to nuclei by combining traditional spherical shell-model states with SU(3) collective configurations. An application to $^{24}$Mg, using the realistic two-body interaction of Wildenthal, is used to explore the validity of this oblique-basis, mixed-symmetry shell-model concept. The applicability of the theory to the lower $pf$-shell nuclei $^{44-48}$Ti and $^{48}$Cr using the Kuo-Brown-3 interaction is also discussed. While these nuclei show strong SU(3) symmetry breaking due mainly to the single-particle spin-orbit splitting, they continue to yield enhanced B(E2) values not unlike those expected if the symmetry were not broken. Other alternative basis sets are considered for future oblique-basis shell-model calculations. The results suggest that an oblique-basis, mixed-symmetry shell-model theory may prove to be useful in situations where competing degrees of freedom dominate the dynamics.

Two dominate but often competing modes characterize the structure of atomic nuclei. One is the single-particle shell structure underpinned by the validity of the mean-field concept; the other is the many-particle collective behavior manifested through nuclear deformation. The spherical shell model is the theory of choice when single-particle behavior dominates [1]. When deformation dominates, the Elliott SU(3) model can be used successfully [2]. This manifests itself in two dominant elements in the nuclear Hamiltonian: the single-particle term, $H_0 = \sum_i \epsilon_i n_i$, and a collective quadrupole-quadrupole interaction, $H_{QQ} = \hat{Q} \cdot \hat{Q}$. It follows that a simplified Hamiltonian $\hat{H} = \sum_i \epsilon_i n_i - \chi \hat{Q} \cdot \hat{Q}$ has two solvable limits associated with these modes.

To probe the nature of such a system, we consider a simpler problem: the one-dimensional harmonic oscillator in a box of size $2L$ [3]. As for real nuclei, this system

![Graph](image)

**Figure 1.** Left graph shows the structure of the interaction potential of a particle in a one-dimensional box subject to a harmonic oscillator restoring force toward the center of the box. Right graph shows the relative deviations from the exact energy eigenvalues for $\omega = 16$, $L = \pi/2$, $\hbar = \hbar = 1$. The open circles represent deviation of the exact energy eigenvalue from the corresponding harmonic-oscillator eigenvalue $(1 - E_{ho}/E_{exact})$, the solid diamonds are the corresponding relative deviation from the energy spectrum of a particle in a 1D box, and the solid squares are the first-order perturbation theory results.
has a finite volume and a restoring force whose potential is of a harmonic oscillator type, \( \omega^2 x^2 / 2 \). For this model, shown in fig.1, there is a well-defined energy scale which measures the strength of the potential at the boundary of the box, \( E_c = \omega^2 L^2 / 2 \). The value of \( E_c \) determines the type of low-energy excitations of the system. Specifically, depending the value of \( E_c \) there are three spectral types:

1. For \( \omega \to 0 \) the energy spectrum is simply that of a particle in a box.
2. At some value of \( \omega \), the energy spectrum begins with \( E_c \) followed by the spectrum of a particle in a box perturbed by the harmonic oscillator potential.
3. For sufficiently large \( \omega \) there is a harmonic oscillator spectrum below \( E_c \) followed by the perturbed spectrum of a particle in a box.

The last scenario (3) is the most interesting one since it provides an example of a two-mode system. For this case the use of two sets of basis vectors, one representing each of the two limits, has physical appeal, especially at energies near \( E_c \). One basis set consists of the harmonic oscillator states; the other set consists of basis states of a particle in a box. We call this combination a mixed-mode / oblique-basis approach. In general, the oblique-basis vectors form a nonorthogonal and overcomplete set. Even thought a mixed spectrum is expected around \( E_c \), our numerical study, that includes up to 50 harmonic oscillator states below \( E_c \), shows that the first order perturbation theory in energy using particle in a box wave functions as the zero order approximation to the exact functions works quite well after

![Figure 2](image-url)

**Figure 2.** Coherent structure with respect to the non-zero components of the 25th, 27th and 29th exact eigenvector in the basis of a free particle in an one-dimensional box. Parameters of the toy Hamiltonian are \( \omega = 16 \), \( L = \pi / 2 \), \( \hbar = m = 1 \). Right graph shows the coherent structure of the first three yrast states in \(^{48}\)Cr calculated using realistic single-particle energies with Kuo-Brown-3 two body interaction (KB3). On the horizontal axis is \( C_2 \) of \( SU(3) \) with contribution of each \( SU(3) \) state to the corresponding yrast state on the vertical axis.
the breakdown of the harmonic oscillator spectrum. This observation is demonstrated in the right graph of fig. 1 which shows the relative deviations from the exact energy spectrum for a particle in a box.

Although the spectrum seems to be well described using first order perturbation theory based on particle in a box wave functions, the exact wave functions near $E_c$ have an interesting structure. For example, the zero order approximation to the wave function used to calculate the energy may not be present at all in the structure of the exact wave function as is the case shown in the left graph of fig. 2. Another feature also seen in fig. 2 is the common shape of the distribution of the non-zero components along the particle in a box basis. The right graph of fig. 2 shows this same effect in nuclei which is usually attributed to coherent mixing [4, 5].

An application of the theory to $^{24}$Mg [6], using the realistic two-body interaction of Wildenthal [7], demonstrates the validity of the mixed-mode shell-model scheme. In this case the oblique-basis consists of the traditional spherical states, which yield a diagonal representation of the single-particle interaction, together with collective SU(3) configurations, which yield a diagonal quadrupole-quadrupole interaction. The results shown in fig. 3 were obtained in a space that spans less than 10% of the full-space. They reproduce, within 2% of the full-space result, the correct binding energy as well as the low-energy spectrum and the dominate structure of the states that have greater than 90% overlap with the full-space results. In contrast, for a $m$-scheme spherical shell-model calculation one needs about 60% of the full space to obtain results comparable with the oblique basis results.

Studies of the lower $pf$-shell nuclei $^{44-48}$Ti and $^{48}$Cr [8], using the realistic Kuo-Brown-3 (KB3) interaction [9], show strong SU(3) symmetry breaking due mainly to the single-particle spin-orbit splitting. Thus the KB3 Hamiltonian could also be considered a two-mode system. This is further supported by the behavior of the yrast band B(E2) values that seems to be insensitive to fragmentation of the SU(3) symmetry. Specifically, the quadrupole collectivity as measured by the B(E2) strengths remains high even though the SU(3) symmetry is rather badly broken. This has been attributed to a quasi-SU(3) symmetry [5] where the observables behave like a pure SU(3) symmetry while the true eigenvectors exhibit a strong

| Number of Basis States | SM ground state | SM+ one SU(3) irrep | SM+ two SU(3) irreps |
|------------------------|-----------------|---------------------|---------------------|
| -94                    | -79             | -79                 | -79                 |
| -91                    | -82             | -82                 | -82                 |
| -88                    | -85             | -85                 | -85                 |
| -85                    | -88             | -88                 | -88                 |
| -82                    | -91             | -91                 | -91                 |
| -99                    | -98             | -98                 | -98                 |

**Figure 3.** Left graph shows the calculated ground-state energy for $^{24}$Mg as a function of various model spaces. SM(n) denotes spherical shell model calculation with up to n particles outside of the $d_{5/2}$ sub-shell. Note the dramatic increase in binding (3.3 MeV) in going from SM(2) to SM(2)+(8,4)&(9,2) (a 0.5% increase in the dimensionality of the model space). Enlarging the space from SM(2) to SM(4) (a 54% increase in the dimensionality of the model space) adds 4.2 MeV in the binding energy. The right graph shows representative overlaps of pure SM(n), pure SU(3), and oblique-basis results with the exact full sd shell eigenstates. A number within a bar denotes the state with the overlap shown by the bar if it is different from the number for the exact full-space calculation shown on the abscissa. For example, for SM(2) the third eigenvector has the largest overlap with the fourth exact eigenstate, not the third, while the fifth SM(2) eigenvector has greatest overlap with the third exact eigenstate.
coherent structure with respect to each of the two bases. This provides strong justification for further study of the implications of two-mode shell-model studies.

Future research may provide justification for an extension of the theory to multi-mode oblique shell-model calculations. An immediate extension of the current scheme might use the eigenvectors of the pairing interaction \[^9\] within the Sp(4) algebraic approach to the nuclear structure \[^10\], together with the collective SU(3) states and spherical shell model states. Hamiltonian driven basis sets can also be considered. In particular, the method may use eigenstates of the very-near closed shell nuclei obtained from a full shell-model calculation to form Hamiltonian driven J-pair states for mid-shell nuclei \[^11\]. This type of extension would mimic the Interacting Boson Model (IBM) \[^12\] and the so-called broken-pair theory \[^11\]. In particular, the three exact limits of the IBM \[^13\] can be considered to comprise a three-mode system. Nonetheless, the real benefit of this approach is expected when the system is far away of any exactly solvable limit of the Hamiltonian and the spaces encountered are too large to allow for exact calculations.

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