Mixed-Mode Shell-Model Calculations

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September 20, 2002

Abstract

A one-dimensional harmonic oscillator in a box is used to introduce the oblique-basis concept. The method is extended to the nuclear shell model by combining traditional spherical states, which yield a diagonal representation of the usual single-particle interaction, with collective configurations that track deformation. An application to $^{24}$Mg, using the realistic two-body interaction of Wildenthal, is used to explore the validity of this mixed-mode shell-model scheme. Specifically, the correct binding energy (within 2% of the full-space result) as well as low-energy configurations that have greater than 90% overlap with full-space results are obtained in a space that spans less than 10% of the full-space. The theory is also applied to lower pf-shell nuclei, $^{44-48}$Ti and $^{48}$Cr, using the Kuo-Brown-3 interaction. These nuclei show strong SU(3) symmetry breaking due mainly to the single-particle spin-orbit splitting. Nevertheless, the results also show that yrast band $B(E2)$ values are insensitive to fragmentation of the SU(3) symmetry. Specifically, the quadrupole collectivity as measured by $B(E2)$ strengths remains high even though the SU(3) symmetry is rather badly broken. The IBM and broken-pair models are considered as alternative basis sets for future oblique-basis shell-model calculations.

Typically, two competing modes characterize the structure of a nuclear system. The spherical shell model is the theory of choice when single-particle
behavior dominates. When deformation dominates, it is the Elliott SU(3) model. This manifests itself in two dominant elements in the nuclear Hamiltonian: the single-particle field, \( H_0 = \sum_i \varepsilon_i n_i \), and a collective quadrupole-quadrupole interaction, \( H_{QQ} = Q \cdot Q \). It follows that a simplified Hamiltonian \( H = \sum_i \varepsilon_i n_i - \chi Q \cdot Q \) has two solvable limits associated with these modes.

To probe the nature of such a system, we first consider the simpler problem of a one-dimensional harmonic oscillator in a box of size \( 2L \). As for real nuclei, this system has a finite volume and a restoring harmonic potential \( \omega^2 x^2 / 2 \). Depending on the value of \( E_c = \omega^2 L^2 / 2 \), which plays the role of a critical energy, there are three spectral types: (1) for \( \omega \to 0 \) the spectrum is simply that of a particle in a box; (2) at some value of \( \omega \), the spectrum begins with \( E_c \) followed by the spectrum of a particle in a box perturbed by the harmonic potential; and (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 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. One basis set consists of the harmonic oscillator states; the other set consists of basis states of a particle in a box. Even though a mixed spectrum is expected around \( E_c \), a numerical study that includes up to 50 harmonic oscillator states below \( E_c \) shows that first order perturbation theory works well after the breakdown of the harmonic spectrum. Although the spectrum seems to be well described in this way, the wave functions near \( E_c \) have an interesting coherent structure.

An application of the theory to \(^{24}\text{Mg}\), using the realistic two-body interaction of Wildenthal, 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 obtained in a space that spans less than 10% of the full-space reproduce the correct binding energy (within 2% of the full-space result) as well as the low-energy spectrum and 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, \(^{44-48}\text{Ti}\) and \(^{48}\text{Cr}\), using the realistic Kuo-Brown-3 (KB3) interaction 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 has been 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 where the observables behave like a pure SU(3) symmetry while the true eigenvectors exhibit a strong coherent structure with respect to each of the two bases. This provides the opportunity for further study of the implications of two-mode calculations.

Future research may extend to multi-mode oblique calculations. An immediate extension of the current scheme might use the eigenvectors of the pairing interaction within the Sp(4) algebraic approach to the nuclear structure, 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. This type of extension would mimic the Interacting Boson Model (IBM) and the so-called broken-pair theory. In particular, the three exact limits of the IBM can be considered to comprise a three-mode system. Nonetheless, the real benefit of this approach is expected when the spaces encountered are too large to allow for exact calculations.

Acknowledgments. We acknowledge support from the U.S. National Science Foundation under Grant No. PHY-9970769 and Cooperative Agreement No. EPS-9720652 that includes matching from the Louisiana Board of Regents Support Fund. V. G. Gueorguiev is grateful to the Louisiana State University Graduate School for awarding him a dissertation fellowship and to the U. S. National Science Foundation for the support for young scientists to attend the International Nuclear Structure Conference on “Mapping the Triangle” held May 22-25, 2002 in Grand Teton National Park, Wyoming, and in so doing allowing him to present the main results of his Ph.D. dissertation.