Implications of Deformation and Shape Coexistence for the Nuclear Shell Model

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The successes of the nuclear shell model in explaining the stability properties of magic nuclei are challenged by the observation of rotational bands for which the sequential filling of single-particle energy levels of the spherical shell model are not respected. This Letter proposes criteria for identifying the shell-model configurations appropriate for describing such bands of states.

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A suggestion by Morinaga [1] that many excited $J^\pi = 0^+$ states of light nuclei are the lowest states of excited rotational bands is now well established. Many low-energy rotational bands and even superdeformed bands have been observed in closed-shell [2,3] and other light nuclei. The appearance of states of different deformation in a single nucleus is known as *shape coexistence* [4].

Morinaga observed that, while the ^{16}O ground state may be predominantly a spherical closed-shell state, excited states are no longer in closed-shell configurations, and, like the states of doubly-open-shell nuclei, they could be seriously deformed.

Many studies have explained why multi-particle-multi-hole states occur at low energies [5–12]. Nevertheless, from a conventional spherical shell-model perspective, the appearance of multi-particle-multi-hole states in the low-energy domain is potentially disturbing. Even if understood, it is disturbing because it suggests that a conventional shell-model calculation with basis states restricted to a single valence shell becomes questionable when there is little or no energy gap between valence- and higher-shell configurations. A commonly accepted way out of this dilemma is to regard the states of rotational bands with deformations very different from those of the valence-shell states as *intruder states* [8,13] that couple only weakly to the valence-shell states.

Insights into shape coexistence, gained from mean-field models [9,11], suggest the use of deformed bases for the shell model. In general, this causes incompleteness problems and the loss of coupling schemes and other machinery associated with conventional harmonic-oscillator bases. However, as this note shows, such problems are circumvented and shape coexistence can be understood by the use of restricted mean-field calculations within the framework of a symplectic-model basis for the shell model. This understanding has important implications for the selection of a truncated shell-model space.

The standard basis for the nuclear shell model is provided by the independent-particle model of nucleons in a spherical-harmonic-oscillator potential. In application to a light nucleus, a many-nucleon Hamiltonian is diagonalized in the finite space of the lowest-energy major shell. For a closed-shell nucleus, such as ^{16}O, the lowest major shell contains only the closed-shell state which can be regarded as a 0p-0h, particle-hole vacuum, state. Thus, for ^{16}O, the standard shell model predicts the lowest-energy excited states to be negative-parity 1p-1h states in which one nucleon is promoted from the occupied $1p$ single-particle shell to the $2s$-$1d$ shell. In fact, the first excited state of ^{16}O, at 6.05 MeV, is of positive parity and is the lowest state of a rotational band. Examination of the properties of this band of states and shell-model calculations in large multishell spaces indicate that the 6.05 MeV state is a 4p-4h state [1,5–12].

It is well known that low-energy states of doubly-open-shell nuclei tend to belong to rotational bands. Thus, if an np-nh state of a closed-shell nucleus is considered as a product of open-shell configurations, a significant lowering of the energies, due to deformation correlations, and the appearance of rotational states is to be expected.

In constructing a model of rotor bands in light open-shell nuclei, Elliott [14] considered a Hamiltonian

$$\hat{H}(\chi) = \hat{H}_0 - \frac{1}{2}\chi \sum_{ij} \hat{Q}(i) \cdot \hat{Q}(j), \tag{1}$$

where $\hat{H}_0$ is an independent-particle spherical-harmonic-oscillator Hamiltonian, $\hat{Q}(i)$ is the mass quadrupole tensor for nucleon i, and χ is a coupling constant. When $\hat{Q}$ is replaced by its restriction, $\hat{\mathcal{Q}}$, to a single harmonic-oscillator shell, and χ is replaced by a suitable effective coupling constant κ, the resulting Hamiltonian,

$$\hat{\mathcal{H}}(\kappa) = \hat{H}_0 - \frac{1}{2}\kappa \sum_{ij} \hat{\mathcal{Q}}(i) \cdot \hat{\mathcal{Q}}(j), \tag{2}$$

has a spectrum of rotorlike bands; this is because $\hat{\mathcal{H}}(\kappa)$ is diagonal in a basis of states with the quantum numbers of the subgroup chain

$$\begin{array}{ccccccc} \mathrm{U}(3) & \supset & \mathrm{U}(1)\times\mathrm{SU}(3) & \supset & \mathrm{SO}(3) & \supset & \mathrm{SO}(2) \\ N(\lambda,\mu) & & N \quad (\lambda,\mu) & & L & & M \end{array} \tag{3}$$

where U(3) is the symmetry group of the spherical harmonic oscillator. The energy-level spectrum of $\hat{\mathcal{H}}(\kappa)$ is determined from the value

$$\langle(\lambda\mu)|\hat{C}_{SU3}|(\lambda\mu)\rangle = 4[\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)] \quad (4)$$

of the SU(3) Casimir invariant

$$\hat{C}_{SU3} = \hat{Q}\cdot\hat{Q} + 3\hat{L}\cdot\hat{L}, \qquad \hat{Q}\cdot\hat{Q} \equiv \sum_{ij}\hat{Q}(i)\cdot\hat{Q}(j). \quad (5)$$

Thus, if $N\hbar\omega$ is an eigenvalue of $\hat{H}_0$, the energy levels of $\hat{\mathcal{H}}(\kappa)$ are given by

$$E_{LM}^{N(\lambda\mu)} = N\hbar\omega - 2\kappa[\lambda^2 + \lambda\mu + \mu^2 + 3(\lambda + \mu)] + \frac{3}{2}\kappa L(L+1). \quad (6)$$

The Hilbert space of the nuclear shell model is a sum of U(3) subspaces combined with corresponding spin-isospin states. This suggests that an appropriate space for a shell-model calculation of nuclear states, which include rotational states, is given by a suitably selected set of U(3) irreps (irreducible representations). Thus, we consider a procedure for assigning an energy-ordering to the U(3) subspaces of the shell model.

The harmonic-oscillator shell-model space also has a natural decomposition into irreducible subspaces of an Sp(3, ℝ) symplectic algebra [15,16]. This Lie algebra includes infinitesimal generators of nuclear deformation and unrestricted nuclear quadrupole moments. From a collective model perspective, each of its irreps comprises an infinite rotational band of states coupled to multiple-phonon giant-monopole and giant-quadrupole excitations. From a shell-model perspective, each Sp(3, ℝ) irrep is an infinite tower of many U(3) irreps based on a *lowest-grade* U(3) irrep of the Elliott type [14], where the grade of a U(3) irrep is given by its harmonic-oscillator energy $N\hbar\omega$. Moreover, every Sp(3, ℝ) irrep in the shell model is uniquely defined by its lowest-grade U(3) subirrep and is characterized by the $N(\lambda\mu)$ quantum numbers of this U(3) irrep. Thus, there is a unique projection from any Sp(3, ℝ) irrep onto its lowest-grade U(3) irrep, and, as a consequence, the U(3) model provides a meaningful *effective shell-model* image of a more complete symplectic model. It follows that a subspace of the shell model that includes a suitable set of lowest-grade U(3) irreps is a tailor-made effective shell-model space for the description of shape coexistence. Note that, in working within an effective model space, effective charges and other renormalizations are required to account for the neglected coupling to higher shell-model configurations.

Variational criteria for ordering the lowest-grade U(3) irreps by increasing energy are now defined as follows. Let $|\varphi_{N(\lambda\mu)}\rangle$ denote the highest-weight state for a lowest-grade U(3) irrep $N(\lambda\mu)$ and let $|\varphi_{N(\lambda\mu)}(a,b,c)\rangle$ denote the same state deformed by a stretching operation applied to each of its spatial coordinates;, i.e., $x_i \to ax_i$, $y_i \to by_i$, $z_i \to cz_i$. The three-dimensional manifold $\mathcal{M}_{N(\lambda\mu)}$ of states $\{|\varphi_{N(\lambda\mu)}(a,b,c)\rangle\}$ with real values of the deformation parameters (a, b, c) is known [17] to span a subspace of the Sp(3, ℝ) irrep based on the U(3) irrep $N(\lambda\mu)$. Now, if $E_{N(\lambda\mu)}$ denotes the minimum value of the expectation value of a realistic nuclear Hamiltonian for the states of $\mathcal{M}_{N(\lambda\mu)}$, it is meaningful to order the U(3) irreps by increasing values of $E_{N(\lambda\mu)}$; this makes it possible to select a subset of low-energy U(3) irreps to form a finite-dimensional effective shell-model space.

Such variational calculations have yet to be attempted. However, we show here that a simple parameter-free model, based on the methods of Ref. [18] and the *coupled SU(3) model* of Ref. [19], indicates the kind of results that can be expected. The model gives a qualitative indication of which np-nh states are likely to contribute to the low-energy states of nuclei.

We consider the Hamiltonian $\hat{H}(\chi)$, which is quadratic in the elements of the sp(3, ℝ) algebra, and recall that the $\hat{Q}\cdot\hat{Q}$ interaction of this Hamiltonian is designed for use within the framework of a mean-field approximation. For the Hamiltonian $\hat{H}(\chi)$, the mean field experienced by nucleon i due all other nucleons when the nucleus is in the minimal-energy state $|\varphi\rangle$ of the manifold $\mathcal{M}_{N(\lambda\mu)}$is given by

$$U(\mathbf{r}_i) = \frac{1}{2}m\omega^2 r_i^2 - \chi Q(i)\cdot\langle\varphi|\sum_j Q(j)|\varphi\rangle, \quad (7)$$

where $\frac{1}{2}m\omega^2 r_i^2$ is the spherical-harmonic-oscillator potential. Thus, if the density distribution ρ of the state $|\varphi\rangle$ is nonspherical, the mean field U will also be nonspherical and be expressible, in terms of Cartesian coordinates (x, y, z) for the vector $\mathbf{r}$, in the form

$$U(\mathbf{r}) = \frac{1}{2}m(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2) \quad (8)$$

of an ellipsoidal harmonic-oscillator potential. For self-consistency, the equipotential surfaces of U should have the same ellipsoidal shape as the equidensity surfaces of ρ. This condition fixes the magnitude of the coupling constant to a value given, to leading order in λ/N, by $\chi = \hbar\omega/(4N)$ [20], where $N = n_1 + n_2 + n_3$ is the number of quanta in the state $|\varphi\rangle$ of harmonic-oscillator energy $n_1\hbar\omega_1 + n_2\hbar\omega_2 + n_3\hbar\omega_3$ (including the zero-point energy).

From the relationship between the symplectic and U(3) models, we now infer a corresponding value of the coupling constant appropriate for the effective U(3) Hamiltonian $\hat{\mathcal{H}}(\chi)$ of Eq. (2). First, as observed above, any state in an sp(3, ℝ) irrep can be mapped, by projection, to its lowest-grade U(3) irrep. Thus, an appropriate value of the effective coupling constant κ is determined such that, when used in the Hamiltonian $\hat{\mathcal{H}}(\kappa)$ restricted to the lowest harmonic-oscillator shell, it will give the same mean-field results as the Hamiltonian $\hat{H}(\chi)$ in the unrestricted shell-model space. Suppose, for example, that $|\varphi_0\rangle$ is the SU(3) state that maps to $|\varphi\rangle$ under the abovementioned scale transformation. Then, the value of the effective SU(3) coupling constant κ is defined by setting

$$\langle\varphi_0|\hat{\mathcal{H}}(\kappa)|\varphi_0\rangle = \langle\varphi|\hat{H}(\chi)|\varphi\rangle. \tag{9}$$

This gives (to leading order in λ/N)

$$\kappa \approx 2\chi = \frac{\hbar\omega}{2N}. \tag{10}$$

Such a self-consistency argument also gives the effective charge for electric quadrupole transitions in the SU(3) model to be twice its unrenormalized value.

Consider, for example, the spectrum of $\hat{\mathcal{H}}(\kappa)$ for some lowest-grade U(3) irreps of ^{16}O. The 0p-0h closed-shell state of ^{16}O spans a one-dimensional lowest-grade U(3) irrep $N(0,0)$ with $N = 36$. Excited 2p-2h states are obtained by tensor coupling the $(2,0) \otimes (2,0)$ SU(3) irreps for two-particles in the $2s1d$ shell with $(0,1) \otimes (0,1)$ irreps for two holes in the $1p$ shell. The leading irrep (the one with largest value of the SU(3) Casimir operator) in this tensor product is the irrep $N(\lambda,\mu) = 38(4,2)$. The leading irreps for 4p-4h, 6p-6h, and 8p-8h excited configurations are listed in Table I.

The table shows that, if the harmonic-oscillator unit of energy is assigned the standard value $\hbar\omega = 41A^{-1/3}$ MeV, required to give observed nuclear radii, the lowest-energy positive-parity excited state of ^{16}O in the model is at $\approx$ 5 MeV and comes from the leading 4p-4h SU(3) irrep [negative-parity excitations are not considered here]. This result is remarkably close to the observed excitation energy, 6.05 MeV, of the first excited state of ^{16}O. The experimental and theoretical spectra, for the predicted value of κ, are shown in Fig. 1. All observed energy levels have counterparts in the model and E2 transition rates between them are predicted with the correct orders of magnitude. However, the observed E2 transitions imply minor mixing of the U(3) irreps as expected for a more realistic interaction. Thus, as a zero-order approximation to the shell model, the model appears to be successful in identifying the essential U(3) irreps required for a description of low-energy positive-parity states in ^{16}O.

TABLE I. Parameters and excitation energies of leading lowest-grade U(3) irreps for ^{16}O.

Nucleus	np-nh	$N(\lambda,\mu)$	$\hat{C}_{\mathrm{SU3}}$	$E_{\mathrm{exc}}^{N(\lambda\mu)}/\hbar\omega$	$E_{\mathrm{exc}}^{N(\lambda\mu)}$ (MeV)
^{16}O	0p-0h	36(0,0)	0	0	0
	2p-2h	38(4,2)	184	0.79	12.9
	4p-4h	40(8,4)	592	0.30	4.9
	6p-6h	42(10,4)	792	1.29	20.9
	8p-8h	44(12,4)	1024	2.18	35.5

We emphasize that the simple no-parameter model presented is not expected to give a quantitative description of the low-energy states of any nucleus. Its purpose is to initiate the development of criteria for the selection of appropriate effective shell-model spaces in which realistic shell-model calculations can be carried out. Thus, the detailed predictions of the model are not intended to be taken literally. A major cause of uncertainty is the sensitivity of the results to the value of κ, as Fig. 2 shows. This figure also shows another lowest-grade U(3) irrep with $N(\lambda,\mu) = 48(24,0)$ whose excitation energy falls extremely rapidly with increasing values of κ and, for the value given by the above self-consistency argument, falls below the energy of the 0p-0h ground state. However, the assumptions on which the above estimate of κ are based make little sense for an irrep with such a large value of λ/N, which is why the 48(24,0) irrep is not included in Table I. Such an irrep corresponds to a highly elongated nuclear shape that is not at all well described by a mean field with only monopole and quadrupole components. Moreover, the leading order self-consistency estimate is clearly an overestimate for an irrep with such a large value of λ/N. A better estimate, for small μ, would appear to be given by $\kappa \approx \frac{\hbar\omega}{2N}(1 - \frac{\lambda}{2N})$. Excitation energies for this adjusted coupling constant are indicated in Fig. 2. The strength of the $Q \cdot Q$ interaction has been analyzed by Dufour and Zuker [21]. However, for present purposes, what is needed is an accurate determination of the way it scales with deformation. A natural strategy, within the framework of the present approach, for determining the appropriate dependence of κ on $N(\lambda,\mu)$ would be to compare the energies given by Eq. (6) as functions of κ with those of mean-field calculations, with realistic interactions, restricted to corresponding Sp(3, $\mathbb{R}$) irreps, as described above.

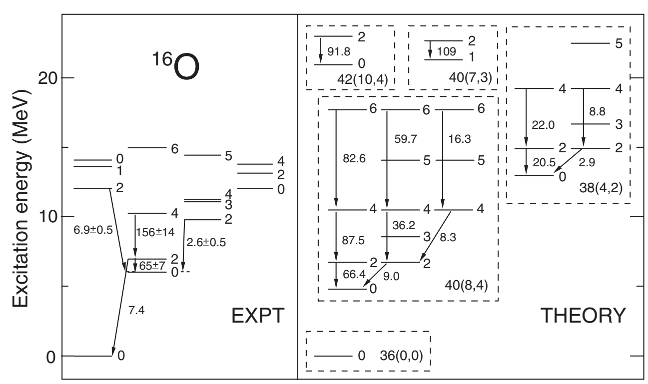

FIG. 1. Positive-parity energy levels of the model with $L \leq 6$ for ^{16}O in comparison with those observed below 15 MeV. Energy levels associated with an irrep $N(\lambda\mu)$ are shown in groups. Reduced $E2$ transition rates are indicated (in e^2fm^4 units) beside the arrows. (The data are extracted from the ENSDF data base, revision of Mar 8, 2002.).

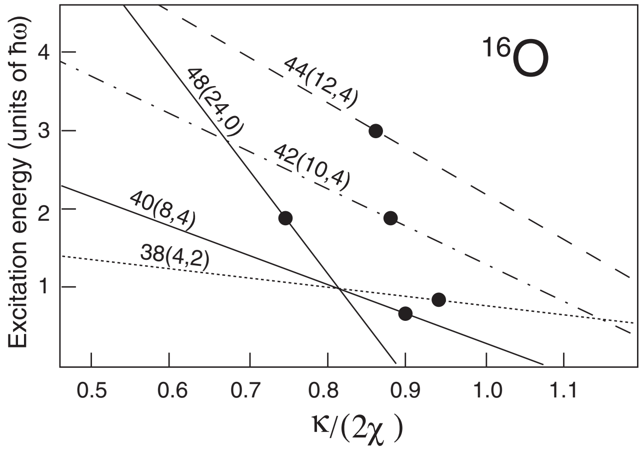

FIG. 2. Spectrum of $E^{N(\lambda\mu)}_{\rm exc}/\hbar\omega$ energies for leading positive-parity lowest-grade U(3) irreps of ^{16}O as functions of κ. The filled circles indicate values of $\kappa = 2\chi[1 - \lambda/(2N)]$.

There is now substantial evidence, independent of the predictions of the model, that particular combinations of 4p-4h states fall lower in energy than even the 1p-1h states in ^{16}O. This is not an isolated example as revealed by the observation of shape coexistence in many nuclei [4]. In heavy nuclei, there is strong evidence to suggest that well-deformed states from high-lying shells fall well below those of the 0p-0h states. For example, Jarrio *et al.* [22] showed that while a deformed independent-particle (Nilsson) model can explain the ground-state rotational bands of the Erbium isotopes, a description of these bands in terms of the spherical shell model must be dominated by states from Sp(3, $\mathbb{R}$) irreps based on lowest-grade U(3) irreps with $(2\lambda + \mu) \sim 200$. Carvalho [18] showed that such SU(3) irreps belong to $N(\lambda, \mu)$ irreps of U(3) with $N \gtrsim N_0 + 10$, where N_0 is the value of N for the 0p-0h spaces of these nuclei. In a symplectic-model calculation of the ^{166}Er ground-state rotational band, Bahri [23] found that the lowest-grade SU(3) components were not even the dominant components of the states that emerged; in fact, the dominant components were from shells of order 8 higher than those of the lowest-grade SU(3) irrep, which was already some 10 shells higher than the 0p-0h shell for this nucleus. Nevertheless, the lowest-grade U(3) irrep, with renormalized parameters, provided a remarkably accurate *effective model* description of this rotational band.

The suitability of an Elliott SU(3) basis [14] for mixed-shell-model calculations in light nuclei has been emphasized by several authors [7,24,25]. Variations of the perspective given in this paper have also been expressed elsewhere [18,22,26]. What is special about this Letter is a demonstration of the insights into nuclear structure to be gained from a study of shape coexistence and what can be achieved by defining an effective shell-model space in terms of U(3) lowest-grade states.

For application to medium and heavy nuclei, the current model needs refinement to take account of the spin-orbit interaction in the definition of spherical shell-model states. The emergence of SU(3) as a relevant coupling scheme for rotational states in heavy nuclei has been observed in the calculations of Sun *et al.* [27]. Obvious possibilities for the extension of the present approach is by use of the pseudo-SU(3) [28] and pseudo-Sp(3, $\mathbb{R}$) models [29] and by the methods of Refs. [18,22].

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