

# Nuclear shape coexistence from the perspective of an algebraic many-nucleon version of the Bohr-Mottelson unified model

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A fully quantal algebraic version of the Bohr-Mottelson unified model is presented with the important property that its quantization is defined by the fully antisymmetric many-nucleon unitary irreps (irreducible representations), which span the many-nucleon Hilbert space of a nucleus. The spatial component of this model, with added spin  $SU(2)_S$  and isospin  $SU(2)_T$  degrees of freedom, is uniquely defined by the requirement that its Lie algebra of observables includes the nuclear quadrupole moments, its angular momenta, and kinetic energy. Thus, it is determined to be an  $Sp(3, \mathbb{R})$  Lie algebra, which is then combined with the spin and isospin algebras of a Lie algebra for an  $Sp(3, \mathbb{R}) \times SU(2)_S \times SU(2)_T$  dynamical group of the desired algebraic unified model. The irreps of this model are uniquely defined by their  $Sp(3, \mathbb{R})$  lowest weights, spins, and isospins, and have the property that observed transitions between rotational states of nuclei can be expressed in terms of these irreps and their mixtures. The algebraic unified model parallels the Bohr-Mottelson version in almost all respects, including the possibility of taking into account the effects of Coriolis and centrifugal forces as subsequent perturbations. In addition, it defines the admissible fully antisymmetric many-nucleon irreps and puts a new perspective on the phenomenon of shape coexistence. It avoids use of an overcomplete set of coordinates and corrects the phenomenological unified model treatment of angular momentum quantization. These changes have significant implications for the dynamics of nuclear rotations, which are hidden when its moments of inertia are considered as adjustable parameters in the standard expression of rotational kinetic energies.

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## I. INTRODUCTION

Nuclei are of special interest among the many-particle systems that have contributed to the development of quantum mechanics. They have shell structures, similar to those of atoms, and rotational states with properties between those of molecules and superfluids. Such properties and the prevalence of deformed nuclei with rotational spectra throughout the nuclear periodic table [1–5] stimulate interest in the dynamics of nuclear rotations and motivate development of the many-nucleon quantum mechanics of the rotational states of deformed nuclei.

It is generally understood that, in the classical mechanics of a many-particle system in a rotating frame of reference, there are perturbations due to centrifugal and Coriolis forces. In accord with Born-Oppenheimer theory [6], it is also understood that these inertial forces can be treated as perturbations of the low angular-momentum rotational states of nuclei in quantum mechanics. Thus, Bohr and Mottelson [7] introduced their highly influential unified model of low-energy rotational states with moments of inertia as adjustable parameters and wave functions expressed as functions of the orientation angles of an intrinsic state that also has higher-energy vibrational excitations. However, there are fundamental differences between translations and rotations in quantum and classical mechanics that were not taken into account in the phenomenological unified model. A particularly significant difference is that, whereas the wave functions of a many-

particle system can be expressed as products of functions that are, respectively, functions of center-of-mass coordinates and intrinsic functions of relative coordinates, there is no such separation of the many-nucleon coordinates into subsets of rotational and complimentary intrinsic coordinates, as presumed in the unified model, other than in a rigid-rotor limit [8].

Another questionable presumption is that the rotational energies of nuclei are kinetic energies as understood, for example [9], in the interpretation of the moments of inertia of the Inglis cranking model [10,11] as linear combinations of those for rigid-body and irrotational flow rotations. More sophisticated cranking models [12] and models with the inclusion of superconducting pairing interactions [13] were similarly interpreted and the moments of inertia of essentially all rotational nuclei have been observed, in support of this cranking model interpretation [14], to lie between those of irrotational superfluid rotations and the rigid-body flows of a viscous fluid.

This paper is concerned with establishing a framework in which the dynamics of nuclear rotations can be explored. The dynamics is expected to be model dependent. However, as this paper shows, it is possible to define an optimal algebraic many-nucleon version of the unified model with the property that there are no isoscalar  $E2$  transitions between the states of its different irreps (irreducible representations). Observed rotational states are then mixtures of its irreps. A useful result, shown in Sec. III, is that this optimal model is the

already well-known symplectic model, which now acquires an enhanced significance.

Early symplectic model calculations were made [15–19] to derive the properties of nuclear rotational states with model interactions in truncated finite-dimensional shell-model spaces. In these applications, fits were obtained to both the energy levels and  $E2$  transitions of  $^{20}\text{Ne}$  [15],  $^{24}\text{Mg}$  [18], and four rare-earth nuclei [19], without the use of effective charges, and it was determined that the so-called rotational energies of the nuclei in these calculations were mixtures of kinetic and potential energies of comparable magnitude. Similar results were later obtained for  $^{166}\text{Er}$  by Bahri [20]. However, while significant and suggestive, these results with model Hamiltonians in truncated spaces could not be considered definitive.

## II. DYNAMICS OF THE BOHR-MOTTelson UNIFIED MODEL

In the Bohr-Mottelson unified model [1,7], the rotations and shape vibrations of a nucleus are characterized by an intrinsic state that corresponds to a classical limit of a rotor at rest. This state has vibrational excitations corresponding to those of quantized normal-mode vibrations and rotational states described by wave functions that are functions of the orientation angles of the intrinsic ground state. All the states of the ground-state rotational band of the unified model were thereby assigned a common intrinsic state and, hence, common potential energies. The rotational energies of the unified model were then presumed to be kinetic energies. The remarkable successes of this unified model, with moments of inertia adjusted to fit the data, then resulted in its widespread acceptance.

Unfortunately, there is negligible experimental information on the nature of nuclear rotations. There was early optimism that the current flows in rotating nuclei could be determined from transverse electron scattering cross sections [21–26]. However, because of the dominance of much larger longitudinal cross sections, the available cross sections proved to be too imprecise to be of much value.

In view of the successes of the Bohr-Mottelson model, there followed numerous theoretical investigations of the many-nucleon kinetic energy of a nucleus [8,10,11,27–38]. Complete decompositions of the nuclear kinetic energy operator were ultimately obtained in terms of collective coordinates and momenta [35,38–40], and summarized in Ref. [41]. The objective was to express the many-nucleon kinetic energy of a nucleus as a sum of intrinsic plus rotational components with a minimal coupling term that could be treated as a perturbation. However, it turned out that only for a rigid-body rotor or a superfluid with zero vorticity could the kinetic energy of a nucleus be expressed as a sum of rotational and complementary intrinsic energies without a strong coupling term. The search was nevertheless rewarding in that it led to the discovery, as reviewed in Refs. [16,42], of a number of algebraic many-nucleon models of nuclear collective motions: one was  $U_i$ 's rigid rotor model [43]; another was the so-called CM(3) model of Weaver, Biedenharn, and Cusson [37],

which included quantized vortex spin degrees of freedom; and another was the symplectic model [15,16].

Meanwhile, a coupling scheme for the spherical shell model based on the  $U(3)$  symmetry group of the spherical harmonic oscillator, with the remarkable ability to reproduce many of the properties of a rotor model with an effective interaction and an effective charge, was provided by Elliott's  $SU(3)$  model [44,45]. This is now understood from the observation that an  $SU(3)$  irrep is the projected image of a rigid-rotor model [46] irrep onto an irreducible  $U(3)$  subspace of the spherical harmonic-oscillator shell model. For, whereas the Lie algebra of the  $U_i$  rigid-rotor model is spanned by angular momentum and quadrupole moment operators, the  $SU(3)$  Lie algebra is spanned by the same angular momentum operators but with the restriction of the quadrupole moment operators to their  $SU(3)$  components. As a result, all the states of an  $SU(3)$  rotor model irrep have identical kinetic energies and provide no information on the dynamics of nuclear rotations.

## III. AN OPTIMAL MODEL OF THE ROTATIONS AND SHAPE VIBRATIONS OF DEFORMED NUCLEI

The collective dynamics of nuclear rotations and shape vibrations is model dependent. However, it is most usefully defined for an algebraic model with a dynamical group having the following properties: (i) its Lie algebra is a subalgebra of that of the group of all one-body unitary transformations of a many-nucleon Hilbert space; (ii) it has a set of irreps that together span the fully anti-symmetric many-nucleon Hilbert space of a nucleus; and (iii) its Lie algebra contains among its elements the many-nucleon kinetic energy, the angular momentum operators, and the monopole/quadrupole moment operators of nuclei. Conditions (i) and (ii) then restrict consideration to the set of admissible many-nucleon representations; i.e., those which are fully antisymmetric as required of a many-fermion model. And, condition (iii) ensures that the decomposition of the Hilbert space of a nucleus into irreducible collective model subspaces, has the essential and invaluable property that there can be no nonzero matrix elements of any of the operators in its Lie algebra between states belonging to different model irreps. While the rotational states of physical nuclei are not expected to satisfy the latter condition, its inclusion in the optimal model enables the physical states to be expressed as mixtures of the model's states to explain observed interband  $E2$  transitions. The properties of such an optimal rotor model are then of primary interest.

A fortuitous result is that the simplest algebraic model with these properties is already known. It is the symplectic model [15,16,42] with an  $\text{Sp}(3, \mathbb{R}) \times \text{SU}(2)_S \times \text{SU}(2)_T$  dynamical group in which  $\text{Sp}(3, \mathbb{R})$  is the symplectic group with Lie algebra spanned, for an  $A$ -nucleon nucleus, by the operators

$$\hat{Q}_{ij} = \sum_{n=1}^A \hat{x}_{ni} \hat{x}_{nj}, \quad \hat{P}_{ij} = \sum_{n=1}^A (\hat{x}_{ni} \hat{p}_{nj} + \hat{p}_{ni} \hat{x}_{nj}), \quad (1)$$

$$\hbar \hat{L}_{ij} = \sum_{n=1}^A (\hat{x}_{ni} \hat{p}_{nj} - \hat{x}_{nj} \hat{p}_{ni}), \quad \hat{K}_{ij} = \sum_{n=1}^A \hat{p}_{ni} \hat{p}_{nj}, \quad (2)$$

where  $\hat{x}_{ni} = x_{ni}$  and  $\hat{p}_{ni} = -i\hbar\partial/\partial x_{ni}$ , with  $i, j = 1, 2, 3$ , are the position and momentum observables of the  $n = 1, \dots, A$  nucleons of a nucleus. The spin-isospin groups  $SU(2)_S \times SU(2)_T$  are included to take account of the neutron and proton spins and ensure that the combined space, spin, and isospin states of an irrep satisfy the antisymmetry requirements of a many-nucleon nucleus. The  $\hat{P}_{ij}$  operators were not among the required elements of the Lie algebra being sought. However, their inclusion is appropriate; not only are they required to close the Lie algebra, they also have an important physical significance as the infinitesimal generators of model shape deformations.

An invaluable property of this  $Sp(3, \mathbb{R}) \times SU(2)_S \times SU(2)_T$  symplectic model is that its totally antisymmetric irreps together span the Hilbert spaces of any nucleus with and without inclusion of the nuclear center-of-mass degrees of freedom. Another important property, as shown in the following section, is that the Bohr-Mottelson unified model emerges as a mean-field expression of this algebraic many-nucleon model.

The group  $Sp(3, \mathbb{R})$  is understood to have elementary unitary representations given, respectively, by the positive and negative parity states of a three-dimensional harmonic oscillator. It similarly has many-nucleon unitary representations defined by a lowest-weight state of some number of nucleons in the states of a spherical harmonic oscillator. A classification of the states of nuclei, in terms of their space, spin, and isospin quantum numbers is then obtained in terms of  $Sp(3, \mathbb{R}) \times SU(2)_S \times SU(2)_T$  irreps on subspaces of many-nucleon harmonic-oscillator shell-model states. A systematic procedure for determining the matrix elements of these irreps in an angular-momentum coupled basis has also been given by so-called vector-coherent-state methods [47–50]. However, for present purposes, I am concerned with the simpler task of constructing the states of an algebraic many-nucleon version of the Bohr-Mottelson unified model.

The Lie algebra of the symplectic model is defined as follows. First, express the position and momentum coordinates of the nucleons in terms of harmonic-oscillator raising and lowering operators,  $\{c_{ni}^\dagger, c_{ni}\}$ , by the standard expressions

$$\hat{x}_{ni} = \frac{1}{\sqrt{2}a}(c_{ni}^\dagger + c_{ni}), \quad \hat{p}_{ni} = i\hbar\frac{a}{\sqrt{2}}(c_{ni}^\dagger - c_{ni}), \quad (3)$$

where  $a = \sqrt{M\omega_0/\hbar}$  is a harmonic-oscillator unit of inverse length. This gives

$$\hat{Q}_{ij} = \frac{1}{2a^2}(2\hat{Q}_{ij} + \hat{A}_{ij} + \hat{B}_{ij}), \quad \hat{P}_{ij} = i\hbar(\hat{A}_{ij} - \hat{B}_{ij}), \quad (4)$$

$$\hat{K}_{ij} = \frac{1}{2}a^2\hbar^2(2\hat{Q}_{ij} - \hat{A}_{ij} - \hat{B}_{ij}), \quad \hat{L}_{ij} = -i(\hat{C}_{ij} - \hat{C}_{ji}), \quad (5)$$

with

$$\hat{A}_{ij} = \hat{A}_{ji} = \sum_{n=1}^A c_{ni}^\dagger c_{nj}^\dagger, \quad \hat{B}_{ij} = \hat{B}_{ji} = \sum_{n=1}^A c_{ni} c_{nj}, \quad (6)$$

$$\hat{C}_{ij} = \sum_{n=1}^A \left( c_{ni}^\dagger c_{nj} + \frac{1}{2}\delta_{i,j} \right), \quad \hat{Q}_{ij} = \frac{1}{2}(\hat{C}_{ij} + \hat{C}_{ji}). \quad (7)$$

Thus, it is apparent that the states of the optimal model are defined on subspaces of many nucleons in the positive- or negative-parity states of a three-dimensional harmonic oscillator.

#### IV. A CLASSICAL MEAN-FIELD PERSPECTIVE

Primary objectives of this paper are to identify the Bohr-Mottelson unified model with a classical representation of the symplectic model and to identify its quantization with an irreducible unitary representation of this algebraic model. This section outlines the relationship between these two representations in terms of mean-field theory.

It has long been understood that classical mechanics can be realized as constrained quantum mechanics [51] in which, for example, the classical states of a finite fermion system are identified with the states of a submanifold of quantum mechanical states known in physics as coherent states. Coherent states were introduced for harmonic-oscillator states by Glauber [52] and subsequently defined for any algebraic model with a dynamical group and unitary irreps with lowest-weight states, by Perelomov and Klauder [53,54], as the states generated by the transformations of a lowest-weight state of the irrep by the set of dynamical group elements. Such coherent states are described in mathematics as elements of a coadjoint orbit [55–58]. Thus, it is apparent that an algebraic model with a dynamical group and a lowest-weight state has a classical representation with a phase space given by the coherent states generated by the group transformations of the lowest-weight state and a quantum mechanical representation defined on the Hilbert space spanned by these coherent states.

The most familiar classical manifolds in many-fermion quantum mechanics, are sets of independent-particle states with Slater determinant wave functions. For these manifolds, the equations of motion of quantum mechanics for the time evolution of a Slater determinant, that is constrained to remain a Slater determinant, are the well-known classical equations of time-dependent HF (Hartree-Fock) theory. The corresponding classical Hamiltonian equations of motion, defined by time-dependent HF theory, are then identical to the corresponding equations of motion of constrained quantum mechanics as shown, for example, in Refs. [59–62]. Thus, a minimum energy HF state in such a manifold is a classical equilibrium state for which the expectation value of the quantum mechanical Hamiltonian is a (possibly local) minimum. Also the classical normal-mode vibrations of a nucleus about its equilibrium state, given by the time-dependent HF equations of motion [63,64], are identical to those of the quantum-mechanical random-phase approximation (RPA) of Bohm and Pines [65]. This becomes apparent when the RPA is expressed in the double-commutator equations-of-motion formalism [66–68], which is the form in which it is now commonly used in nuclear physics [69].

The embedding of classical mechanics in quantum mechanics by such mean-field methods is insightful for understanding the physics of quantum systems from a classical perspective; e.g., for exploring the topography of the classical potential energy surface, as a landscape, in the neighbourhood of its lowest-energy equilibrium state. This was initiated by

Rowe, Basserman [59,70] and Marumori [71], who studied the valley floor of its classical potential energy surface and by Reinhard and Goeke [72], who studied its fall lines. It is apparent [73,74] that, in proceeding upwards along the valley floor, starting from its lowest point, a high point of the valley is reached, following which the valley path begins a descent to another low-energy point. It follows that the HF minimisation procedure could converge to such a local minimal-energy state if the iterative HF procedure were initiated from a state in its neighborhood. Such a possibility has been considered by Matsuyanagi and colleagues [75]. However, the properties of local minimum-energy HF excited states have yet to be explored.

A promising application relates to the many minima of very different deformations given by the algebraic many-nucleon version of the unified model, as discussed in the following section in which it is shown that, when the Lie group of one-body operators is restricted to its  $\text{Sp}(3, \mathbb{R}) \times \text{SU}(2)_S \times \text{SU}(2)_T$  symplectic model subgroup, the classical HF potential-energy surface separates into a sum of disconnected energy surfaces, each of which is defined for an irrep of the symplectic model subgroup. It would not be surprising then to find that, if a general HF calculation were initiated from the minimum-energy state of one these symplectic model irreps, it converged to a local minimum-energy state of essentially the same general form. For example, if an HF calculation for  $^{16}\text{O}$  were initiated from a closed-shell state of spherical harmonic oscillator states, it would most likely converge to a closed-shell state of single-nucleon states with modified radial wave functions. Likewise, if it were initiated from a deformed four-particle–four-hole symplectic model minimum-energy state, it might converge to a modified but related four-particle–four-hole state relative to the closed-shell solution. It would then be meaningful to interpret the minimum-energy state as an intrinsic state of a unified model, as pursued in the following for the symplectic model, for which its low-energy rotational states are generated by its rotations and its intrinsic vibrational excited states are defined by its small-amplitude time-dependent normal mode vibrations.

## V. AN ALGEBRAIC MANY-NUCLEON (AMN) UNIFIED MODEL

Following the definition in Sec. III, an optimal model of nuclear rotations and shape vibrations can be constructed with an  $\text{Sp}(3, \mathbb{R}) \times \text{SU}(2)_S \times \text{SU}(2)_T$  dynamical group in an AMN version of the Bohr-Mottelson unified model. Its essential properties are exhibited by its irreps of minimal spin and isospin, which are also of maximal space symmetry and, hence, are the most deformed. As now shown, the states of this model are substantially lowered in energy by corresponding deformations of the shell-model potential and end up with energy levels surrounded by those of less deformation and lower spherical harmonic-oscillator energies. This perspective provides an understanding of the emergent phenomenon of shape-coexistence of strongly deformed states among spherical states of much lower spherical shell-model energy [4,5]. Thus, for simplicity in establishing the principles underlying the approach presented, the focus in this paper is restricted

to the properties of fully antisymmetric  $\text{Sp}(3, \mathbb{R}) \times \text{SU}(2)_S \times \text{SU}(2)_T$  irreps with  $S = 0$  and  $T = T_0$  with the expectation that an extension to other irreps will be straightforward.

A symplectic model irrep is conventionally defined, within the many-nucleon Hilbert space of a nucleus, by a lowest-weight state  $|\sigma, \omega\rangle$  that satisfies the equations

$$\hat{B}_{ij}|\sigma, \omega\rangle = 0, \quad \text{for } i, j = 1, 2, 3, \quad (8)$$

$$\hat{C}_{ij}|\sigma, \omega\rangle = 0, \quad \text{for } i < j, \quad (9)$$

$$\hat{C}_{ii}|\sigma, \omega\rangle = \sigma_i|\sigma, \omega\rangle, \quad \text{for } i = 1, 2, 3, \quad (10)$$

where  $|\sigma, \omega\rangle$  is a spherical shell-model state and, therefore an eigenstate of a many-nucleon spherical harmonic-oscillator Hamiltonian

$$\hat{H}_{\text{sho}}|\sigma, \omega\rangle \equiv \hbar\omega \sum_{i=1}^3 \hat{C}_{ii}|\sigma, \omega\rangle = \hbar\omega \sum_{i=1}^3 \sigma_i|\sigma, \omega\rangle, \quad (11)$$

with a value of  $\omega$  such that the volume of the state  $|\sigma, \omega\rangle$  is that of essentially incompressible nuclear matter. However, a symplectic model calculation can be carried out more meaningfully and, for present purposes, more usefully in a triaxial harmonic-oscillator basis of eigenstates of a Hamiltonian  $\hat{H}_{\text{tho}}$  for which the state  $|\sigma, \omega\rangle$  is the lowest-energy eigenstate

$$\hat{H}_{\text{tho}}|\sigma, \omega\rangle \equiv \sum_{i=1}^3 \hbar\omega_i \hat{C}_{ii}|\sigma, \omega\rangle = \sum_{i=1}^3 \hbar\omega_i \sigma_i|\sigma, \omega\rangle \quad (12)$$

with frequencies chosen to minimize the energy  $\langle \sigma, \omega | \hat{H} | \sigma, \omega \rangle$  of a nuclear Hamiltonian among states that are now eigenstates of a generally triaxial harmonic oscillator  $\hat{H}_{\text{tho}}$ . The required state  $|\sigma, \omega\rangle$  is then given by the self-consistency property of HF theory, which is that the values of  $(\omega_1, \omega_2, \omega_3)$  are determined by the condition that the potential-energy component

$$V(x) = \frac{1}{2}M \sum_n (\omega_1^2 x_{n1}^2 + \omega_2^2 x_{n2}^2 + \omega_3^2 x_{n3}^2), \quad (13)$$

of the mean-field Hamiltonian  $\hat{H}_{\text{tho}}(\omega)$ , of which the state  $|\sigma, \omega\rangle$  is an eigenstate, has maximal overlap as a function of the  $x_i$  coordinates with the density of the minimum-energy state  $|\sigma, \omega\rangle$  (subject to the constraint that the volume of the nucleus is consistent with that of essentially incompressible nuclear matter).

The surfaces of constant  $V(x)$  potential energy are seen to be ellipsoidal. Also the mean values of  $\sum_n x_{ni}^2$  in the lowest-energy state of the independent-particle Hamiltonian with this potential energy are given by

$$\langle x_i^2 \rangle_{\omega(\sigma)} = \langle \sigma, \omega | \sum_n x_{ni}^2 | \sigma, \omega \rangle = \frac{\hbar\sigma_i}{M\omega_i}, \quad i = 1, 2, 3. \quad (14)$$

It follows that the closest approach to an ellipsoidal equidensity surface for the minimal energy state, is defined by the equation

$$\frac{x_1^2}{\langle x_1^2 \rangle_{\omega(\sigma)}} + \frac{x_2^2}{\langle x_2^2 \rangle_{\omega(\sigma)}} + \frac{x_3^2}{\langle x_3^2 \rangle_{\omega(\sigma)}} = \text{const.}, \quad (15)$$

i.e., by

$$\frac{\omega_1 x_1^2}{\sigma_1} + \frac{\omega_2 x_2^2}{\sigma_2} + \frac{\omega_3 x_3^2}{\sigma_3} = \text{const.} \quad (16)$$

For this equidensity surface to have the same ellipsoidal shape as the equipotential surface for the potential  $V(x)$  given by the equation

$$\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2 = \text{const.} \quad (17)$$

it is then required that

$$\sigma_1 \omega_1 = \sigma_2 \omega_2 = \sigma_3 \omega_3. \quad (18)$$

Such a shape-consistency relationship has also been used for other purposes; e.g., by Bohr and Mottelson [1,9] and Castel *et al.* [76]. In addition to satisfying the shape consistency of the harmonic-oscillator field and the density of its lowest-weight state, it also corresponds to an equipartition of the three components of the generally triaxial harmonic oscillator energy which is also a desirable property of a minimal energy equilibrium state.

When  $\sigma_1 = \sigma_2 = \sigma_3$ , it follows that  $\omega_1 = \omega_2 = \omega_3$  and that the corresponding lowest-weight state of the symplectic model is rotationally invariant and in a state of zero orbital angular momentum. It is then a many-nucleon  $L = S = J = 0$ ,  $T = T_0$  ground state of a spherical harmonic oscillator Hamiltonian and has one-phonon monopole and quadrupole vibrational excitations given by the random phase approximation. This is what one would expect for a doubly closed-shell nucleus. However, when  $\sigma_1 > \sigma_2$  and/or  $\sigma_2 > \sigma_3$ , the shape-consistent lowest-energy lowest-weight state for an irrep of the  $\text{Sp}(3, \mathbb{R})$  dynamical group is nonspherical and has an interpretation as an intrinsic state of an algebraic many-nucleon version of the Bohr-Mottelson unified model.

Following the Nambu-Goldstone interpretation [77,78], a nonrotationally invariant (broken-symmetry) minimum-energy state is understood to be a combination of the many states of good angular momentum that can be obtained by angular-momentum projection methods as developed, for example, by Lee, Cusson [79,80], Kamlah [81], and others [82,83]. Low-energy rotational states for the model are then obtained by diagonalization of a nuclear Hamiltonian in the space of these projected states of good angular momentum, which then have an interpretation as the rotational states of a unified model.

In concluding this section, it is instructive to consider the relationship of the symplectic model of a rotor to that of Elliott's SU(3) model. The SU(3) model was introduced as a coupling scheme for the spherical shell model of nuclei and was observed to exhibit many rotor model properties. These properties can be understood, as noted in Sec. I, from the observation that the SU(3) model is the image of a genuine rigid-rotor model [46] irrep when projected onto an irreducible U(3) subspace of the spherical harmonic-oscillator shell model. As such it has an interpretation as a model of a rigid rotor with an effective Hamiltonian and an effective charge. Thus, the kinetic rotational energy of the rigid rotor is effectively replaced by a potential energy and both the neutrons and the protons are assigned

large effective charges. Clearly, many characteristics of the rigid rotor are lost in its projection to a single spherical harmonic oscillator shell. For example, a rigid rotor model is infinite dimensional whereas an SU(3) model is finite.

The symplectic model has sometimes been considered to be an extension of the SU(3) model. However, as shown in Sec. III the symplectic model is more appropriately considered to be an advance on the rigid-rotor model of which the SU(3) model is a projected image. Moreover, as model calculations illustrate [19] and as the following section confirms, the low-lying rotational states of the symplectic model description of well-deformed nuclei generally have essentially zero overlaps with low-lying SU(3) states. Nevertheless, in spite of their differences, symplectic model calculations benefit substantially from the many developments of the SU(3) tensor algebra [84,85].

It is also significant that massive shell-model calculations of nuclear rotational states with realistic interactions in the symmetry-adapted no-core shell model [86], determine them to be mixtures of numerous SU(3) irreps from many different spherical harmonic oscillator shells. However, as recently shown [87], these many SU(3) irreps belong to just a few symplectic model irreps. It follows that the symplectic model not only provides a fully quantal many-nucleon version of the successful Bohr-Mottelson unified model, it also identifies the symplectic symmetry that underlies the shape coexistence of nuclei as an emergent phenomenon.

## VI. AN ENERGY ORDERING OF SYMPLECTIC MODEL IRREPS AND SHAPE COEXISTENCE

In the standard spherical shell model, an energy-ordered basis of independent-particle states is defined by the energies of single neutron and single proton states in a spherical harmonic-oscillator field with a spin-orbit interaction and a minor angular-momentum-dependent term with strengths adjusted to fine tune the required sequences of states. Such an ordering of single-nucleon states is then used in the selection of active valence-shell spaces for shell-model calculations of the many-nucleon states of nuclei. This is no doubt appropriate for doubly closed-shell nuclei and for states that give no evidence of belonging to rotational sequences. However, even for spherical nuclei, there are frequent occurrences of strongly deformed states at low excitation energies. For example, the first excited state of  $^{16}\text{O}$  is understood to be the  $J = 0$  ground state of a band of a strongly deformed rotational states with an intrinsic state given by a four-particle-four-hole excitation of the spherical  $^{16}\text{O}$  closed-shell state [88,89]. Consistent with the widespread observation of nuclear shape coexistence [4,5,90], Hartree-Fock calculations [91,92] also indicate that most nuclei have deformed lowest-energy mean-field states. This is easily understood.

Table I lists the leading positive parity  $S = 0$ ,  $T = T_0 = \frac{1}{2}(N - Z)$  AMN symplectic-model irreps available for three nuclei. The irreps of each nucleus are ordered by increasing values of the mean-field energies  $E_\sigma$  of their lowest-weight states as determined, in units of  $\hbar\omega_0$ , by the mean-field shape-

TABLE I. Comparison of the minimum lowest-weight energies  $E_\sigma = \langle \sigma, \omega | \hat{\mathcal{H}} | \sigma, \omega \rangle / \hbar\omega_0$  of positive parity symplectic model irreps of three nuclei, given in increasing order in units of  $\hbar\omega_0$  as defined by Eq. (19), and the corresponding values of  $N$ ,  $\lambda = \sigma_1 - \sigma_2$ , and  $\mu = \sigma_2 - \sigma_3$ , for a range of values of  $N = \sigma_1 + \sigma_2 + \sigma_3$  increasing from the minimum value allowed by the Pauli exclusion principle for states of spin  $S = 0$  and isospin  $T = T_0$ . The spurious contributions of the center-of-mass states to the results shown have been removed. The relative magnitudes of ellipsoidal deformations of the shape-consistent  $\text{Sp}(3, \mathbb{R})$  lowest-weight states are characterized by the values of  $(\lambda + \mu)^2$ . The representations are ordered by increasing values of  $E_\sigma = 3(\sigma_1\sigma_2\sigma_3)^{1/3}$ . The tables show that the irreps with strongly deformed lowest-weight states, as characterized by large values of  $(\lambda + \mu)^2$ , have significantly lower values of  $E_\sigma$  relative to  $N$  than those that are closer to spherical harmonic-oscillator irreps with relatively small values  $(\lambda + \mu)^2$ . (Similar results without removal of the center-of-mass energies were presented in Ref. [93].)

$^{12}\text{C}$					$^{16}\text{O}$					$^{166}\text{Er}$				
$N$	$\lambda$	$\mu$	$(\lambda + \mu)^2$	$E_\sigma$	$N$	$\lambda$	$\mu$	$(\lambda + \mu)^2$	$E_\sigma$	$N$	$\lambda$	$\mu$	$(\lambda + \mu)^2$	$E_\sigma$
24.5	0	4	16	23.8	34.5	0	0	0	34.5	812.5	30	8	1444	811.05
28.5	12	0	144	24.3	38.5	8	4	144	35.7	824.5	96	20	13,456	811.38
26.5	6	2	64	24.7	36.5	4	2	36	35.8	822.5	82	26	11,664	811.47
30.5	10	2	144	26.9	46.5	24	0	576	36.3	826.5	104	20	15,376	811.49
32.5	12	2	196	27.9	42.5	16	2	324	36.6	814.5	40	16	3,136	811.51
					40.5	10	4	196	36.9	820.5	70	28	9,604	811.53
										816.5	52	20	5,184	811.58
										818.5	60	26	7,396	811.59
										828.5	114	16	16,900	811.66

consistency relationship equation (18), which implies that

$$\begin{aligned}
 E_\sigma \hbar\omega_0 &= \langle \sigma, \omega | \hat{\mathcal{H}}(\omega) | \sigma, \omega \rangle \\
 &= \sum_i \hbar\omega_i \sigma_i = 3(\sigma_1\sigma_2\sigma_3)^{1/3} \hbar\omega_0, \text{ with } \omega_0^3 = \omega_1\omega_2\omega_3,
 \end{aligned}
 \tag{19}$$

for a range of  $N = \sigma_1 + \sigma_2 + \sigma_3$  values.

The mean-field energy  $E_\sigma \hbar\omega_0$  of a lowest-weight state in these tables is equal to  $N\hbar\omega_0$  for a spherical state, for which  $\lambda = \sigma_1 - \sigma_2$  and  $\mu = \sigma_2 - \sigma_3$  are both zero, as seen for the lowest-energy state of  $^{16}\text{O}$ . However, the  $N = 38.5$  state of  $^{16}\text{O}$ , which would be at an excitation energy of  $\approx 4\hbar\omega_0$  if it were spherical, is understood to be the intrinsic state of a strongly deformed  $N(\lambda, \mu) = 38.5(8, 4)$  rotational band at 6.05 MeV [88,89,94]. Similarly, the lowest three states obtained for  $^{12}\text{C}$ , include that of the rotational band of states, based on the highly deformed Hoyle state, with  $N(\lambda, \mu) = 28.5(12, 0)$  and another with  $N(\lambda, \mu) = 26.5(6, 2)$  in accord with observations and the calculations of Dreyfuss *et al.* [95].

A notable prediction of the shape-consistent mean-field ordering of states, by increasing values of  $E_\sigma$ , is clearly very different to that of the spherical harmonic oscillator for the rare-earth nucleus  $^{166}\text{Er}$ ; for this nucleus and many others with the exception of the lowest-energy states of closed and singly closed-shell nuclei, there is clearly a major departure from the spherical shell-model ordering of states. Recall also that  $E_\sigma \hbar\omega_0$  has an interpretation, in the AMN version of the unified model, as the intrinsic energy of a rotational band and that the lowest-energy  $J = 0$  rotational state of a rotational band of states has considerably lower energy than the energy of its deformed intrinsic state.

Thus, the results of the table are a clear indication that the ordering of independent-particle basis states, as given by the spherical shell model, is only relevant for the relatively few spherical states of nuclei. In particular, the spherical shell

model is inappropriate for a many-nucleon theory of deformed nuclei for which a shape-consistent Nilsson model [96,97] expression of the intrinsic state of a rotor model is more relevant.

In concluding this section it is recalled that, whereas a Hartree-Bogolyubov generalization of HF calculations to take account of short-range pairing correlations is known to result in a partial restoration of spherical symmetry, it can be expected that a parallel extension of the AMN unified model to take account of pair correlations could result in reduced deformations and, in particular, the enhancement of axial symmetric relative to triaxial rotational states. This remains to be explored in the context of the AMN symplectic model.

## VII. MEAN-FIELD ALGEBRAIC MANY-NUCLEON UNIFIED MODEL CALCULATIONS

A fundamental property of the symplectic model is that, because its spatial  $\text{Sp}(3, \mathbb{R})$  Lie group and its complementary  $\text{SU}(2)_S$  spin and  $\text{SU}(2)_T$  isospin groups are semisimple, its many-nucleon irreps are uniquely defined by their lowest weights. Thus, its irreps can be explored in mean-field theory one at a time more usefully and much more insightfully than in the single independent-particle model irrep of standard HF theory. In this section, rotational energies of various kinds are determined for an  $S = 0$ ,  $T = T_0$  symplectic-model irrep of  $^{166}\text{Er}$ .

An essential observation, as shown in Sec. V, is that the properties of a symplectic model irrep are given by identifying its minimum lowest-energy, lowest-weight state with the intrinsic state of an AMN version of the Bohr-Mottelson unified model. It was then shown that the required lowest-energy state is obtained in mean-field theory if the lowest-weight state is the ground state of a generally triaxial harmonic oscillator that satisfies the shape-consistency equation (18) and if  $\omega_0$ , defined by Eq. (19), has a value such that the lowest-weight state has

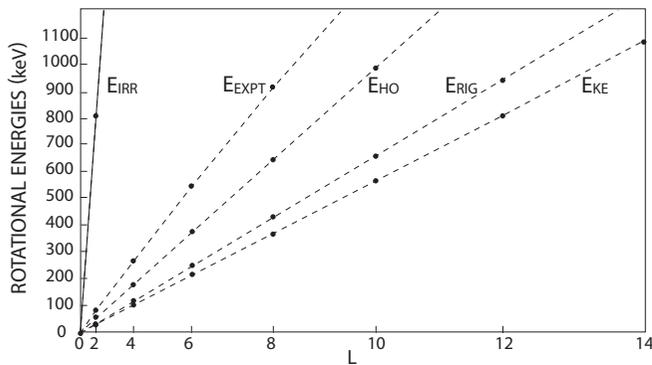


FIG. 1. The figure shows energy levels, labeled by  $E_{\text{EXPT}}$ , of the ground-state rotational band of  $^{166}\text{Er}$  and corresponding energies  $E_{\text{IRR}}$  for irrotational flow and  $E_{\text{RIG}}$  for rigid-body rotations of the shape-consistent (lowest-weight) intrinsic state for the  $\text{Sp}(3, \mathbb{R})$   $S = 0$  irrep  $(327\frac{1}{2}, 249\frac{1}{2}, 249\frac{1}{2})$ . (The half-odd integer weights of the  $\text{Sp}(3, \mathbb{R})$  irrep label are due to the exclusion of the center-of-mass zero-point energy contribution to the energies of states.) The kinetic energies,  $E_{\text{KE}}$ , are those of the states angular momentum projected from the shape-consistent intrinsic state as defined in the text. The energy levels  $E_{\text{HO}}$  are those which, in addition to the kinetic energies, include the harmonic-oscillator potential energies of the angular-momentum-projected states. The results show that, for a nuclear Hamiltonian consisting of a many-nucleon kinetic energy plus a potential energy interaction term adjusted to fit the experimental energies, more than half of each excitation energy would be potential energy, consistent with the results of Refs. [19,20].

the volume for the nucleus under consideration as required of essentially incompressible nuclear matter. The rotational states of the AMN unified model are then obtained, in accord with the Nambu-Goldstone interpretation of a broken symmetry in mean-field theory [77,78], by angular-momentum projection from the lowest-energy lowest-weight state.

As a first study of the dynamics of the AMN unified model obtained in this way, I consider an irrep with an axially symmetric lowest-weight state. This has the distinct advantage that the angular-momentum projected rotational states of the model can then be obtained explicitly by the algebraic methods given in Ref. [98].

Figure 1 shows the excitation energies of a few states of low angular momentum  $L$  of an axially symmetric  $S = 0$ ,  $T = T_0$  symplectic-model rotational band as they would be for different model moments of inertia. The  $\text{Sp}(3, \mathbb{R})$  irrep considered was used previously [20] in a fit to the lower-energy rotational states of  $^{166}\text{Er}$  and the  $E2$  transitions between them with a schematic interaction but without the use of an effective charge. According to the estimates of Jarrío *et al.* [99], the experimentally most-appropriate irreps for this nucleus are weakly triaxial. However, an axially symmetric representation was chosen for a first study of the dynamics of nuclear rotations because its multiplicity-free angular momentum wave functions are uniquely defined, independently of the Hamiltonian, and can be explicitly determined for a given irrep by known algebraic methods [98]. They are also the most useful because other rotor model studies, with which

comparisons can be made, have been for axially symmetric irreps.

The entries in the figure were obtained as follows:

- (i) The experimental energies,  $E_{\text{EXPT}}$ , were obtained from the Brookhaven NuDat 2.7 compilation.
- (ii) The irrotational  $E_{\text{IRR}}$  and rigid-body  $E_{\text{RIG}}$  rotational energies were obtained from the expression for rotational energies about a  $z$  axis given by  $E = \frac{\hbar^2}{2\mathcal{I}}L(L+1)$  with moments of inertia (given in Ref. [1], p. 78)

$$\mathcal{I}_{\text{IRR}} = M \frac{\left( \sum_n (x_n^2 - y_n^2) \right)^2}{\left( \sum_n (x_n^2 + y_n^2) \right)}, \quad \mathcal{I}_{\text{RIG}} = M \left\langle \sum_n (x_n^2 + y_n^2) \right\rangle. \quad (20)$$

- (iii) The energies  $E_{\text{HO}}$  and  $E_{\text{KE}}$  are the expectation values of the spherical harmonic oscillator Hamiltonian and the many-nucleon kinetic energy operator, respectively, in the states angular momentum projected from the intrinsic state of the AMN unified model. The AMN model intrinsic state for the results of Fig. 1 was chosen to be axially symmetric. The kinetic energies of the rotational states could then be calculated, without resorting to numerical approximations, because the kinetic energy observable of nuclear states is an element of the  $\text{Sp}(3, \mathbb{R})$  Lie algebra and because rotational states of good angular momentum can be analytically projected from an axially symmetric intrinsic state, as shown in Ref. [98]. The calculations were repeated for other axially symmetric irreps and determined to be characteristic of any axially symmetric irrep.

Several conclusions emerge from these results. A primary conclusion is that they are inconsistent with the presumption that nuclear rotational energies are kinetic energies as suggested based on the observation that the observed rotational energies can be fitted, phenomenologically as linear combinations of rigid-body and irrotational flow kinetic energies [1,9]. Another is that with a residual interaction or a slightly larger value of  $\lambda > 327.5$ , a close fit to the experimental rotational energies could be obtained with rotational energies given by  $E_{\text{HO}}$ . A desirable characteristic of the results shown is that they were obtained without the use of any particular nuclear Hamiltonian. Thus, they can be expected to hold for any nucleon-nucleon interaction that satisfies the shape-consistency condition. It would nevertheless be useful to ascertain that a reasonable nuclear interaction, could supply the additional potential energy needed to fit the observed rotational energies.

Regardless of the choice of Hamiltonian, it is worth recalling, as mentioned above, that because the nuclear kinetic energy is an element of the symplectic model Lie algebra the expectation values of the nuclear kinetic energies for the states of mixed symplectic model irreps can only be the averages of those of the unmixed irreps.

### VIII. SUMMARY AND CONCLUSIONS

The primary objectives of the investigations pursued in this paper were to define a fully quantal algebraic many-nucleon version of the Bohr-Mottelson unified model and determine the dynamical properties of nuclear rotations; e.g., whether or not nuclear rotational energies are the kinetic energies of linear combinations of rigid-body and irrotational superfluid flows or combinations of rotational and potential energies.

In pursuing these objectives, an optimal algebraic many-nucleon version of the Bohr-Mottelson unified model has been constructed with unitary irreps, given by the symplectic model [15,16,42] with an  $\text{Sp}(3, \mathbb{R}) \times \text{SU}(2)_S \times \text{SU}(2)_T$  dynamical group that spans the Hilbert spaces of nuclei. This model has an important property that there can be no isoscalar  $E0$  or  $E2$  transitions between the states of its inequivalent irreps. Thus, an observation of such transitions between states signifies that the states either belong to common symplectic model irreps or that they are mixtures of symplectic model irreps with one or more irrep in common.

A new development, exploited in deriving the results of Sec. VII, is based on the observation that  $\text{Sp}(3, \mathbb{R})$  is the dynamical group of the positive- and negative-parity states of a many-nucleon, generally triaxial, three-dimensional harmonic oscillator. As a result, every  $S = 0$ ,  $T = T_0$  unitary irreps of the many nucleon symplectic model is characterized by a lowest weight  $\sigma = (\sigma_1, \sigma_2, \sigma_3)$  and harmonic-oscillator frequencies  $\omega = (\omega_1, \omega_2, \omega_3)$ , as defined by Eq. (19) to minimize the expectation value  $\langle \sigma, \omega | \hat{H} | \sigma, \omega \rangle$  of an appropriate nuclear Hamiltonian and satisfy a mean-field shape-consistency condition. The generally triaxial lowest-energy, lowest-weight state for the symplectic model was then shown to have an interpretation as the intrinsic state of an AMN version of the Bohr-Mottelson unified model.

A generally nonspherical many-nucleon harmonic-oscillator ground state has been determined and shown to have a physical interpretation as the intrinsic state of a many-nucleon unified model, in which the low-energy rotational states are generated by its rotations and its intrinsic shape vibrational states are generated by its symplectic model raising operators. Thus, a proposed new method for determining the spectrum of a symplectic model is to start by identifying its minimum energy lowest-weight state as a mean-field state of a generally triaxial lowest-energy lowest-weight state. Then, in accord with the Nambu-Goldstone interpretation [77,78] of the generally broken rotational symmetry of this minimum energy state, rotational states are determined that span the vector space of states generated by its rotations. The intrinsic vibrational states of the AMN unified model can also be determined in time-dependent mean-field theory or, equivalently, in the random phase approximation [68,69].

The above approach enables a nuclear shell model to be constructed, which, unlike the standard spherical shell model, provides an appropriate framework for describing the states of deformed nuclei. In particular, it provides an order-of-magnitude simpler approach to that of previous symplectic-model calculations [42], in which basis states were expressed in the space of spin 1/2 neutrons and protons occupying

subspaces of states of a three-dimensional spherical harmonic oscillator. Most significantly, the basis states of the new approach have an interpretation as algebraic many-nucleon states of the Bohr-Mottelson unified model, which enables simple comparisons of phenomenological and many-nucleon unified model interpretations of nuclear data.

In reflecting on what has been achieved, it is instructive to contrast the current expression of a symplectic model irrep with its expression in terms of the spherical shell model. The standard lowest-weight state of an  $\text{Sp}(3, \mathbb{R})$  irrep is traditionally taken to be the  $\text{U}(3)$  highest-weight state among a degenerate set of lowest spherical harmonic-oscillator energy, where  $\text{U}(3) \subset \text{Sp}(3, \mathbb{R})$  is the symmetry group of the three-dimensional spherical harmonic oscillator. This practice has its origins in the recognition that  $\text{U}(3)$  is the maximal compact subgroup of  $\text{Sp}(3, \mathbb{R})$  and, because of the introduction of a  $\text{U}(3) \supset \text{SU}(3) \supset \text{SO}(3)$  coupling scheme for the spherical shell model [44], its properties have been well studied. The downside of this practice is that an expansion of rotor model states in terms of a sequence of  $\text{SU}(3) \subset \text{U}(3)$ -coupled basis states is slowly convergent and, hence, not so efficient for understanding the dynamics of nuclear rotations. In contrast, the single lowest-weight state of a generally triaxial harmonic oscillator irrep is uniquely defined for that irrep and has a physical interpretation as the intrinsic state of the unified model. Another advantage is that the  $\beta$ - and  $\gamma$ -vibrational states of the emergent unified model are obtained by standard Tamm-Dancoff and RPA excitations of this same lowest-weight state [68,69]. A third advantage is that a realistic Hamiltonian for a nucleus can be diagonalized in a space of many symplectic model irreps, with many different lowest weights, in an independent-particle basis. This enables the binary structure of computers to be exploited, as recognized by Whitehead [100,101] and now used, with considerable success, in huge NCSM (no-core shell-model) calculations [102,103] and, in symmetry adapted NCSM calculations in mixed  $\text{SU}(3)$  model bases [86,104]. A useful and particularly remarkable result is the emergence of states with unexpectedly little mixing of states belonging to different  $\text{Sp}(3, \mathbb{R}) \times \text{SU}(2)_S \times \text{SU}(2)_T$  irreps [87].

In conclusion, it is admitted that only the maximally deformed subset of spin  $S = 0$  and minimum isospin  $T = T_0 = \frac{1}{2}(N - Z)$  irreps have been considered in this paper. Hopefully, an extension to states of nonzero spin and nonminimal isospin  $T > \frac{1}{2}(N - Z)$  will be straightforward. It is also possible that there is a common coherent coupling of many symplectic model irreps, such as a mixing of pair-coupled states, as in the shell-model seniority coupling scheme and HF Bogolyubov theory, which could go some way to restoring the spherical symmetries of symplectic model states. In particular, it might be that a restriction to unmixed symplectic model irreps could result in partially restoring the axial symmetry and even the spherical symmetry of some otherwise strongly deformed triaxial nuclei. A promising procedure is to extend the program to study the many-nucleon states of deformed nuclei in spaces of multiple symplectic model irreps within the framework of the symmetry-adapted no-core shell model [87] with, for example, a mixture of quadrupole plus pairing interactions.

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