Sp(3,R) mean field theory for heavy deformed nuclei

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Algebraic mean field theory (AMFT) for the symplectic sp(3,R) algebra is used to derive collective rotational bands in the Riemann ellipsoidal approximation. AMFT is formulated in terms of symplectic density matrices that are defined by the quantum mechanical expectations of the sp(3,R) operators. The mean field approximation restricts the densities to a coadjoint orbit of the canonical transformation group Sp(3,R). For principal axis rotation, a system of three algebraic equations is derived from energy minimization on an orbit surface. The system is solved self-consistently for the axis lengths and the potential tensor.

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I. INTRODUCTION

This paper presents a new many-body quantum theory of the Riemann model of rotating ellipsoids. The Riemann model is a classical theory of self-gravitating systems that have an ellipsoidal boundary and a linear velocity field [1,2]. This model allows for rotational dynamics on a continuum from rigid rotation to irrotational fluid flow. The quantized Riemann theory can model successfully geometrical collective rotation in atomic nuclei.

The dynamical symmetry algebra of the Riemann ellipsoidal model is the general collective motion algebra gcm(3) [3], which is a noncompact subalgebra of the real symplectic algebra sp(3,R) [4–14]. The only Casimir of gcm(3) [15] is the length C of the Kelvin circulation vector [16]. The Kelvin circulation is a conserved quantity for classical fluid flow [17]. In its modern differential geometric formulation, the classical theory of Riemann ellipsoids is a gauge theory in which the nonholonomic constraints to irrotational flow or a "falling cat" are particular connections on a principal GL(3,R) bundle and the Kelvin circulation is a conserved gauge invariant [18].

An irreducible unitary representation (irrep) of gcm(3) defines a quantum Riemann ellipsoidal model. These irreps are indexed by the Kelvin circulation which is quantized to nonnegative integral multiples of \hbar [19–23]. The original Bohr-Mottelson liquid drop model is indistinguishable from the gcm(3) irrep with vanishing circulation, which corresponds to irrotational flow. The irrotational flow model describes the giant quadrupole resonance [24]. In the domain of rapidly rotating triaxial nuclei, the Kelvin circulation is approximately constant and equals the critical angular momentum at which the nucleus bifurcates to a Jacobi triaxial shape from a spheroidal one [25]. But the low-energy states of the yrast band of a deformed rotating nucleus do not share a common value for the circulation [26]. Typically the rigidity parameter [3], which is approximately proportional to the ratio of the Kelvin circulation to the angular momentum, is almost constant for the yrast band, and, therefore, gcm(3) dynamical symmetry is strongly broken in the low-energy domain. The rigidity parameter r varies continuously from r=0 (irrotational flow) to r = 1 (rigid rotation) [3]. Among the rare earth even-even nuclei, the rigidity is approximately a quadratic function of the ground state quadrupole deformation, a fact which implies a simple formula for the energy of their 2^+ states as a function of the deformation [27]. An explanation for the γ -ray staggering in the deexcitation of some superdeformed bands in the ¹⁵⁶Gd region with a period of $4\hbar$ is achieved when the ratio of the Kelvin circulation *C* to the angular momentum *I* is about one-half [28,29].

The nuclear Kelvin circulation and rigidity can be determined experimentally from inelastic electron scattering measurements of the transverse *E*2 form factor [30–36]. This form factor for a Riemann rotor is a weighted interpolation of the rigid rotor and irrotational flow form factors [37]. There is to date no published measurement of transverse form factors in the heavy deformed region. But projected Hartree-Fock calculations of the transverse *E*2 form factor of ¹⁵⁶Gd [38] imply a rigidity $r \approx 0.12$.

There are three established ways to derive a microscopic quantum theory of the Riemann model. By making a change of variables from Cartesian coordinates to collective and intrinsic coordinates, the space of antisymmetrized manynucleon wave functions may be decomposed into gcm(3) irreps [39]. This method determines the necessary and sufficient theoretical conditions for good gcm(3) symmetry, derives rigorously the quantum collective kinetic energy corresponding to the classical Riemann model from the manyparticle Laplacian [40], and creates a relationship with hyperspherical harmonics theory [41]. The disadvantages of this realization of the classical Riemann model are that exact gcm(3) symmetry is required and that a GL(3,R) intrinsic wave function is tedious to calculate for practical applications.

The second method to derive the Riemann model uses the known decomposition of shell model space into holomorphic discrete series irreps of sp(3,R) as an intermediate step [5,8]. Each irrep of the symplectic algebra that arises in the shell model decomposition must be reduced subsequently into irreps of gcm(3). The gcm(3) reduction of discrete series irreps of sp(3,R) is governed by a reciprocity theorem [42]: each symplectic irrep is associated with an irrep of the Elliott su(3) algebra; the spectrum of the Kelvin circulation, including multiplicity, in a given symplectic shell model irrep equals the angular momentum reduction of the associated su(3) irrep. Although this theorem determines the gcm(3)

irreps that occur in a sp(3,R) irrep, the vectors that span a gcm(3) irrep are not constructed explicitly. Because the Kelvin circulation is a complicated five-body operator [15], its matrix elements in a symplectic irrep space have not been evaluated to date. As a consequence, an explicit gcm(3) reduction of a sp(3,R) discrete series irrep has not been attained. Nevertheless, the $sp(3,R) \downarrow gcm(3)$ reduction theorem does determine the strong limitations imposed by the shell model on the possible values of the Kelvin circulation in yrast rotational bands.

The Kelvin circulation operator simplifies when it is evaluated in the rotating principal axis frame. The third tractable microscopic realization of the Riemann theory is achieved by cranking the Hamiltonian in the rotating frame simultaneously with the angular and vortex velocities [43– 45]. The angular momentum is conjugate to the angular velocity, and the Kelvin circulation is conjugate to the vortex velocity. When the anisotropic harmonic oscillator models the nuclear Hamiltonian in the rotating frame and the axis lengths and oscillator frequencies are chosen selfconsistently, the "Inglis" cranking energy in perturbation theory for small angular and vortex velocities equals the classical Riemann ellipsoidal kinetic energy [43]. An improved microscopic realization is attained when the anisotropic harmonic oscillator is replaced by a self-consistent Hartree-Fock mean field that corresponds to a realistic interaction [45,46].

The physical effects of cranking the anisotropic oscillator with the vortex velocity are similar to the effects of adding the monopole pairing interaction to the deformed oscillator Hamiltonian. As the strength of the monopole pairing interaction increases, the expectation of the Kelvin circulation operator in the BCS approximation diminishes until finally, at a critical pairing strength, the circulation vanishes and the system becomes an irrotational superfluid [47].

The "cranking" realization of the Riemann model assumes a determinantal wave function. Although this ansatz produces a tractable theory, the simplicity is attained by severely restricting the admissible model states. For applications to geometrical collective states, the determinantal ansatz is troubling because a collective mode must be a coherent superposition of many single-particle excitations.

This paper's realization of the Riemann model is a submodel of the symplectic theory that is neither intractable nor restricted to determinantal wave functions. The relevant mathematics is the theory of coadjoint orbits of Lie groups. A coadjoint orbit is a manifold contained in the space of densities of the Lie algebra. A density corresponding to a wave function is defined by the expectations of the Lie algebra's operators. An orbit surface that contains the density of a highest weight vector of a semisimple Lie algebra is called an integral coadjoint orbit.

Geometric quantization is a mathematical technique for the construction of irreducible representations of Lie groups [48–51]. The starting point for this construction is a Lie group's coadjoint orbits. According to Kirillov [52], for every Lie representation theory concept, a corresponding (and ultimately equivalent) idea exists for integral coadjoint orbits. All information about an irreducible representation of a Lie group is encoded in the symplectic geometry of a coadjoint orbit. This Kirillov metatheorem of coadjoint orbit theory means that the physical properties of a quantum system governed by a Lie dynamical symmetry can be calculated in two ways. The direct way is by explicit construction of the irreducible representations of the dynamical symmetry group; the indirect method is via a geometrical analysis of the Lie group's coadjoint orbits. Prior applications to the Elliott su(3) [53–55] and symplectic sp(3,R) [27,56] models demonstrate a close relationship between irrep and coadjoint orbit results.

Hartree-Fock mean field theory is a special case of coadjoint orbit theory [57-59]. The relevant Lie group is the group U(n) of all unitary transformations of an *n*-dimensional single-particle space, the Lie algebra u(n) is the set of all one-body operators, and the coadjoint orbit is the manifold of all idempotent density matrices. The Hartree-Fock-Bogoliubov mean field theory corresponds similarly to the Lie group O(2n) [60]. When applied to many-body physics, coadjoint orbit theory is naturally called algebraic mean field theory (AMFT).

The fundamental ansatz of AMFT is that the densities of model states lie on one coadjoint orbit of the Lie group. This ansatz is the mean field expression of dynamical symmetry. The parallel ansatz in representation theory is that the model states are vectors in one unitary irreducible representation of the Lie group. Although the only nontrivial unitary representations of a noncompact Lie algebra such as sp(3,R) are infinite dimensional, the mean field approximation limits the theoretical investigation to a finite-dimensional manifold. In fact, sp(3,R) mean field theory requires only matrix computations with 6×6 real matrices.

The ideal AMFT coadjoint orbit for nuclear applications contains the density of the exact ground state. Due primarily to spin-orbit and pairing forces, the exact ground state of a heavy deformed nucleus is a sum of vectors from several irreducible sp(3,R) representations, and it is not a single Slater determinant. As a practical matter the ideal orbit cannot be identified precisely. In the case of heavy deformed isotopes, we argue in Sec. IV that the various coadjoint orbits corresponding to the different symplectic irreps that mix to form the ground state have very similar properties. The predictions of sp(3,R) mean field theory are consequently rather insensitive to the exact choice of the orbit in the heavy deformed region. A physically reasonable choice for the coadjoint orbit is estimated in this paper from the deformed harmonic oscillator Hamiltonian [61–63].

The Hohenberg-Kohn theorem of density functional theory [64] was generalized to prove that there exists an energy functional of the density (relative to a given Lie algebra) whose absolute minimum is the algebraic density of the exact ground state [65]. At least in principle, AMFT is an exact theory, just like the density functional theory. The existence theorems of the density functional theory and the AMFT do not construct the exact energy functional.

This paper presents the basic definitions and notations in the following section. In Sec. III, the energy functional is assumed to be the sum of the harmonic oscillator and a collective quadrupole potential energy. We derive the equations for the critical points on a coadjoint orbit of this energy functional when the rotation axis is aligned with a principal axis. The solutions to the equations yield the density of a Riemann rotor with good angular momentum and Kelvin circulation. In Sec. IV the theory is applied to the heavy deformed isotope ¹⁶⁶Er.

II. Sp(3,R) COADJOINT ORBITS

This section defines the symplectic sp(3,R) Lie algebra, its dual space of densities, the coadjoint action of the symplectic group on the dual space, the sp(3,R) Casimirs, and determines the coadjoint orbits. The definitions and notation follow that of Ref. [27].

Let $(x_{\alpha j}, p_{\alpha j})$ denote the dimensionless Cartesian components of the position and momentum vectors of particle α in a finite system of particles. They obey the canonical commutation relation $[x_{\alpha j}, p_{\beta k}] = i \delta_{\alpha \beta} \delta_{jk}$. The symplectic generators are the Hermitian one-body operators,

$$\hat{Q}_{jk} = \sum_{\alpha} x_{\alpha j} x_{\alpha k}, \quad \hat{T}_{jk} = \sum_{\alpha} p_{\alpha j} p_{\alpha k},$$
$$\hat{N}_{jk} = \sum_{\alpha} \left(x_{\alpha j} p_{\alpha k} - \frac{1}{2} i \,\delta_{jk} \right). \tag{2.1}$$

The observables \hat{Q}_{jk} and \hat{T}_{jk} are the monopole-quadrupole tensors in position and momentum space, respectively. The nine components \hat{N}_{jk} generate the Lie algebra gl(3,*R*) of the general linear group. The antisymmetric parts of *N*, $\hat{L}_i = \varepsilon_{ijk}\hat{N}_{jk}$ are the vector orbital angular momentum components. The gcm(3) algebra is spanned by the operators \hat{Q}_{jk} and \hat{N}_{ik} .

The 21-dimensional sp(3,R) matrix algebra consists of all 6×6 real matrices,

$$S = \begin{pmatrix} X & -U \\ V & -X^T \end{pmatrix}, \tag{2.2}$$

where X, U, V are 3×3 real matrices and U, V are symmetric. The operator representation σ of the algebra of matrices is defined by

$$\sigma(S) = i \sum_{jk} \left(X_{jk} \hat{N}_{jk} + \frac{1}{2} U_{jk} \hat{Q}_{jk} + \frac{1}{2} V_{jk} \hat{T}_{jk} \right).$$
(2.3)

When *S* is a matrix in the symplectic Lie algebra, the operator $\sigma(S)$ is a skew-adjoint one-body operator. The set of operators is an sp(3,R) representation, $[\sigma(S_1), \sigma(S_2)] = \sigma([S_1, S_2])$.

The symplectic density matrix ρ corresponding to a normalized wave function Ψ is

$$\rho = \begin{pmatrix} n^T & t \\ -q & -n \end{pmatrix},$$
(2.4)

where the 3×3 real dimensionless matrices n,q,t are the expectations of the algebra generators: $q_{jk} = \langle \Psi | \hat{Q}_{jk} | \Psi \rangle$,

 $t_{jk} = \langle \Psi | \hat{T}_{jk} | \Psi \rangle$, and $n_{jk} = \langle \Psi | \hat{N}_{jk} | \Psi \rangle$. The quantum mechanical expectation of a symplectic Lie algebra representation $\sigma(S)$ is

$$\langle \rho, S \rangle \equiv \frac{1}{2} \operatorname{tr}(\rho S) = -i \langle \Psi | \sigma(S) | \Psi \rangle.$$
 (2.5)

For a physical density, i.e., one that is defined by the expectations of sp(3,R) Hermitian operators with respect to some quantum mechanical state, the matrix ρ of Eq. (2.4) has restrictions on it. For example, the matrices q and t are real, symmetric, and positive definite, and the expectation $\frac{1}{2}tr(t + q)$ of the oscillator number operator is bounded from below by a half integer or an integer that depends on the number of neutrons and protons.

When the symplectic group $\operatorname{Sp}(3,R)$ acts on an arbitrary many-body wave function Ψ , the unitarily transformed vector $\Psi \mapsto \exp[\sigma(S)]\Psi$ is difficult to compute explicitly. However, the corresponding symplectic density transforms simply according to the coadjoint action, $\rho \mapsto \operatorname{Ad}_g^* \rho = g\rho g^{-1}$. The coadjoint orbit \mathcal{O}_ρ is a smooth surface consisting of the density ρ and all transformed densities $\operatorname{Ad}_g^* \rho$ as g ranges over the entire symplectic group $\operatorname{Sp}(3,R)$.

The symplectic Casimirs $C_{2s}[\rho]$ are real-valued functions of the density,

$$C_{2s}[\rho] = \frac{(-1)^s}{2} \operatorname{tr}(\rho^{2s}), \quad s = 1, 2, 3.$$
 (2.6)

The Casimirs are constant on each coadjoint orbit, $C_{2s}[\rho] = C_{2s}[Ad_g^*\rho]$ for $g \in Sp(3,R)$. The trace of an odd power of the density is identically zero. Only the quadratic, quartic, and sextet Casimirs can be functionally independent.

The geometrical model provides a physical interpretation for the quadratic sp(3,*R*) Casimir. In terms of the density components, this Casimir is $C_2 = \text{tr}(tq - n^2)$. For a linear velocity field, as the Riemann model postulates, the kinetic tensor simplifies to $t_{\text{coll}} = n^T q^{-1}n$, cf. Eq. (48) of Ref. [3]. The squared length of the Kelvin circulation vector is C^2 $= \text{tr}(n^T q^{-1}nq - n^2)$ [16]. Therefore the quadratic sp(3,*R*) Casimir is

$$C_2 = C^2 + tr[(t - t_{coll})q].$$
 (2.7)

When a system is rotating purely collectively and the intrinsic kinetic tensor $t_{intr} = t - t_{coll}$ vanishes, the quadratic sp(3,*R*) Casimir simplifies to the squared length of the Kelvin circulation. More typically in a rotational band, the circulation increases as the angular momentum increases, and the intrinsic kinetic energy must correspondingly decrease to maintain a constant value for the quadratic symplectic Casimir.

Almost every symplectic coadjoint orbit contains a matrix in the normal form,

$$\varrho = \begin{pmatrix} 0 & t \\ -q & 0 \end{pmatrix}, \quad t = q = \operatorname{diag}(N_1, N_2, N_3). \quad (2.8)$$

By "almost every," we mean that, with the exception of a set of measure zero, all symplectic densities can be transformed by a symplectic group transformation to the normal form (2.8) [66]. The situation is entirely equivalent to the fact that almost every random phase approximation matrix can be diagonalized. Two such normal form densities lie on two different coadjoint orbits unless the N_k for one density are merely a permutation of the other density's N_k . The normal forms label distinct orbits when an ordering is adopted, say $N_3 \ge N_2 \ge N_1$.

The symplectic density of a sp(3,R) shell model highest weight vector is in normal form. Moreover, for a highest weight density, $\lambda = N_3 - N_2$ and $\mu = N_2 - N_1$ are nonnegative integers defining the su(3) irrep, and $N_0 = N_1 + N_2$ $+N_3$ is an integer or half integer that equals the total number of oscillator quanta. Yet not every density in the normal form is defined by a sp(3,R) highest weight vector. For a normal form density, the expectations of the oscillator number operators in the 1,2, and 3 directions equal N_1, N_2 , and N_3 , respectively, but these are not necessarily half integers. Although the expectations of the angular momentum, Kelvin circulation, and other sp(3,R) operators are required to vanish for a normal form density, the corresponding quantum state vector is not required to be an eigenstate of the oscillator number operators, angular momentum, circulation, etc. Thus, the density theory we describe here is not limited to one symplectic irreducible representation, and the quantum state corresponding to a normal form density may be a superposition of vectors from many symplectic irreps. This flexibility is important because pairing and spin-orbit forces break exact sp(3,R) dynamical symmetry in the shell model space of a real nucleus.

For the orbit \mathcal{O}_{ϱ} , labeled by (N_1, N_2, N_3) , the values of the symplectic Casimirs are the constants,

$$\mathcal{C}_{2s}[\varrho] = \sum_{k} N_k^{2s}.$$
(2.9)

In general, an algebraic variety is defined as the set of points in the real \mathbb{R}^n satisfying a system of polynomial equations, $f_i(x_1, x_2, \ldots, x_n) = 0$ for $i = 1, 2, \ldots$ [67]. Because each symplectic Casimir is a polynomial function of the components q_{jk}, t_{jk}, n_{jk} of the density ρ , the orbit \mathcal{O}_{ϱ} is contained in the algebraic variety consisting of all densities ρ , Eq. (2.4), which satisfy the three algebraic equations (2.9). In the typical case of distinct N_k , the three Casimirs are functionally independent, and the algebraic variety is 18 dimensional. The algebraic variety associated with the Casimirs has the same dimension as a coadjoint orbit, but, in general, the coadjoint orbit is contained properly as a smooth connected component of the variety, cf. the Appendix of Ref. [27].

The subgroups of the symplectic group are transformation groups on each coadjoint orbit. The orthogonal subgroup SO(3) rotates the matrices of the symplectic density, Eq. (2.4), as follows: for $R \in SO(3)$, $n \mapsto RnR^T$, $t \mapsto RtR^T$, and $q \mapsto RqR^T$. Each orbit of the rotation subgroup contains a diagonal monopole-quadrupole tensor $q = \text{diag}(a_1^2, a_2^2, a_3^2)$, where $a_k > 0$, k = 1,2,3. In the classical rotor model the a_k are interpreted as the axis lengths of the abstract inertia ellipsoid. When the system is a real classical fluid with an ellipsoidal boundary and uniform mass distribution, the a_k are proportional to this ellipsoid's axis lengths.

When q is diagonal, the symplectic density represents the system in the rotating principal axis frame, and it is denoted by $\tilde{\rho}$. In the rotating principal axis frame, the angular momentum \vec{I} and Kelvin circulation \vec{C} vectors are inferred from the off-diagonal entries of n: for i, j, k cyclic, $I_i = n_{ik} - n_{ki}$ and $C_i = (a_k/a_j)n_{jk} - (a_j/a_k)n_{kj}$. We call this vector quantity \tilde{C} the "Kelvin circulation" of a symplectic density because its definition coincides with the expression for the Kelvin circulation vector of a classical Riemann ellipsoid, cf. Eq. (39) of Ref. [3]. The definition has useful properties. The squared length C^2 of the Kelvin circulation of a symplectic density is invariant with respect to the GCM(3) transformation subgroup of the symplectic group, and, therefore, it is a gcm(3) Casimir function. The range of C^2 on an integral coadjoint orbit of Sp(3,R) was proven recently to match the range of the expectation of the corresponding quantum gcm(3) Casimir in the orbit's associated irreducible unitary representation [27,42]. In prior work on the quantum geometrical model before its relationship with the Riemann model was understood fully, the Kelvin circulation was called the vortex momentum [39].

III. EQUILIBRIUM STATES

This section derives Eqs. (3.13) for the critical points of the energy functional on the algebraic variety defined by the symplectic Casimirs in the space of symplectic densities when the rotation axis is aligned with a principal axis and there is no vibration of the axis lengths. These equations must be solved self-consistently for the axis lengths and the potential tensor. We show that the total kinetic energy is a sum of the Riemann collective kinetic energy and an intrinsic kinetic energy for which a concrete formula is attained (3.11). When $\mu = 0$, the I=0 ground state is a prolate spheroid, and we derive a simple condition (3.15) relating its deformation to the strength of the collective potential energy. For heavy deformed nuclei, when the angular momentum is much less than λ and N_0 , the equations for a critical point simplify in perturbation theory.

The symplectic energy $E[\rho]$ is a rotational scalar functional of the density. A simple sp(3,*R*) energy functional that has been used in prior symplectic representation theory applications [7] is the sum of the harmonic oscillator and a quadrupole collective potential energy, $E[\rho]=E_0[\rho]$ + $V[\rho]$. The isotropic harmonic oscillator energy is

$$E_0[\rho] = \frac{1}{2} \text{tr}(t+q)$$
(3.1)

in units of $\hbar \omega_0$. A quadrupole potential energy functional depends on the quadratic and cubic rotational scalars,

$$v_2 = \frac{1}{2} \operatorname{tr}(q^{(2)})^2,$$

 $v_3 = \frac{1}{3} \operatorname{tr}(q^{(2)})^3 = \det q^{(2)},$ (3.2)

where $q_{ij}^{(2)} = q_{ij} - 1/3 \,\delta_{ij} \operatorname{tr} q$. Because v_2 and v_3 are rotational scalars, these potential terms may be evaluated in the principal axis frame in which $q = \operatorname{diag}(q_1, q_2, q_3)$ is the diagonal,

$$v_{2} = (q_{1}^{2} + q_{2}^{2} + q_{3}^{2} - q_{2}q_{3} - q_{1}q_{3} - q_{1}q_{2})/3,$$

$$v_{3} = (2q_{1} - q_{2} - q_{3})(2q_{2} - q_{1} - q_{3})(2q_{3} - q_{1} - q_{2})/27.$$
(3.3)

These scalars may be expressed in terms of the quadrupole deformation parameters β and γ ,

$$v_2 = \frac{3}{4} f^2 \beta^2,$$

 $v_3 = \frac{1}{4} f^3 \beta^3 \cos 3\gamma,$ (3.4)

where $f = (1/\sqrt{5\pi})A(R_0/b)^2$, with *A* equal to the mass number, $R_0 = 1.2A^{1/3}$ fm is the nuclear radius, and $b = \sqrt{\hbar/m\omega_0}$ is the oscillator length. An elementary collective potential (in units of $\hbar \omega_0$) is

$$V[\rho] = b_2 v_2 + b_3 v_3 + b_4 v_2^2, \qquad (3.5)$$

where b_2 , b_3 , and b_4 are dimensionless real constants.

Consider the special case of rotation about a principal axis, say the 1-axis. The nonzero components of the angular momentum and the Kelvin circulation are $I_1 = I$ and $C_1 = C$. For rotors in equilibrium, the axis lengths are not vibrating, and therefore, the diagonal components of *n* vanish. The kinetic tensor *t* in the principal axis frame is diagonal for an ellipsoidal body. Thus, the model sp(3,R) energy $E[\tilde{\rho}]$ simplifies to a function of the axis lengths of the inertia ellipsoid, the diagonal components of the kinetic tensor, the angular momentum, and the Kelvin circulation.

As measured in the rotating frame, the energy is the difference between the laboratory frame energy and the collective kinetic energy of a Riemann ellipsoid with angular momentum I and Kelvin circulation C,

$$T_{\text{coll}}[\tilde{\rho}] = \frac{1}{2} \text{tr}(n^{T}q^{-1}n) = \frac{1}{4} \left[\frac{(I+C)^{2}}{(a_{2}+a_{3})^{2}} + \frac{(I-C)^{2}}{(a_{2}-a_{3})^{2}} \right],$$
(3.6)

in units of $\hbar \omega_0$. Riemann rotor solutions with angular momentum *I* and Kelvin circulation *C* are critical points of the rotating frame energy,

$$\mathcal{E}_{IC}[\tilde{\rho}] = E[\tilde{\rho}] - T_{\text{coll}}[\tilde{\rho}] - \sum_{k=1,2,3} m_{2k} \mathcal{C}_{2k}[\tilde{\rho}], \quad (3.7)$$

on the space of all principal axis frame symplectic densities $\tilde{\rho}$ with fixed *I* and *C*, where m_{2k} are Lagrange multipliers enforcing the constraint to the algebraic variety associated with the sp(3,*R*) Casimirs. An equilibrium density satisfies the six energy minimization conditions

$$\frac{\partial \mathcal{E}_{IC}}{\partial a_i} = \frac{\partial \mathcal{E}_{IC}}{\partial t_{ii}} = 0, \qquad (3.8)$$

and the three polynomial equations $C_{2s}[\tilde{\rho}] = \sum N_i^{2s}$.

Energy minimization determines analytically the Lagrange multipliers, which can be eliminated, and the kinetic tensor in the rotating frame

$$t_{11} = a_1^2 - W_{11},$$

$$t_{22} = a_2^2 - W_{22} + \frac{(a_2 C - a_3 I)^2}{(a_3^2 - a_2^2)^2},$$

$$t_{33} = a_3^2 - W_{33} + \frac{(a_3 C - a_2 I)^2}{(a_3^2 - a_2^2)^2},$$
(3.9)

in terms of the potential tensor W in the principal axis frame

$$W_{ii} = -a_i \frac{\partial V}{\partial a_i} = -2 q_i \frac{\partial V}{\partial q_i}.$$
 (3.10)

For a self-gravitating system, W is called the Chandrasekhar potential tensor [2]. Thus, the sp(3,R) kinetic energy T of an equilibrium density is the sum of collective and intrinsic energies,

$$T = \frac{1}{2} \operatorname{tr} t = T_{\text{coll}} + T_{\text{intr}},$$

$$T_{\text{intr}} = \frac{1}{2} \sum_{k} (a_{k}^{2} - W_{kk}).$$
 (3.11)

The axis lengths are determined by solving the three Casimir equations. In terms of the forces

$$z_i = \frac{W_{ii}}{q_i} = -2\frac{\partial V}{\partial q_i},\tag{3.12}$$

the Casimir equations simplify to

$$3\sqrt{1-z_1}q_1 = N_0 - \lambda - 2\mu,$$

$$3\sqrt{1-z_2}q_2 = (P - \sqrt{Q})^{1/2},$$

$$3\sqrt{1-z_3}q_3 = (P + \sqrt{Q})^{1/2},$$
(3.13)

where $P = N_0^2 + N_0 (\lambda + 2 \mu) + 5\lambda^2/2 + \lambda \mu + \mu^2 - 9C^2/2$ and $Q = 9 (\lambda^2 - C^2)[(2N_0 + \lambda + 2\mu)^2 - 9C^2]/4$. Note that $\sqrt{P^2 - Q} = (N_0 - \lambda + \mu) (N_0 + 2\lambda + \mu)$. In addition to system (3.13) for rotation about the short axis, there are similar equation systems corresponding to rotation about the long and middle axes.

Disregarding exceptional circumstances, Eqs. (3.13) cannot be solved analytically for the deformations q_i because the force quantities z_i depend on (q_1, q_2, q_3) in a complicated way. This system of equations must be solved self-consistently for the deformations and forces. All other conditions have been satisfied for energy minimization on the algebraic variety defined by the sp(3,R) Casimirs and the final step is to solve system (3.13) numerically.

When there is no collective potential energy V, the force quantities vanish, $z_i=0$, and the total energy is just the harmonic oscillator energy, $E[\rho]=E_0[\rho]$. In this special case, system (3.13) is easily solved. When the circulation vanishes, the deformations reduce to their su(3) single oscillator-shell values for the ground state.

A. Ground state

For a nonrotating ground state, the angular momentum and Kelvin circulation are zero. Equations (3.13) relate the axis lengths to the potential energy,

$$3\sqrt{1-z_{1}q_{1}} = N_{0} - \lambda - 2\mu,$$

$$3\sqrt{1-z_{2}}q_{2} = N_{0} - \lambda + \mu,$$

$$3\sqrt{1-z_{3}}q_{3} = N_{0} + 2\lambda + \mu.$$
 (3.14)

A pure quadrupole potential energy has the invariance property $V(q_1 + \epsilon, q_2 + \epsilon, q_3 + \epsilon) = V(q_1, q_2, q_3,)$ for all real ϵ , which implies the identity $z_1 + z_2 + z_3 = 0$. When $\mu = 0$ the ground state is a prolate spheroid, $q_1 = q_2 < q_3$, $z_1 = z_2 < 0$ $< z_3 = -2z_1$, and Eqs. (3.14) specialize to

$$3\sqrt{1-z_1}q_1 = N_0 - \lambda,$$

 $3\sqrt{1+2z_1}q_3 = N_0 + 2\lambda$ (3.15)

for $-\frac{1}{2} < z_1 \le 0$. Thus the ground state deformation of a prolate spheroid depends parametrically on one force parameter z_1 . The su(3) limit of the sp(3,*R*) theory is attained when $z_1=0$. Since the quadrupole deformation of a well-deformed prolate ground state is considerably greater than the theoretical su(3) prediction, the value of z_1 is certainly negative for such states.

B. Low-energy states

When N_0 and λ are large compared to the circulation *C*, accurate solutions to the equilibrium equations are obtained in perturbation theory. The right hand sides of Eqs. (3.13) are given for small *C* by the Maclaurin series,

$$(P - \sqrt{Q})^{1/2} = (N_0 - \lambda + \mu) [1 + MC^2 + \cdots],$$

$$(P + \sqrt{Q})^{1/2} = (N_0 + 2\lambda + \mu) [1 - MC^2 + \cdots], \quad (3.16)$$

where $M=3/[2\lambda(2N_0+\lambda+2\mu)]$. Let q_k denote the ground state deformation, and $q_k(\epsilon)=q_k+\epsilon_k$ be the deformation when C>0. For small ϵ_k , a first-order Maclaurin series yields the force terms

$$z_{1}(\boldsymbol{\epsilon}) = z_{1} - R\boldsymbol{\epsilon}_{1} - S\boldsymbol{\epsilon}_{2} + T\boldsymbol{\epsilon}_{3},$$

$$z_{2}(\boldsymbol{\epsilon}) = z_{2} - S\boldsymbol{\epsilon}_{1} - R\boldsymbol{\epsilon}_{2} + T\boldsymbol{\epsilon}_{3},$$

$$z_{3}(\boldsymbol{\epsilon}) = z_{3} + T(\boldsymbol{\epsilon}_{1} + \boldsymbol{\epsilon}_{2} - 2\boldsymbol{\epsilon}_{3}),$$
(3.17)

where $u = q_3 - q_1$ and

$$R = \frac{4}{9} (3 b_4 u^2 - b_3 u + 3 b_2),$$

$$S = \frac{2}{9} (4 b_3 u - 3 b_2),$$

$$T = R + S.$$
(3.18)

Thus, equilibrium equations (3.13) for small circulation simplify to

$$\frac{R\epsilon_{1}+S\epsilon_{2}-T\epsilon_{3}}{2(N_{0}-\lambda-2\mu)^{2}} + \frac{\epsilon_{1}}{9q_{1}^{3}} = 0,$$

$$\frac{S\epsilon_{1}+R\epsilon_{2}-T\epsilon_{3}}{2(N_{0}-\lambda+\mu)^{2}} + \frac{\epsilon_{2}}{9q_{2}^{3}} = \frac{MC^{2}}{9q_{2}^{2}},$$

$$\frac{-T(\epsilon_{1}+\epsilon_{2}-2\epsilon_{3})}{2(N_{0}+2\lambda+\mu)^{2}} + \frac{\epsilon_{3}}{9q_{3}^{3}} = -\frac{MC^{2}}{9q_{3}^{2}}.$$
(3.19)

These linear equations may be solved for the shifts ϵ_k in the ground state deformations q_k as the circulation *C* changes. In the following section, we are able to solve for the low-energy states of a heavy deformed nucleus using these perturbation formulas.

IV. APPLICATION TO A HEAVY DEFORMED NUCLEUS

To apply the Riemann approximation of symplectic mean field theory to a heavy deformed isotope, e.g., ¹⁶⁶Er, a coadjoint orbit must be selected based on physical considerations. Our pragmatic choice for ¹⁶⁶Er is the coadjoint orbit corresponding to the leading sp(3,*R*) irrep that has the highest weight quantum numbers N_0 =813, λ =108, and μ =0. This highest weight vector is an eigenstate of the deformed harmonic oscillator Hamiltonian [62,63].

A better choice for the orbit could be calculated from the Nilsson model Hamiltonian that adds the spin-orbit force to the deformed oscillator Hamiltonian. The eigenvectors of the Nilsson model are a mixture of vectors from several inequivalent sp(3,*R*) irreps. Adding the pairing interaction will induce further mixing of sp(3,*R*) irreps into the ground state configuration. Certainly the coadjoint orbit containing the density of the real ¹⁶⁶Er ground state is not an integral orbit, i.e., it does not correspond to a unique irreducible representation of the symplectic algebra.

Suppose a quantum mechanical state Ψ is selected to model the nuclear deformed ground state, e.g., Ψ is an eigenstate of the Nilsson Hamiltonian. The density ρ corresponding to Ψ is calculated from the expectations of the one-body sp(3,*R*) operators using Eq. (2.4). To identify the coadjoint orbit \mathcal{O}_{ϱ} that contains ρ , the matrix ρ can be transformed to the normal form ϱ by a symplectic group transformation, $\operatorname{Ad}_{g}^{*}\rho = \varrho$ for some $g \in \operatorname{Sp}(3,R)$. A simple method to find the normal form (2.8) is to evaluate the real eigenvalues, $\pm N_1, \pm N_2, \pm N_3$, of the complex matrix $i\rho$.

The calculation of the density matrix ρ simplifies when Ψ lies entirely in one major oscillator shell, i.e., Ψ is an eigenstate of the isotropic harmonic oscillator Hamiltonian H_0 . In this case the matrix n is antisymmetric and is determined completely by the expectations of the angular momentum operators. This simplifying observation follows from the commutation relation $\hat{N}_{jk} + \hat{N}_{kj} = i[\hat{H}_0, \hat{Q}_{jk}]$. In addition, the expectations of the momentum and position tensors are equal, $t_{jk} = q_{jk}$.

The different sp(3,*R*) irreps that contribute substantially to the heavy deformed ¹⁶⁶Er ground state have similar quantum numbers $(N_0, \lambda, \mu) \approx (813, 108, 0)$. This assertion is supported by experiment and is predicted by the Nilsson model. Note that the quantum number N_0 must be large for a heavy nucleus because the nuclear radius is large. Indeed, in the isotropic oscillator shell model, the value of $N_0 \approx 0.9A^{4/3}$ when $\hbar \omega_0 \approx 41/A^{1/3}$ MeV [68]. For a heavy deformed prolate nucleus, the dominant contributions to the ground state must have a large value for the quantum number λ . The reason is that a substantial excess of quanta in the direction of the long axis relative to the short axis is necessary to produce the experimentally observed quadrupole deformation. The value of μ must be small or zero for a prolate spheroid.

For an AMFT application to the low-energy states of ¹⁶⁶Er, it is not imperative to adopt the exact values of the quantum numbers (N_0, λ, μ) for this isotope's ground state. The expectation values of the sp(3,*R*) Casimirs [Eq. (2.9)] and the AMFT equations themselves [Eqs. (3.13)], are rather insensitive to the precise choice of coadjoint orbit quantum numbers.

To be well defined, symplectic representation theory requires a single sp(3,R) irrep with a precise integral highest weight. When spin-orbit and pairing forces break symplectic dynamical symmetry, a pure sp(3,R) algebraic structure must be abandoned, and the full shell model (augmented with symplectic core excitations) should be invoked. This is a more realistic theory, but it is unnecessarily complicated to explain many properties of geometrical collective states. In essence, the shell model constructs state vectors which, in principle, allow for the prediction of the expectations of all Hermitian N-body operators. AMFT only makes predictions about the expectations of symplectic algebra operators; details about the mixing of sp(3,R) irreps are not required to achieve this limited aim. Thus, although one leading sp(3,R)irrep provides a poor approximation to the ¹⁶⁶Er ground state wave function, the symplectic density of one leading coadjoint orbit can yield an excellent approximation to the symplectic density of the exact ground state. Similar considerations apply to any heavy deformed nucleus. The theoretical situation is similar to the Hartree-Fock one. A Hartree-Fock determinant may have a very small overlap with a shell



FIG. 1. The theoretical quadrupole deformation of the prolate ground state of ¹⁶⁶Er is plotted against the potential tensor component W_{11} in MeV. AMFT yields the experimental ground state $\beta = 0.342$ when the component of the potential tensor is $W_{11} = -24.7$ MeV.

model wave function, yet the Hartree-Fock density matrix may approximate accurately the expectations of one-body operators with respect to the shell model wave function.

For the isotope ¹⁶⁶Er, the oscillator frequency is $\hbar \omega_0$ = 7.36 MeV, the oscillator length b = 2.37 F, the nuclear radius $R_0 = 6.60$ F, and the parameter of Eq. (3.4) is f = 323. When $z_1 = 0$, Eqs. (3.15) determine the dimensionless deformations $q_1 = q_2 = 235$ and $q_3 = 343$ of the prolate ground state in the su(3) approximation. Using Eq. (3.4), the quadrupole deformation in the su(3) limit is calculated to be β =0.223. Because the experimental quadrupole deformation is $\beta = 0.342$ [69] and effective charges are not used in the sp(3,R) theory, a nonzero value for z_1 is required. In Fig. 1 the theoretical quadrupole deformation of the prolate ground state is plotted versus the potential tensor component W_{11} using Eqs. (3.15). The measured ground state deformation, $q_1 = q_2 = 223$ and $q_3 = 389$, is fitted when $W_{11} = -24.7$ MeV and $z_1 = -0.111$. This value for z_1 in the ground state imposes a constraint on the potential parameters of the collective potential energy (3.5),

$$-997b_2 - (5.52 \times 10^4)b_3 - (1.83 \times 10^7)b_4 = 1.$$
 (4.1)

The monopole moment is proportional to tr(q). To maintain a constant value for the nuclear radius, the monopole moment of excited yrast band states must equal the monopole moment of the ground state. In the perturbation theory, this invariance is assured when $\Sigma \epsilon_k = 0$, or, using Eqs. (3.19),

$$T = \frac{2 (q_3 - q_1)(N_0 - \lambda)^2 (N_0 + 2\lambda)^2}{27 q_1 q_3 [q_3^2 (N_0 - \lambda)^2 - q_1^2 (N_0 + 2\lambda)^2]}.$$
 (4.2)

Thus, a constant monopole moment imposes the following constraint on the collective potential parameters of ¹⁶⁶Er:

$$907 b_2 + (1.00 \times 10^5) b_3 + (5.00 \times 10^7) b_4 = 1. \quad (4.3)$$



FIG. 2. The collective potential energy $V(\beta, \gamma)$ in MeV is plotted versus β for several values of γ .

Since a physical collective quadrupole potential is bounded from below, the coefficient b_4 of the highest power in β is positive. For prolate solutions, the coefficient b_3 of $\cos(3\gamma)$ is negative. For simplicity, we set b_2 equal to zero. Then Eqs. (4.1) and (4.3) imply $b_3 = -7.43 \times 10^{-5}$, $b_4 = 1.69 \times 10^{-7}$, and

$$V(\beta, \gamma) = 1041 \,\beta^4 - 628 \,\beta^3 \cos(3\,\gamma). \tag{4.4}$$

This potential is drawn in Fig. 2. The prolate ground state deformation $\beta = 0.342$ does not coincide with the minimum of the quadrupole potential because the sp(3,*R*) Casimirs impose constraints on the energy minimization. From a physical perspective, these constraints are a consequence of the nuclear shell structure.

The circulation of a Riemann ellipsoid is proportional to the angular momentum, with a factor that is a function of the rigidity and the axis lengths perpendicular to the rotation axis [3],

$$C = \frac{2a_2a_3(a_2^2 + a_3^2)r}{(a_2^2 - a_3^2)^2 + 4a_2^2a_3^2r}I.$$
 (4.5)

To complete the analysis, a value for the rigidity must be adopted. Energy levels and deformations for the yrast rotational band can then be calculated using Eqs. (3.13) and (4.5). The energy of the 2^+ excited state of ¹⁶⁶Er is fitted when the rigidity r=0.125. In Fig. 3, the theoretical energy



FIG. 3. The yrast band spectrum of ¹⁶⁶Er is compared with the theoretical spectrum of a rigid rotor r=1 and a Riemann ellipsoid with r=0.125.

levels are compared to experiment and to the compressed spectrum of a rigid rotor.

The quadrupole deformation $\beta = 0.342$ decreases less than 0.1% from I=0 to I=8. Similarly, the shape remains a prolate spheroid, $\gamma = 0^{\circ}$. Equation (4.5) then implies a constant ratio of the Kelvin circulation to the angular momentum, C/I=0.635. This constant ratio in our calculations is in harmony with the explanation of γ -ray staggering made by Mikhailov and Quentin [28].

The expectations of the harmonic oscillator excitation number operator $N-N_0$ for the yrast band of ¹⁶⁶Er are listed in Table I. The su(3) limit corresponds to $N-N_0=0$, and wave functions in this limit are restricted to vectors from the $0 \hbar \omega_0$ harmonic oscillator major shell. The nonzero expectation (≈ 3.4) for the oscillator excitation number in the sp(3,*R*) calculations shows that significant admixtures of core-excited vectors are necessary to build the observed quadrupole deformation. The mean field expectation for the oscillator excitation number is consistent with prior symplectic representation theory calculations [61,62].

Table I also shows the breakdown of the total excitation energy of yrast states into collective kinetic energy, intrinsic kinetic energy, and potential energy. The energies of this table are zeroed at the ground state. The collective kinetic energy accounts for most of the excitation energy. Indeed, it overshoots the total energy by about 10%, while the other energy terms lower the total energy by 10%.

The intrinsic kinetic energy for yrast band states is nearly

TABLE I. Sp(3,R) principal axis Riemann rotor for ¹⁶⁶Er.

$I(\hbar)$	$N - N_0$	$T_{\rm coll}~({\rm keV})$	$T_{\rm intr}$ (keV)	T (keV)	E_0 (keV)	V (keV)	E (keV)
0	3.36	0	0	0	0	0	0
2	3.37	88.6	-6.9	81.7	75.3	5.5	80.8
4	3.39	295	-23.1	272	251	18.4	269
6	3.43	620	-48.5	572	527	38.6	565
8	3.48	1063	-83.1	980	903	66.3	969

a constant negative 8% of the total kinetic energy. The intrinsic kinetic energy is the difference between the total kinetic energy and the collective kinetic energy. The latter is the kinetic energy due to the collective rotational and vortex motion of a Riemann ellipsoid. The calculation demonstrates that the total kinetic energy is dominated by geometrical collective motion. The qualitative conclusion is that the potential energy fixes the quadrupole deformation, while the collective kinetic energy determines the excitation energy.

V. CONCLUSION

The geometrical collective model plays an important role in the Riemann approximation to sp(3,R) AMFT. The geometrical model motivates the mathematical assumptions in the derivation of Eqs. (3.13), e.g., the energy is minimized in the rotating frame, the potential energy is a function of the quadrupole deformation parameters (β, γ) , and the potential tensor W and force quantities z_i are defined by the gradient of the collective potential. Yet, sp(3,R) AMFT differs significantly from the simple geometrical collective model. The ground state density in AMFT does not minimize the potential energy unless $z_i = 0$, which is the su(3) limit. The reason is that the energy minimum in AMFT is constrained to lie on a coadjoint orbit surface. The constraints imposed by the three symplectic Casimirs depend on the labels (N_0, λ, μ) that, in turn, depend on the Nilsson model and the Pauli exclusion principle. Thus, microscopic quantum physics is an essential part of AMFT. Another difference between sp(3,R) AMFT and the collective model is that the sp(3,R)kinetic energy is the exact microscopic kinetic energy-not just the collective Riemann kinetic energy. Yet another difference with the geometrical model is that the Riemann model's kinetic energy is a fixed function of the Kelvin circulation, angular momentum, and axis lengths with no adjustable mass parameter.

An earlier paper [27] investigated the class of sp(3,R) AMFT solutions corresponding to the cranked anisotropic oscillator Hamiltonian of conventional mean field theory. This paper shows that the AMFT method can be used for a rotational scalar Hamiltonian that is the sum of the isotropic harmonic oscillator Hamiltonian plus a collective quadrupole potential energy. This is just the Hamiltonian that has been used in prior sp(3,R) shell model applications; e.g., see Ref. [8]. One significant difference between AMFT and shell model studies is that the Kelvin circulation can be evaluated

in AMFT, while its calculation is beyond the reach of shell model technology.

The application of sp(3,R) AMFT in the Riemann ellipsoid approximation shows that the Kelvin circulation, which is sensitive to the collective nuclear current, is proportional to the angular momentum among yrast band states in heavy deformed nuclei. The model's assertion about the vortex dynamics of nuclear collective rotation, as characterized by the rigidity parameter, needs to be tested independently and directly via inelastic electron scattering measurements of the transverse *E*2 form factor in the heavy deformed region [30–36]. There is a simple formula for the transverse *E*2 form factor in the Riemann ellipsoidal approximation [37].

One of the benefits of the algebraic mean field method is its computational simplicity compared to the representation theory. Although this paper used a simple potential energy [Eq. (3.5)], to study the ground band, very complicated potential energy surfaces $V(\beta, \gamma)$ present no substantial theoretical or computational impediments. The application of AMFT to γ bands requires a nonzero μ for the coadjoint orbit.

The symplectic mean field Hamiltonian is, in general, a density-dependent element of the sp(3,R) Lie algebra. In a subsequent paper we plan to derive the sp(3,R) mean field Hamiltonian from the energy functional using the symplectic geometry of a coadjoint orbit. The mean field Hamiltonian can be applied to the description of normal mode oscillations of symplectic equilibrium states. For su(3) dynamical symmetry, the mean field Hamiltonian and normal mode theory have been determined already [54,55].

The AFMT method may be applied to other group theoretical models to derive simple approximations to representation theory results. At the present time, based on this paper and prior applications to su(3) and sp(3,R), there seems to be no serious obstruction that prevents the method's practical application to any Lie algebra. The algebraic mean field method may prove to be especially useful in cases where the representation theory is intractable because either matrix elements of generators are unavailable or the dimension of the representation is infinite or prohibitively large.

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