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LETTER TO THE EDITOR

Sp(3, R) coadjoint orbit theory

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Abstract

The algebraic mean field method is applied to the symplectic Lie algebra sp(3, R) that describes geometrical collective states in atomic nuclei. The expectations of sp(3, R) generators define a symplectic density matrix. The mean field approximation restricts the densities to a manifold that is a coadjoint orbit of the transformation group Sp(3, R) and a level surface of the symplectic Casimir functions. Compared to representation theory, mean field theory is technically simpler, but yields similar predictions for physical properties of collective states. The critical points of the energy functional on a coadjoint orbit surface define rotational bands. The deformation, kinetic energy and Kelvin circulation of principal axis symplectic rotors are determined as a function of the angular momentum. Illustrative applications of coadjoint orbit theory are reported for the yrast rotational bands of a light ^{20}Ne and a heavy ^{166}Er deformed isotope.

The one-body Hermitian operators that are quadratic in the Cartesian position and momentum coordinates generate the noncompact 21-dimensional symplectic Lie algebra sp(3, R) [1, 2]. The total number of oscillator quanta in the three Cartesian directions (N_1, N_2, N_3) of an Elliott su(3) highest weight vector labels an sp(3, R) irreducible representation (irrep). In addition to the su(3) irrep, an sp(3, R) infinite-dimensional irrep space includes *np–nh* core-excited shell model configurations for all whole numbers n. Repeated applications of the microscopic mass quadrupole and monopole operators to the vectors in the Elliott su(3) irrep space create these symplectic core excitations. The addition of symplectic configurations to the su(3) model space enables the explanation of collective E2 and E0 transition rates using only bare nucleon charges. The sp(3, R) model can also predict transverse E2 form factors that are sensitive to the collective nuclear current [3].

The 15-dimensional general collective motion algebra gcm(3) is a Lie subalgebra of sp(3, R). The gcm(3) Casimir is the length C of the Kelvin circulation vector that is an important degree of freedom of the geometrical model. Its value, in conjunction with the angular momentum, determines the character of nuclear rotation, namely, irrotational flow, rigid rotation, or, more typically, an intermediate collective rotation. The infinite-dimensional unitary irreps of gcm(3) are labelled by the integral values of C. The representation with

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zero circulation is indistinguishable from the irrotational flow model of Bohr and Mottelson. Representations $C > 0$ correspond to the quantum Riemann ellipsoid model. The multiplicity of the circulation C in an sp(3, R) irrep equals the multiplicity of the angular momentum $L = C$ in the generating su(3) irrep [4].

The symplectic sp(3, R) model unifies the geometrical collective model, associated with the gcm(3) subalgebra, and the harmonic oscillator shell model, associated with the u(3) subalgebra. But some important physical questions cannot be framed and answered with precision in irreducible representation theory. For example, given a wavefunction from an irrep of a dynamical symmetry model, does it correspond physically to the collective rigid rotation of a prolate spheroid about its short principal axis? Another vexing problem for the symplectic model is that the gcm(3) Casimir operator is a five-body operator that challenges computation.

Algebraic mean field theory (AMFT) is an alternative way of formulating a dynamical symmetry model. The rotating body-fixed frame is well defined in sp(3, R) AMFT. In this noninertial frame, the shape, rotation axis and circulation are evaluated easily. Moreover, the model space of AMFT is a finite-dimensional manifold while the unitary irreps of sp(3, R) are infinite dimensional. Hartree–Fock and Hartree–Fock–Bogoliubov may be viewed as AMFTs associated with the unitary and orthogonal groups, respectively [5, 6]. Recently, AMFT was developed for the Elliott su(3) algebra [7–9]. This letter applies the algebraic mean field method to sp(3, R). Assuming principal axis rotation, results are reported for the circulation, deformation, kinetic energy and total energy as a function of the angular momentum.

For any Lie algebra, the AMFT space consists of the density matrices that are defined by the expectations of the algebra's operators. The Lie group of the algebra acts as a transformation group on the densities via the coadjoint action. The mean field approximation limits the densities to a single coadjoint orbit which is a surface contained in the space of all densities. The Casimirs of the algebra are constant on each coadjoint orbit. The restriction to a coadjoint orbit is the mathematical expression of dynamical symmetry in AMFT. The energy is a real-valued function of the density; its critical points on a coadjoint orbit are the equilibrium mean field densities.

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 $[x_{\alpha j}, p_{\beta k}] = \mathrm{i}\delta_{\alpha\beta}\delta_{jk}$. The symplectic generators are the Hermitian one-body operators

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

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 angular momentum components. The gcm(3) algebra is spanned by the operators $\hat{Q}_{jk}$ and $\hat{N}_{jk}$.

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

$$S = \begin{pmatrix} X & -U \\ V & -X^T \end{pmatrix} \tag{2}$$

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

$$\sigma(S) = \mathrm{i} \sum_{jk} \left(X_{jk}\hat{N}_{jk} + \frac{1}{2}U_{jk}\hat{Q}_{jk} + \frac{1}{2}V_{jk}\hat{T}_{jk} \right). \tag{3}$$

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 wavefunction Ψ is

$$\rho = \begin{pmatrix} n^T & t \\ -q & -n \end{pmatrix} \tag{4}$$

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

$$\langle\rho, S\rangle \equiv \tfrac{1}{2}\operatorname{tr}(\rho S) = -\mathrm{i}\langle\Psi|\sigma(S)|\Psi\rangle. \tag{5}$$

Denote the symplectic density of an sp(3, R) highest weight vector by

$$\varrho = \begin{pmatrix} 0 & t \\ -q & 0 \end{pmatrix} \qquad t = q = \operatorname{diag}(N_1, N_2, N_3). \tag{6}$$

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

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

$$\mathcal{C}_{2s}[\rho] = \frac{(-1)^s}{2}\operatorname{tr}(\rho^{2s}) \qquad s = 1, 2, 3. \tag{7}$$

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

For the orbit $\mathcal{O}_\varrho$, labelled by (N_1, N_2, N_3), that contains the density of a highest weight vector, the values of the symplectic Casimirs are

$$\mathcal{C}_{2s}[\varrho] = \sum_k N_k^{2s}. \tag{8}$$

Thus, the common level surface of the symplectic Casimir functions consists of all densities ρ, equation (4), that satisfy the three algebraic equations (8). In the typical case of distinct N_i, the three Casimir functions are functionally independent, and the level surface is 18-dimensional.

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, equation (4), as follows: for $R \in \mathrm{SO}(3)$, $n \mapsto RnR^T$, $t \mapsto RtR^T$ and $q \mapsto RqR^T$. Each orbit of the rotation subgroup contains a diagonal inertia tensor, $q = \operatorname{diag}(a_1^2, a_2^2, a_3^2)$, where $a_k > 0$, $k = 1, 2, 3$, are proportional to the axis lengths of the inertia ellipsoid.

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 $\vec{C}$ components are inferred from the off-diagonal components of n: for i, j, k cyclic, $I_i = n_{jk} - n_{kj}$ and $C_i = (a_k/a_j)n_{jk} - (a_j/a_k)n_{kj}$.

1. Applications

The symplectic energy is a rotational scalar functional of the density. A simple sp(3, R) energy functional 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

$$E_0[\rho] = \tfrac{1}{2}\operatorname{tr}(t + q) \tag{9}$$

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

$$v_2 = \tfrac{1}{2}\,\mathrm{tr}(q^{(2)})^2 \qquad v_3 = \tfrac{1}{3}\,\mathrm{tr}(q^{(2)})^3 = \det q^{(2)} \tag{10}$$

where $q^{(2)}_{ij} = q_{ij} - 1/3\delta_{ij}\,\mathrm{tr}\,q$. The scalars v_2 and v_3 are proportional to β^2 and $\beta^3\cos 3\gamma$, respectively. An elementary collective potential, in units of $\hbar\omega_0$, that has been used in prior sp(3, R) representation theory applications is

$$V[\rho] = b_2 v_2 + b_3 v_3 + b_4 v_2^2 \tag{11}$$

where b_2, b_3, b_4 are dimensionless real constants [1, 2]. Because it is a rotational scalar, the energy functional may be evaluated conveniently in the principal axis frame.

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 isotropic system. The sp(3, R) energy $E[\tilde{\rho}]$ of a principal axis rotor with good I and C simplifies to a function of the axis lengths of the inertia ellipsoid and the diagonal components of the kinetic tensor.

As measured in the rotating frame of a principal axis rotor, the energy is the difference between the sp(3, R) laboratory frame energy E and the collective kinetic energy of a Riemann ellipsoid with angular momentum I and Kelvin circulation C,

$$T_{\mathrm{coll}}[\tilde{\rho}] = \frac{1}{4}\left[\frac{(I+C)^2}{(a_2+a_3)^2} + \frac{(I-C)^2}{(a_2-a_3)^2}\right] \tag{12}$$

in units of $\hbar\omega_0$. Equilibrium solutions with angular momentum I and Kelvin circulation C are critical points of the rotating frame energy on a coadjoint orbit surface. Such equilibria are critical points of the functional

$$\mathcal{E}_{IC}[\tilde{\rho}] = E[\tilde{\rho}] - T_{\mathrm{coll}}[\tilde{\rho}] - \sum_{k=1,2,3} m_{2k}\mathcal{C}_{2k}[\tilde{\rho}] \tag{13}$$

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

$$\frac{\partial\mathcal{E}_{IC}}{\partial a_i} = \frac{\partial\mathcal{E}_{IC}}{\partial t_{ii}} = 0 \tag{14}$$

and the three level surface equations, $\mathcal{C}_{2s}[\tilde{\rho}] = \sum N_i^{2s}$.

Energy minimization in the rotating frame determines analytically the kinetic tensor

$$t_{11} = a_1^2 - W_{11} \qquad t_{22} = a_2^2 - W_{22} + \frac{(a_2C - a_3I)^2}{\left(a_2^2 - a_3^2\right)^2} \qquad t_{33} = a_3^2 - W_{33} + \frac{(a_3C - a_2I)^2}{\left(a_2^2 - a_3^2\right)^2} \tag{15}$$

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

$$W_{ii} = -a_i\frac{\partial V}{\partial a_i}. \tag{16}$$

Thus, the sp(3, R) kinetic energy T of an equilibrium density is the sum of intrinsic and collective energies,

$$T = \frac{1}{2}\,\mathrm{tr}\,t = T_{\mathrm{intr}} + T_{\mathrm{coll}} \qquad T_{\mathrm{intr}} = \sum_k \left(a_k^2 - W_{kk}\right). \tag{17}$$

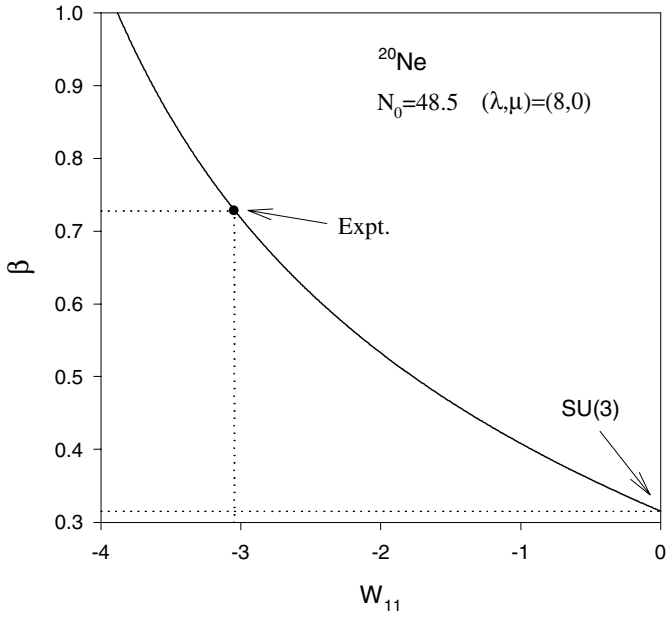

Figure 1. For ^{20}Ne, the quadrupole deformation of its prolate sp(3, R) ground state is plotted versus the component of the potential tensor in the direction of the rotation axis.

The axis lengths are solutions to the three Casimir equations. Suppose the coadjoint orbit labels are ordered as $N_3 \geqslant N_2 \geqslant N_1$ and set the u(3) labels $N_0 = N_1 + N_2 + N_3$, $\lambda = N_3 - N_2$, $\mu = N_2 - N_1$. The Casimir equations simplify to

$$\begin{aligned} 3\sqrt{a_1^2 - W_{11}}a_1 &= N_0 - \lambda - 2\mu \\ 3\sqrt{a_2^2 - W_{22}}a_2 &= \sqrt{P + \sqrt{Q}} \\ 3\sqrt{a_3^2 - W_{33}}a_3 &= \frac{(N_0 - \lambda + \mu)(N_0 + 2\lambda + \mu)}{\sqrt{P + \sqrt{Q}}} \end{aligned} \tag{18}$$

where $P = N_0^2 + N_0(\lambda + 2\mu) + 5\lambda^2/2 + \lambda\mu + \mu^2 - 9C^2/2$, $Q = 9(\lambda^2 - C^2)((2N_0 + \lambda + 2\mu)^2 - 9C^2)/4$. Note that W_{kk} is a function of the axis lengths. The axis lengths in (18) must be determined self-consistently with the potential tensor.

1.1. Coadjoint orbits with $\mu = 0$

When μ vanishes, a principal axis rotational band exists for angular momentum $0 \leqslant I \leqslant \lambda$. There are no real positive solutions to equations (18) for the axis lengths when $I > \lambda$. As illustrations of Sp(3, R) AMFT, we study the yrast rotational band of a light (^{20}Ne) and a heavy (^{166}Er) deformed nucleus. For ^{20}Ne the leading Elliott su(3) representation is used: $N_0 = 48.5$, $(\lambda, \mu) = (8, 0)$ and $\hbar\omega_0 = 13.1$ MeV. In figure 1 the quadrupole deformation β of the prolate ground state of ^{20}Ne is plotted versus the potential tensor component W_{11}. When the collective potential vanishes and the total energy reduces to the harmonic oscillator, the deformation is the su(3) value, $\beta = 0.32$. Since the experimental deformation of ^{20}Ne is $\beta = 0.73$, the required value of the potential tensor is $W_{11} = -3.0$. Solutions for $0 < I < \lambda$ are parametrized by the rigidity r that is defined as the ratio of the Kelvin circulation to its

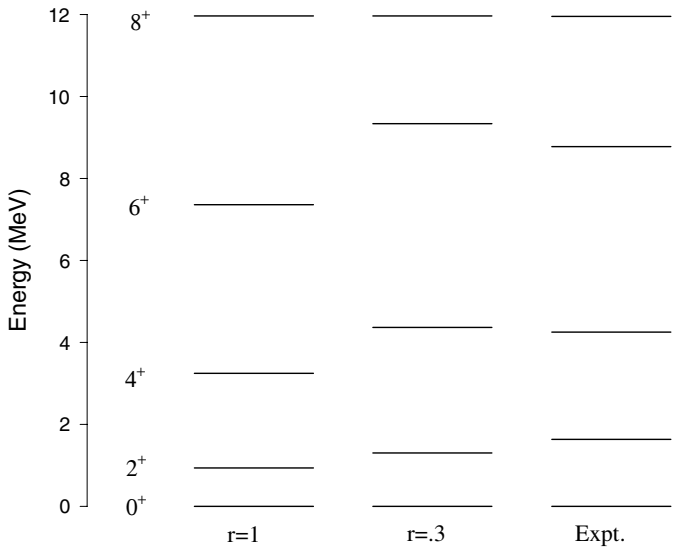

Figure 2. ^{20}Ne yrast energy levels are compared to the sp(3, R) energies of a rigid rotor ($r = 1$) and a Riemann rotor ($r = 0.3$).

Table 1. Sp(3, R) principal axis rotor for ^{20}Ne.

I	C	β	γ	N
0	0.0	0.73	0	50.0
2	1.6	0.72	0.2	50.0
4	2.9	0.68	0.7	50.1
6	4.5	0.61	2.1	50.0
8	8.0	0.22	60	48.6

rigid body value. In figure 2 the experimental yrast energy levels of ^{20}Ne are compared to a rigid body $r = 1$ and a symplectic rotor with rigidity $r = 0.3$ when the potential parameters $b_2 = -0.026$, $b_3 = 0$ and $b_4 = 2.4 \times 10^{-5}$. Table 1 reports the circulation, quadrupole deformation and the expectation N of the oscillator number operator when the rigidity $r = 0.3$.

For a heavy deformed nucleus the rotational band solutions have a nearly constant moment of inertia that depends on the rigidity and deformation. The potential determines the deformation but it has a minor effect on the energies of yrast band members for small angular momentum. For ^{166}Er, the sp(3, R) labels are $N_0 = 813$, $\lambda = 108$, $\mu = 0$ and $\hbar\omega_0 = 7.82$ MeV. When the potential parameters are $b2 = 0$, $b3 = -0.0006$, $b4 = 1.65 \times 10^{-6}$, the quadrupole deformation of the prolate ground state matches experiment, $\beta = 0.34$. When the rigidity $r = 0.14$, the calculated symplectic and experimental moments of inertia of the yrast rotational band are similar.

2. Conclusion

From a physical perspective, good dynamical symmetry for densities is a weaker assertion than good symmetry for wavefunctions. Even when wavefunctions that form a band are a superposition of vectors from many irreducible representations, the densities of band members

can share approximately common values for the algebra's Casimirs. For most deformed nuclei, mixing of symplectic representations is expected due to pairing and spin–orbit forces, yet the values of the symplectic Casimirs can be approximately constant among band members. Symplectic irreducible representation theory makes strong claims about nuclear wavefunctions that are irrelevant to the description of geometrical states. Sp(3, R) coadjoint orbit theory can explain geometrical collective properties, but it does not try to construct wavefunctions that incorporate all the degrees of freedom in phase space.

The method of this letter may be applied to any dynamical symmetry model. Many properties of the irreducible representations of a Lie group may be inferred from the geometry of its coadjoint orbits [10].

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