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Solutions to a time-dependent $su(3)$ mean field Hamiltonian

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Abstract

The time-dependent $su(3)$ mean field equations are solved for a particular energy function relevant to nuclear structure. The model energy in the $su(3)$ enveloping algebra is the sum of two terms which are the squared length of the angular momentum vector $\vec{l}\cdot\vec{l}$ and the cubic rotational scalar $X_3 = \mathrm{tr}(lql)$. The mean field solutions for this energy have constant intrinsic quadrupole moments q. In the three-dimensional space of all angular momentum components in the rotating principal axis frame, a trajectory is defined by the intersection of a sphere and a hyperboloid. This conclusion is similar to the classical rigid rotor for which a solution is the intersection of a sphere and the inertia ellipsoid.

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1. Introduction

This paper reports solutions to the time-dependent $su(3)$ mean field equations in an important special case relevant to nuclear structure physics. In prior work the $su(3)$ mean field Hamiltonian was derived [1] and applied to small amplitude wobbling motions in atomic nuclei [2]. The paper contains three main sections. The introduction reviews the algebraic mean field method and establishes notation for $su(3)$. Section 2 solves the time-dependent $su(3)$ equations for a particular rotationally invariant energy function, equation (3), using the principal axis frame concept. The conclusion discusses other potential applications of the mean field method to algebraic models of nuclear collective motion.

The two fundamental examples of mean field theory in A-particle fermion science are Hartree–Fock, which is based on the Lie algebra $u(n)$ of all one-body operators acting on the exterior product of A-copies of a quantum mechanical n-dimensional single-particle valence space [3, 4], and Hartree–Fock–Bogoliubov theory, which is founded on the Lie algebra

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$o(2n)$ [5]. The Lie algebras underlying the two pre-eminent mean field theories are not always stressed in some presentations; nonetheless, the algebras play essential roles in these two theories. The Lie algebraic structures and associated physical interpretations of the two paradigms generalize to any algebra of many-body observables.

Suppose that $\mathfrak{g}$ is a Lie algebra, which I assume for simplicity is an algebra of matrices, and $\mathfrak{g}^*$ denotes its dual space, which can also be identified with a space of matrices. The dimension of the dual space equals the dimension of the Lie algebra. When $\mathfrak{g}$ is semisimple, the dual space may be identified with the algebra itself via the nondegenerate Killing form. The nondegenerate pairing between a dual space element ρ and a Lie algebra element Z is assumed to be the real number

$$\langle \rho, Z \rangle \equiv \operatorname{tr}(\rho Z). \tag{1}$$

Let σ be a representation of $\mathfrak{g}$ by Hermitian operators on a quantum mechanical Hilbert space $\mathcal{H}$. Corresponding to every normalized vector Ψ of $\mathcal{H}$ is a unique element ρ of the dual space given by the expectation value

$$\langle \rho, Z \rangle = \langle \Psi | \sigma(Z) | \Psi \rangle. \tag{2}$$

Not every dual element is associated with a quantum mechanical state. Those that do are called density matrices. In the typical situation many distinct quantum state vectors yield the same density matrix.

The $su(3)$ Lie algebra consists of all Hermitian traceless 3×3 complex matrices[1]. Since $su(3)$ is semisimple, the dual space $su(3)^*$ is identified with $su(3)$. Thus an $su(3)$ density matrix is a Hermitian traceless 3×3 matrix $\rho = q - \frac{1}{2}\,\mathrm{i}l$, where q is a real symmetric traceless matrix and l is an antisymmetric matrix. The real part q is interpreted as the quadrupole moment expectation and the imaginary part l is the angular momentum expectation [6]. The components of the angular momentum pseudovector $\vec{l}$ are related to the entries of the antisymmetric matrix l via $l_{ij} = \varepsilon_{ijk} l_k$.

The representation that defines these expectations may correspond to any of the various physical realizations of $su(3)$ in nuclear physics by irreducible representations, e.g., the Elliott model for light nuclei [7], the $su(3)$ limit of the interacting boson model [8], pseudo-$su(3)$ symmetry in medium mass isotopes [9–12] and cluster model $su(3)$ symmetry [13, 14]. Quasi-dynamical $su(3)$ symmetry applies to heavy nuclei [15] for which spin–orbit splitting and the pairing force strongly break exact $su(3)$ symmetry. The $su(3)$ representation space is not irreducible in the quasi-dynamical theory [16, 17]. Thus, rotational bands in nuclei are often modelled using some $su(3)$ representation space. But the precise physical interpretation of a density matrix depends on the chosen representation. The application presented in this paper is relevant to any of these models of nuclear rotation.

The ubiquity of nuclear rotational bands throughout the periodic table shows that their existence is neither dependent on the details of the strong interaction, nor on the many-fermion shell model Hilbert space. The band members are characterized simply by their intrinsic quadrupole moments, moments of inertia and angular momenta. Thus the degrees of freedom that the $su(3)$ algebra contains are just exactly what are required to provide a useful 'Ockham's razor' description of these bands. The essential advantage to an $su(3)$ density matrix ρ is that it ignores secondary nuclear degrees of freedom, which the exact wavefunction Ψ describes, and zeros in on the primary collective rotational modes.

[1] Strictly speaking the real algebra consists of the skew-Hermitian matrices, but the correspondence with physics is enhanced using Hermitian matrices.

1.1. Energy and coadjoint orbits

The energy of a physical system that is characterized primarily by some Lie algebra $\mathfrak{g}$ of observables must be an approximate function of its generators. This will be true when the primary degrees of freedom that are part of the algebra are decoupled from other secondary degrees of freedom. In most group theoretical models in physics, a model Hamiltonian is chosen that is an element of the universal enveloping algebra $U(\mathfrak{g})$. In this favourable situation, $\mathfrak{g}$ is called a spectrum generating algebra [18].

Casimirs are elements of the centre of $U(\mathfrak{g})$. The Casimirs commute, therefore, with the Hamiltonian of a spectrum generating algebra. In quantum mechanics, such a Hamiltonian is represented by a self-adjoint operator that leaves invariant a simultaneous eigenspace of the Casimir operators. A simultaneous eigenspace of the Casimirs is not generally irreducible, but, for a compact Lie algebra, it is a direct sum of irreducible subspaces, each of which carries the same equivalent representation. Thus, the Hamiltonian eigenvalue problem for a compact spectrum generating algebra simplifies to a diagonalization on irreducible finite-dimensional subspaces of $\mathfrak{g}$.

In mean field theory, the Casimirs are real-valued functions on the dual space. When $\mathfrak{g}$ is spectrum generating, the model energy is also a real-valued function on $\mathfrak{g}^*$. In this case, the model densities are limited to a simultaneous level surface of the Casimirs, i.e., a surface contained in the dual space on which each Casimir function has a constant value. The analogous concept in quantum mechanics is the restriction to a simultaneous eigenspace of the Casimir operators.

A simultaneous level surface of the Casimirs may not be connected. A connected submanifold is given by a coadjoint orbit $\mathcal{O}$ of the Lie group G, defined as a covering group of $\exp(\mathfrak{g})$. The analogous concept to a coadjoint orbit in mean field theory is an irreducible representation space in quantum mechanics. A coadjoint orbit is defined as follows: the matrix Lie group G acts on its matrix Lie algebra $\mathfrak{g}$ by the adjoint action, $\mathrm{Ad}_g(Z) = gZg^{-1}$ for all $g \in G$ and $Z \in \mathfrak{g}$. The group G then acts on the dual space $\mathfrak{g}^*$ by the coadjoint action that satisfies, $\langle \mathrm{Ad}^*_g(\rho), Z\rangle = \langle \rho, \mathrm{Ad}_{g^{-1}}(Z)\rangle$ for all $g \in G$, $\rho \in \mathfrak{g}^*$ and $Z \in \mathfrak{g}$. The coadjoint orbit $\mathcal{O}$ containing the density ρ consists of ρ and all the transformed densities $\mathrm{Ad}^*_g(\rho)$ as g ranges over the entire group G.

The algebra $su(3)$ is spectrum generating for the following model energy in $U(su(3))$:

$$\mathcal{E}(\rho) = a\vec{l}\cdot\vec{l} + bX_3 \qquad \text{for} \quad \rho = q - \tfrac{1}{2}\,\mathrm{i}l \tag{3}$$

where the squared length of the angular momentum is $\vec{l}\cdot\vec{l} = -(1/2)\mathrm{tr}(l^2)$, the cubic rotational scalar $X_3 = \mathrm{tr}(lql)$ and a, b are real constants. By itself the squared angular momentum term yields a constant moment of inertia rotational band. The X_3 term is necessary to distinguish among densities with the same angular momentum [19, 20]. In deformed even–even isotopes, two low energy angular momentum $L^\pi = 2^+$ states are often found experimentally with quite different energies, one belongs to the yrast band and the other is the head of a γ band. The inclusion of the X_3 term in the $su(3)$ model energy allows for agreement with experiment in such cases [21]. The mean field equations corresponding to the energy function (3) are constructed and solved in the following section.

The simply connected Lie group $SU(3)$ consists of the complex 3×3 unitary matrices with unit determinant. On the dual space, the coadjoint action is $\mathrm{Ad}^*_g\rho = g\rho g^{-1}$ for $g \in SU(3)$ and $\rho \in su(3)^*$. Because any Hermitian matrix can be diagonalized by a unitary matrix, each $SU(3)$ coadjoint orbit contains a real traceless diagonal matrix that is unique except for the ordering of the eigenvalues. For a pair of non-negative real numbers (λ, μ) and a choice of

eigenvalue ordering, each orbit contains a unique diagonal matrix of the form

$$\varrho = \frac{1}{3}\begin{pmatrix} -\lambda+\mu & 0 & 0 \\ 0 & -\lambda-2\mu & 0 \\ 0 & 0 & 2\lambda+\mu \end{pmatrix}. \tag{4}$$

The pair (λ, μ) labels the coadjoint orbits and each such diagonal matrix ϱ is an orbit representative. This particular indexing of the orbits is chosen because, whenever λ and μ are non-negative integers, equation (4) is the density corresponding to a highest weight vector of an irreducible $SU(3)$ representation [7].

The coadjoint orbit, denoted by $\mathcal{O}_\varrho$, containing the diagonal density ϱ, is

$$\mathcal{O}_\varrho = \{\rho = \mathrm{Ad}^*_g \varrho = g\varrho g^{-1} \in su(3)^* \mid g \in SU(3)\}. \tag{5}$$

The dual space $su(3)^*$ is a disjoint union of the coadjoint orbits $\mathcal{O}_\varrho$ as ϱ ranges over the orbit representatives (4). When both λ and μ are nonzero, the coadjoint orbit is in general position, and $\mathcal{O}_\varrho$ is a six-dimensional surface contained in the eight-dimensional dual space.

The $su(3)$ algebra has two-independent Casimirs of quadratic and cubic orders,

$$\begin{aligned} \mathcal{C}_2(\rho) &= \mathrm{tr}\,\rho^2 = \mathrm{tr}\,q^2 - \tfrac{1}{4}\,\mathrm{tr}\,l^2 \\ \mathcal{C}_3(\rho) &= \mathrm{tr}\,\rho^3 = \mathrm{tr}\,q^3 - \tfrac{3}{4}\,\mathrm{tr}\,(lql). \end{aligned} \tag{6}$$

These functions are trivially constant on each coadjoint orbit, $\mathcal{C}_r(\mathrm{Ad}^*_g\rho) = \mathcal{C}_r(\rho)$ for $r = 2, 3$; their values at the orbit representatives (4) are

$$\begin{aligned} \mathcal{C}_2(\varrho) &= \tfrac{2}{3}(\lambda^2 + \lambda\mu + \mu^2) \\ \mathcal{C}_3(\varrho) &= \tfrac{1}{9}(2\lambda^3 + 3\lambda^2\mu - 3\lambda\mu^2 - 2\mu^3). \end{aligned} \tag{7}$$

The simultaneous level surface in general position for the two $su(3)$ Casimirs, $\mathcal{C}_2(\rho) = \mathcal{C}_2(\varrho)$ and $\mathcal{C}_3(\rho) = \mathcal{C}_3(\varrho)$, is the coadjoint orbit $\mathcal{O}_\varrho$.

1.2. Hamiltonian vector fields on $\mathcal{O}_\varrho$

An important mathematical result is that the coadjoint orbits of any Lie group are symplectic manifolds [22–24]. The symplectic geometry of a coadjoint orbit determines the mean field Hamiltonian from the energy function.

Each element Z of the $su(3)$ Lie algebra determines a tangent vector field $\overline{Z}$ to each coadjoint orbit. Consider the curve $\zeta(\epsilon) = \exp(\mathrm{i}\epsilon Z)$ in the group $SU(3)$. Given any point ρ in the dual space, the curve $\epsilon \mapsto \mathrm{Ad}^*_{\zeta(\epsilon)}\rho = \exp(-\mathrm{i}\epsilon Z)\rho\exp(\mathrm{i}\epsilon Z)$ lies in the coadjoint orbit through ρ. The tangent to this curve at ρ is denoted by $\overline{Z}[\rho]$.

The annihilator $\mathcal{A}_\rho$ at ρ is the subalgebra

$$\mathcal{A}_\rho = \{Z \in su(3) \mid [Z, \rho] = 0\}. \tag{8}$$

When Z is an element of the annihilator at ρ, $\overline{Z}[\rho]$ is a zero tangent vector at ρ because the curve $\mathrm{Ad}^*_{\zeta(\epsilon)}\rho$ is a fixed point. When the difference between two Lie algebra elements is an element of the annihilator at ρ, the corresponding tangent vectors are equal: $\overline{Z}[\rho] = \overline{W}[\rho]$ if and only if $Z - W \in \mathcal{A}_\rho$. Therefore, the tangent space to the coadjoint orbit at ρ can be identified with the vector space $su(3)$ modulo the annihilator $\mathcal{A}_\rho$.

For two tangent vectors, $\overline{Z}[\rho]$ and $\overline{W}[\rho]$, to the coadjoint orbit at ρ, define the symplectic form

$$\omega_\rho(\overline{Z}[\rho], \overline{W}[\rho]) = -\mathrm{i}\langle\rho, [Z, W]\rangle. \tag{9}$$

This antisymmetric bilinear form is well defined on the tangent space to the coadjoint orbit at ρ since, $\langle\rho, [Z, W]\rangle = \langle\rho, [Z', W']\rangle$ when $Z - Z' \in \mathcal{A}_\rho$ and $W - W' \in \mathcal{A}_\rho$. The form ω

Table 1. Hamiltonian vector fields in $su(3)$.

Function f	Hamiltonian vector field $Z_f[\rho]$
$\lambda(Z)$	Z
l_{ij}	$-\mathrm{i}(E_{ij} - E_{ji})$
q_{ij}	$(E_{ij} + E_{ji})/2 - (1/3)\delta_{ij}\mathrm{Id}$
$\mathcal{C}_r$	0
$\mathrm{tr}(q^2)$	$2q$
$\vec{l}\cdot\vec{l}$	$-2\mathrm{i}l$
$\mathrm{tr}(lql)$	$4(q^2 - (1/3)\mathrm{tr}(q^2)\mathrm{Id})$

is nondegenerate, i.e., $\omega_\rho(\overline{Z}[\rho], \overline{W}[\rho]) = 0$ for all W in the $su(3)$ Lie algebra if and only if $\overline{Z}[\rho]$ is a null tangent vector at ρ.

Suppose f is any smooth real-valued function on the coadjoint orbit $\mathcal{O}_\rho$. The derivative of f at ρ in the direction of $\overline{W}[\rho]$ is defined by

$$\mathrm{d}f(\overline{W})(\rho) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} f(\exp(-\mathrm{i}\epsilon W)\rho\exp(\mathrm{i}\epsilon W))\mid_{\epsilon=0}. \tag{10}$$

Each function f defines a vector field $\overline{Z}_f$ on each coadjoint orbit satisfying

$$\omega_\rho(\overline{Z}_f[\rho], \overline{W}[\rho]) = \mathrm{d}f(\overline{W})(\rho) \tag{11}$$

for all directions $\overline{W}[\rho]$ tangent to the coadjoint orbit at ρ. The solution $\overline{Z}_f[\rho]$ to this equation is unique because the symplectic form is nondegenerate. The vector field $\overline{Z}_f$ is called the Hamiltonian vector field associated with the smooth function f. There exists a Lie algebra element $Z_f[\rho]$ whose corresponding tangent vector is $\overline{Z}_f[\rho]$. The assignment of the Lie algebra element $Z_f[\rho]$ to the function f at ρ is not unique, but the difference between two such Lie algebra elements must lie in the annihilator $\mathcal{A}_\rho$. When the function f is the energy itself, the vector field $\overline{Z}_f[\rho]$ is the mean field Hamiltonian $\overline{h}[\rho]$. For simplicity of notation, the 'bars' over the algebra elements will be omitted, but understood, whenever confusion between algebra elements and vector fields is unlikely.

For each Lie algebra element Z there is an elementary function $\lambda(Z)$ on the dual space defined by $\lambda(Z)(\rho) = \langle\rho, Z\rangle$. The value of the function $\lambda(Z)$ at ρ is the expectation of the physical observable corresponding to Z when the system state has the $su(3)$ density ρ. It is easily shown that the Hamiltonian vector field associated with $\lambda(Z)$ is Z. The Hamiltonian vector fields associated with various smooth functions are provided in table 1.

In this table, the functions l_{ij} and q_{ij} are the 'coordinate functions' that map $\rho = q - (\mathrm{i}/2)l$ into the i, j real entries of the matrices l and q, respectively. E_{ij} denotes the elementary matrix whose only nonzero entry is one at the intersection of row i and column j. $\mathrm{Id} = E_{11} + E_{22} + E_{33}$ is the identity matrix.

The Poisson bracket on $\mathcal{O}_\varrho$ is defined by the symplectic form. The bracket of two smooth real-valued functions f, g on $\mathcal{O}_\varrho$ is

$$\{f, g\}(\rho) = \omega_\rho(\overline{Z}_f[\rho], \overline{Z}_g[\rho]). \tag{12}$$

2. Dynamics on $\mathcal{O}_\varrho$

The time evolution of an $su(3)$ density is determined by a geometrical condition: a solution $\rho(t)$ must be an integral curve of the $su(3)$ Hamiltonian vector field $\overline{h}[\rho]$ or

$$\mathrm{i}\dot{\rho} = [h[\rho], \rho]. \tag{13}$$

The $su(3)$ mean field dynamical equation is formally identical to the time-dependent Hartree–Fock equation. Equation (13) is a finite-dimensional Lax equation [25, 26]. When $\rho = q - \frac{1}{2}\,\mathrm{i}l$ and $h[\rho] = \mathrm{Re}\,h + \mathrm{i}\,\mathrm{Im}\,h$ are decomposed into their real and imaginary parts, the dynamical system becomes

$$\dot{q} = \tfrac{1}{2}[l, \mathrm{Re}\,h] - [q, \mathrm{Im}\,h] \tag{14}$$

$$\dot{l} = -2[q, \mathrm{Re}\,h] - [l, \mathrm{Im}\,h]. \tag{15}$$

Dynamics may be expressed equivalently using the Poisson bracket. When f is any smooth function on a coadjoint orbit, its time rate of change along a solution curve is

$$\dot{f} = \{\mathcal{E}, f\}. \tag{16}$$

For example, when $f = \lambda(Z)$, the time rate of change of the observable corresponding to Z along a solution curve is

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\lambda(Z) = \langle\dot{\rho}, Z\rangle &= \mathrm{itr}([\rho, h[\rho]]Z) = \omega_\rho(\overline{h}[\rho], \overline{Z}) \\ &= \{\mathcal{E}, \lambda(Z)\}(\rho).\end{aligned} \tag{17}$$

The last line can be written alternatively as the derivative of $\mathcal{E}$ in the direction $\overline{Z}$, $\{\mathcal{E}, \lambda(Z)\}(\rho) = \mathrm{d}\mathcal{E}(\overline{Z})(\rho)$.

2.1. Rotational invariance

The rotation group $SO(3)$ is a subgroup of the special unitary group $SU(3)$. A density $\rho = q - \frac{1}{2}\,\mathrm{i}l$ in $su(3)^*$ is transformed by a rotation $R \in SO(3)$ into the density $\mathrm{Ad}^*_R\rho = R\rho R^T = RqR^T - \frac{1}{2}\,\mathrm{i}RlR^T$. The energy function (3) is invariant under rotations, $\mathcal{E}(\mathrm{Ad}^*_R\rho) = \mathcal{E}(\rho)$ for all $R \in SO(3)$. As a consequence the angular momentum vector $\vec{l}$ is constant along each solution curve

$$\dot{l}_{ij} = \{\mathcal{E}, l_{ij}\}(\rho) = \mathrm{d}\mathcal{E}(-\mathrm{i}(E_{ij} - E_{ji}))(\rho) = \frac{\mathrm{d}}{\mathrm{d}\theta}\mathcal{E}(R(-\theta)\rho R(\theta)|_{\theta=0} = 0 \tag{18}$$

where $R(\theta) = \exp(\theta(E_{ij} - E_{ji}))$ is a rotation in the $i - j$ plane through an angle θ.

The set of three functions $\{\mathcal{E}, \vec{l}\cdot\vec{l}, l_3\}$ Poisson commute. On a six-dimensional orbit $\mathcal{O}_\varrho$ in general position, these three functions are independent. Therefore, $\{\mathcal{E}, \vec{l}\cdot\vec{l}, l_3\}$ is a complete involutive set in the sense of Liouville. A solution curve to the time-dependent mean field equations, equation (13), lies on a level surface of the involutive set. This level set is a three-dimensional torus lying in the compact manifold $\mathcal{O}_\varrho$ and the solution curves are windings on the torus. But explicit solution curves are difficult to derive and another tactic is useful.

2.2. Principal axis frame

The dynamical system defined by (3) on $\mathcal{O}_\varrho$ is rather stiff with many constants of the motion. Since $\mathcal{E}$ and $\vec{l}\cdot\vec{l}$ are constants of the motion, so is X_3. Because the Casimirs are constant on $\mathcal{O}_\varrho$, the functions $\mathrm{tr}\,q^2$ and $\mathrm{tr}\,q^3$ are also constant on solution curves. The real eigenvalues q_1, q_2, q_3 of the traceless symmetric matrix q are constants of the motion too because $\mathrm{tr}\,q^2$ and $\mathrm{tr}\,q^3$ are the coefficients of the secular equation. This suggests transforming the dynamical system to the principal axis frame.

Any real symmetric matrix can be diagonalized by a rotation matrix. Hence, there is an $R \in SO(3)$ such that the rotated quadrupole moment is diagonal

$$\tilde{q} = RqR^T = \mathrm{diag}(q_1, q_2, q_3). \tag{19}$$

The eigenvalues are unique, up to their order, which we fix to be $q_3 \geqslant q_1 \geqslant q_2$. From a physical viewpoint, R rotates the laboratory frame into the rotating body-fixed frame in which, by definition, the system quadrupole moment $\tilde{q}$ is diagonal. At the same time the conserved laboratory angular momentum l is transformed to $I = RlR^T$, which is the system angular momentum projected onto the rotating body-fixed principal axes.

The angular momentum in the body-fixed frame is a pseudovector $\vec{I}$ with components $I_i = \frac{1}{2}\varepsilon_{ijk}I_{jk}$. The rotation of the vector angular momentum $\vec{I} = R\vec{l}$ is equivalent to the matrix transformation $I = RlR^T$. When two of the three components of $\vec{I}$ are zero, the body is rotating around a principal axis. A tilted rotation in a principal plane requires that one component of $\vec{I}$ is zero. In general, all three components of the angular momentum $\vec{I}$ are nonzero, and the matrix I is antisymmetric, but otherwise arbitrary.

Let $\mathcal{M}_\varrho$ denote the surface of all principal axis densities contained in the coadjoint orbit $\mathcal{O}_\varrho$. The points $\tilde{\rho} = \tilde{q} - \frac{1}{2}\,\mathrm{i}\,I$ of $\mathcal{M}_\varrho$ consist of a real diagonal part, $\tilde{q}$, and an imaginary part I. Each point of $\mathcal{M}_\varrho$ is defined by a set of six real variables $(q_1, q_2, q_3; I_1, I_2, I_3)$ that satisfy an algebraic system

$$\begin{aligned}
&\sum_k q_k = 0 \\
&\sum_k q_k^2 + \frac{1}{2}\vec{I}\cdot\vec{I} = \mathcal{C}_2(\varrho) \\
&\sum_k q_k^3 - \frac{3}{4}\sum_k q_k I_k^2 = \mathcal{C}_3(\varrho).
\end{aligned} \tag{20}$$

The principal axis surface $\mathcal{M}_\varrho$ is three dimensional when λ and μ are nonzero.

Let $R(t) \in SO(3)$ be a smooth time-dependent rotation that transforms a solution curve of the dynamical system (13) into the submanifold of principal axis densities. Define the time-dependent antisymmetric matrix $\Omega(t) = \dot{R}R^T$ in the Lie algebra $so(3)$ of the rotation group. The pseudo-vector $\vec{\omega}$ corresponding to the matrix Ω is the angular velocity. Let $\tilde{\rho} = R\rho R^T \in \mathcal{M}_\varrho$ denote the density in the principal axis frame. The Hamiltonian dynamical system on the coadjoint orbit, equation (13), is equivalent to the following dynamical equation on $\mathcal{M}_\varrho$:

$$\mathrm{i}\frac{\mathrm{d}\tilde{\rho}}{\mathrm{d}t} = [h_\Omega[\tilde{\rho}], \tilde{\rho}] \tag{21}$$

where $h_\Omega[\tilde{\rho}] = Rh[\rho]R^T + \mathrm{i}\Omega$ is the $su(3)$ Routhian. When the mean field Hamiltonian is a polynomial in the density, the projection to the body-fixed frame is simply $Rh[\rho]R^T = h[\tilde{\rho}]$. In terms of the body-fixed quadrupole moment and angular momentum, the dynamical equation of a rotationally invariant energy function becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}I = [\Omega, I] \tag{22}$$

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\tilde{q} &= [\Omega, \tilde{q}] + R\dot{q}R^T \\
&= [\Omega, \tilde{q}] + \tfrac{1}{2}[I, R(\mathrm{Re}\,h)R^T] - [\tilde{q}, R(\mathrm{Im}\,h)R^T]
\end{aligned} \tag{23}$$

where $R\dot{q}R^T$ is given by equation (14). These dynamical equations on the principal axis submanifold $\mathcal{M}_\varrho$ differ from the equations on the coadjoint orbit by a Coriolis terms, namely, the commutator involving the angular velocity matrix.

On the principal axis submanifold, the time rate of change of the body-fixed angular momentum obeys the Euler precession equation

$$\dot{I} = [\Omega, I] \qquad \frac{\mathrm{d}}{\mathrm{d}t}\vec{I} = -\vec{\omega} \times \vec{I}. \tag{24}$$

The vibration of the quadrupole deformation in the principal axis frame is given by the diagonal components of equation (23)

$$\frac{\mathrm{d}}{\mathrm{d}t}q_k = \frac{1}{2}[I, R(\mathrm{Re}\, h)R^T]_{kk}. \tag{25}$$

Since $\tilde{q}$ is diagonal, the off-diagonal components on the right-hand side of equation (24) must vanish,

$$\Omega_{ij} = \frac{1}{2(q_i - q_j)}[I, R(\mathrm{Re}\, h)R^T]_{ij} - (R(\mathrm{Im}\, h)R^T)_{ij} \qquad \text{for} \quad i \neq j. \tag{26}$$

The solution of the last equation determines the angular velocity as a function of the angular momentum I and the body-fixed deformation $\tilde{q}$.

For the energy function $\mathcal{E}$ of equation (3), the mean field Hamiltonian according to the table is

$$h[\rho] = -2\mathrm{i}\, al + 4b(q^2 - (1/3)\,\mathrm{tr}(q^2)\mathrm{Id}). \tag{27}$$

The principal axis lengths, as previously argued, are constants of the motion for this energy, and equation (25) yields this result by explicit calculation,

$$\frac{\mathrm{d}}{\mathrm{d}t}q_k = 2b[I, \tilde{q}^2]_{kk} = 0. \tag{28}$$

The angular velocity equation (26) simplifies to

$$\Omega_{ij} = 2(a - b(q_i + q_j))I_{ij}, \text{ or } \omega_k = 2(a + bq_k)I_k. \tag{29}$$

Thus the angular momentum components are proportional to the angular velocity components, $I_k = \mathcal{I}_k\omega_k$, where the constant moments of inertia in the principal axis frame are $\mathcal{I}_k = (2(a + bq_k))^{-1}$. The energy function is the rotor energy, $\mathcal{E} = \sum_k I_k^2/(2\mathcal{I}_k)$. The differential equations to be solved are the precession equations, equation (24), or

$$\begin{aligned} \dot{I}_1 &= -2b(q_2 - q_3)I_2I_3 \\ \dot{I}_2 &= -2b(q_3 - q_1)I_3I_1 \\ \dot{I}_3 &= -2b(q_1 - q_2)I_1I_2. \end{aligned} \tag{30}$$

The solution curves to the precession equations conserve the energy $\mathcal{E}$ and the square of the angular momentum vector $\vec{I} \cdot \vec{I} = \vec{l} \cdot \vec{l}$. The values of the energy and the length of the angular momentum vector determine $X_3 = (\mathcal{E} - a\vec{I} \cdot \vec{I})/b$. On the principal axis manifold $\mathcal{M}_\varrho$ the two Casimirs equations, equations (20), determine the constant traceless quadrupole moment $\tilde{q} = \mathrm{diag}(q_1, q_2, q_3)$. A solution to the precession equations in the three-dimensional space of angular momentum components (I_1, I_2, I_3) must lie in the intersection of the surface of a sphere of radius $\sqrt{\vec{I} \cdot \vec{I}}$, $I_1^2 + I_2^2 + I_3^2 = \vec{I} \cdot \vec{I}$, and the surface of the conic section

$$q_1I_1^2 + q_2I_2^2 + q_3I_3^2 = X_3. \tag{31}$$

The coefficients of this equation for a conic section cannot all have the same sign because the quadrupole moment is traceless, $\sum_k q_k = 0$. When two coefficients are positive and one is negative, the shape is oblate like; when two are negative and one is positive, the shape is prolate like. Therefore, the solution curves to the precession equation in the angular momentum space

lie on the one-dimensional curve defined by the intersection of a sphere and a hyperboloid. This $su(3)$ dynamical system is integrable.

Although both a rotating classical rigid body and rotating $su(3)$ system obey the Euler precession equation, there is a significant difference. The classical rigid body always has positive moments of inertia and the conserved energy equation defines an ellipsoid. Classical rotor solutions are defined by the intersection of a sphere with the inertia ellipsoid.

3. Conclusion

The quantum mechanical wavefunctions of the Hamiltonian self-adjoint operator corresponding to the energy function $\mathcal{E}$ used in this paper are challenging to both calculate numerically and interpret physically and geometrically. The $su(3)$ mean field method for this energy is a simple mathematical problem whose analytic solutions are easy to understand and relate to a classical rotor [27].

These compelling advantages persist for more complicated $su(3)$ energy functions, albeit the very simple physical picture of periodic mean field solutions is lost. Suppose the energy function $\mathcal{E}' = a\vec{l}\cdot\vec{l} + bX_3 + cX_4$ includes the quartic term from the integrity basis, $X_4 = \mathrm{tr}(lq^2l) + (\vec{l}\cdot\vec{l})(q\cdot q)$. The Hamiltonian vector field corresponding to the function $f = X_4$ is

$$Z_f[\rho] = l^2q + ql^2 - \tfrac{2}{3}X_3Id + 2(\vec{l}\cdot\vec{l})q + 2\mathrm{i}(lq^2 + q^2l - \mathrm{tr}(q^2)l). \tag{32}$$

The energy function $\mathcal{E}'$ is a rotational scalar so it is integrable in the sense of Liouville. The mean field solutions are conditionally periodic windings on the three-dimensional torus that is the level surface in the six-dimensional compact manifold $\mathcal{M}_\varrho$ of the involutive set of independent functions $\{\mathcal{E}', (\vec{l}\cdot\vec{l}), l_3\}$. A transformation to the principal axis submanifold $\mathcal{M}_\varrho$ yields the dynamical system of equations (23). Equation (26) determines the angular velocity; it is a function of both the quadrupole deformations q_k and the angular momentum components I_k. But, the precession equation (24) is now coupled nontrivially to the axis length equation because the axis lengths are not constant. From equation (25) the vibrations of the axis lengths are not zero when the real constant $c \neq 0$,

$$\frac{\mathrm{d}}{\mathrm{d}t}q_k = \frac{c}{2}(I^2[I,\tilde{q}] + [I,\tilde{q}]I^2)_{kk}. \tag{33}$$

Any dynamical symmetry algebra $\mathfrak{g}$ determines a mean field theory. The model densities are the points of one coadjoint orbit $\mathcal{O}_\varrho$ of the dynamical symmetry group in the algebra dual space $\mathfrak{g}^*$. The symplectic structure on this coadjoint orbit yields the mean field Hamiltonian $h[\rho]$ from a model energy function $\mathcal{E}(\rho)$. The time development of the density is a Hamiltonian dynamical system on the coadjoint orbit. This semi-classical description for any dynamical symmetry algebra $\mathfrak{g}$ offers advantages similar to $su(3)$ mean field applications, i.e., a transparent physical picture and a tractable mathematical theory.

When the dimension of the algebra $\mathfrak{g}$ is large, representation theory may become intractable and the mean field approximation is the only useful method available. For a noncompact algebra, the irreducible representations are infinite dimensional, while the dimension of a coadjoint orbit is less than the finite dimension of the algebra. For a matrix algebra, calculations in the mean field approximation involves only matrix multiplications; $su(3)$ mean field theory requires matrix operations with 3×3 matrices.

What is the relationship between the semi-classical mean field method and the quantum mechanical representation theory of a dynamical symmetry algebra $\mathfrak{g}$? Starting from integral coadjoint orbits, the unitary irreducible representations of $\mathfrak{g}$ may be constructed via geometric quantization [22–24]. The integral orbits satisfy a generalization of the Bohr–Sommerfeld

quantization rules. For example, the $su(3)$ integral coadjoint orbits are those for which λ and μ are non-negative integers.

Kirillov's metatheorem asserts that all the properties of a unitary irreducible representation are encoded in the symplectic geometry of its integral coadjoint orbits. A typical problem in representation theory is to decompose an irreducible representation of an algebra into a direct sum of irreducible subspaces of some compact subalgebra. The assertion of Kirillov about solving such a problem for the most general Lie algebra may be too optimistic [28], yet there are many encouraging results [22]. One result for $su(3)$ is that the range of the angular momentum in a coadjoint orbit is bounded from above by $\lambda + \mu$ which agrees with representation theory for integral orbits. Yet an unsolved problem for $su(3)$ is to determine the multiplicity of a given angular momentum value in a representation space from the coadjoint orbit data. The solution to the multiplicity problem is, of course, well known using standards methods of representation theory. But an understanding of the problem from a strictly coadjoint orbit perspective might shed significant light on the mean field method's relationship with quantum mechanics. Such understanding would not only clarify matters for $su(3)$, but also for other algebraic mean field models and Hartree–Fock.

The energy function in group theoretical models is approximated usually by a rotationally invariant polynomial of the algebra generators. The polynomial coefficients are chosen to attain a good fit to experimental energy levels and transition rates. The generalized Hohenberg–Kohn theorem [29, 30] shows that there *exists* an energy function on any dual space $\mathfrak{g}^*$ whose global minimum is the density of the exact ground state wavefunction. But the theorem does not provide a method for the energy function's explicit construction. This theorem indicates that the coadjoint orbit method has the potential to be an exact theory in some respects. The construction of the exact energy function in traditional Hohenberg–Kohn density functional theory continues to stimulate the efforts of many researchers, especially in quantum chemistry.

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