$SU(3)$ mean field Hamiltonian

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Abstract
The $su(3)$ mean field approximation describes collective nuclear rotation in a density matrix formalism. The densities $\rho = q - \mathrm{i}\,l/2$ are 3×3 Hermitian matrices in the $su(3)$ dual space, where q is the expectation of the quadrupole moment and l is the expectation of the angular momentum. The mean field approximation restricts these densities to a level surface of the $su(3)$ Casimirs. Each level surface is a coadjoint orbit of the canonical transformation group $SU(3)$. For each density ρ, the $su(3)$ mean field Hamiltonian $h[\rho]$ is an element of the $su(3)$ Lie algebra. A model $su(3)$ energy functional and the symplectic structure on the coadjoint orbit determine uniquely the $su(3)$ mean field Hamiltonian. The densities in time-dependent $su(3)$ mean field theory obey the dynamical equation $\mathrm{i}\,\dot{\rho} = [h[\rho], \rho]$ on a coadjoint orbit. The cranked mean field Hamiltonian is $h_\Omega = h + \mathrm{i}\,\Omega$, where Ω is the angular velocity of the rotating principal axis frame. A rotating equilibrium density $\tilde{\rho}$ in the body-fixed frame is a self-consistent solution to the equation $[h_\Omega[\tilde{\rho}], \tilde{\rho}] = 0$.

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1. Introduction

Any dynamical symmetry algebra determines two different group theoretical models. One of them is based on the unitary irreducible representations of the algebra where the physical states are vectors in a Hilbert space. The other is mean field theory, where the states are density matrices in the algebra's dual space.

The Lie algebra $u(n)$ of all one-body operators in an n-dimensional single-particle valence space illustrates best the two approaches [1, 2]. It is the fundamental algebraic structure underlying both the shell model and Hartree–Fock theory. In the shell model the quantum states span the fully antisymmetrized unitary irreducible representation of the group $U(n)$. In Hartree–Fock the role of the unitary group and its Lie algebra has three essential aspects. First, the densities are elements of the dual space of the Lie algebra. A density matrix ρ is defined by the expectations of the $u(n)$ generators. Second, $U(n)$ is a transformation group on the dual space. A density ρ is transformed by $g \in U(n)$ into the density $g\rho g^{-1}$. Third, the mean field approximation restricts the model densities to one coadjoint orbit of the unitary group.

The orbit containing the density ρ consists of ρ and all the transformed densities $g\rho g^{-1}$ as g ranges over the entire group $U(n)$. The idempotent density matrices, $\rho^2 = \rho$, which correspond to Slater determinants, form a single coadjoint orbit. These three essential ingredients may be used to construct a mean field theory for the densities of any group theoretical model.

A $su(3)$ 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. 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 dual space $su(3)^*$ of the Lie algebra consists of all such density matrices.

The Lie group $SU(3)$ consists of the complex 3×3 unitary matrices with unit determinant. On the dual space, the coadjoint action is the $SU(3)$ group transformation, $\mathrm{Ad}_g^*\rho \equiv g\rho g^{-1}$ for $g \in SU(3)$ and $\rho \in su(3)^*$ [3]. Because any Hermitian matrix can be diagonalized by a unitary matrix, each $SU(3)$ 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

$$\varrho = \frac{1}{3}\begin{pmatrix} -\lambda + \mu & 0 & 0 \\ 0 & -\lambda - 2\mu & 0 \\ 0 & 0 & 2\lambda + \mu \end{pmatrix}. \tag{1.1}$$

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 (1.1) is the density corresponding to a highest-weight vector of an irreducible $SU(3)$ representation [4, 5]. On the other hand, starting from such integral coadjoint orbits, the unitary irreducible representations of $su(3)$ can be constructed via geometric quantization [3, 6–9].

The $su(3)$ mean field approximation restricts the model densities to one coadjoint orbit, denoted by $\mathcal{O}_\varrho$, containing the diagonal density ϱ,

$$\mathcal{O}_\varrho = \{\rho = \mathrm{Ad}_g^*\varrho = g\varrho g^{-1} \in su(3)^* | g \in SU(3)\}. \tag{1.2}$$

The dual space $su(3)^*$ is a disjoint union of the coadjoint orbits $\mathcal{O}_\varrho$ as ϱ ranges over the orbit representatives (1.1). The restriction to a single coadjoint orbit in the density space is the mathematical expression of $SU(3)$ dynamical symmetry in a mean field theory. It is analogous to the restriction to a single irreducible representation for a dynamical symmetry in the shell model.

An energy functional $\mathcal{E}[\rho]$ is a real-valued functional of the density. According to the generalized Hohenberg–Kohn theorem of density functional theory, there exists a $su(3)^*$ energy functional whose minimum is the exact $su(3)$ ground state density [10, 11]. It was shown in an earlier companion paper [12] that the critical points of an $su(3)$ energy functional $\mathcal{E}$ restricted to the surface $\mathcal{O}_\varrho$ determine rotational bands. The aim of this paper is to derive the $SU(3)$ mean field Hamiltonian $h[\rho]$ from the energy functional. For each point ρ, the mean field Hamiltonian $h[\rho]$ is an $su(3)$ Lie algebra element.

The symplectic geometry of a coadjoint orbit is crucial to the determination of the mean field Hamiltonian [13]. An important mathematical result, developed and used by Souriau [6], Kostant [7] and Kirillov [8], is that the coadjoint orbits of a Lie group are symplectic manifolds. The relevance of symplectic geometry to many-body quantum physics is evident in Hartree–Fock [1, 2]. Given two Hermitian one-body operators $\hat{A}$ and $\hat{B}$ and a normalized Slater determinant Φ, define the form ω at Φ as the expectation of the one-body commutator $[\hat{A}, \hat{B}]$ in the state Φ,

$$\omega_\Phi(\hat{A}, \hat{B}) = -\mathrm{i}\langle\Phi| [\hat{A}, \hat{B}] |\Phi\rangle. \tag{1.3}$$

This form is real valued, bilinear and antisymmetric in $\hat{A}$ and $\hat{B}$. If $\hat{H}$ is the exact Hamiltonian, the Hartree–Fock Hamiltonian $\hat{h}$ at Φ is a one-body Hermitian operator satisfying

$$\omega_\Phi(\hat{A}, \hat{h}) = -\mathrm{i} \langle \Phi | [\hat{A}, \hat{H}] | \Phi \rangle \tag{1.4}$$

for all one-body Hermitian operators $\hat{A}$. The one-body operator $\hat{h}$ is not determined uniquely because any pure particle–particle or hole–hole one-body operator may be added to it without altering the equality in equation (1.4). The nonuniqueness of the Hartree–Fock Hamiltonian has a geometrical interpretation.

Choose some orthonormal basis for the n-dimensional single-particle valence space and let A denote the Hermitian matrix in $u(n)$ associated with the one-body operator $\hat{A}$. With respect to the basis, let ρ denote the idempotent density matrix corresponding to the determinant Φ. The form (1.3) can be expressed alternatively as

$$\omega_\rho(A, B) = -\mathrm{i}\,\mathrm{tr}\,(\rho\,[A, B]). \tag{1.5}$$

Any traceless Hermitian matrix A defines a curve

$$\rho(\epsilon) = \exp(-\mathrm{i}\epsilon A)\,\rho\,\exp(\mathrm{i}\epsilon A) \qquad -\infty < \epsilon < \infty \tag{1.6}$$

through the point ρ in the orbit of idempotent densities. Let $\bar{A}$ denote the tangent to this curve. A pure particle–particle plus hole–hole one-body operator $\hat{A}$ determines a zero-tangent vector because the curve $\rho(\epsilon) = \rho$ becomes a fixed point. Such null vectors correspond to the Hermitian matrices A that commute with ρ. The algebra elements associated with the null tangent vectors form a subalgebra of $u(n)$, called the isotropy subalgebra at ρ:

$$u(n)_\rho = \{A \in u(n) \mid [A, \rho] = 0\}. \tag{1.7}$$

A vector is null, $\bar{A} = 0$, if and only if the matrix $A \in u(n)_\rho$. When A and B differ by an element of $u(n)_\rho$, they determine the same tangent vector at ρ. The form ω_ρ is well defined on the tangent space at ρ because $\omega_\rho(A_1, B_1) = \omega_\rho(A_2, B_2)$ whenever $A_1 - A_2$ and $B_1 - B_2$ are elements of the isotropy subalgebra.

The form ω_ρ may be regarded geometrically as a rank two covariant tensor,

$$\omega_\rho(\bar{A}, \bar{B}) = -\mathrm{i}\,\mathrm{tr}(\rho\,[A, B]) \tag{1.8}$$

for each pair of tangent vectors $\bar{A}$ and $\bar{B}$ at the idempotent density ρ. The tensor ω_ρ is nondegenerate, i.e.

$$\omega_\rho(\bar{A}, \bar{B}) = 0 \quad \text{for all } \bar{A} \quad \Leftrightarrow \quad \bar{B} = 0. \tag{1.9}$$

Hence, at the point ρ, the tangent vector $\bar{h}$ corresponding to the Hartree–Fock Hamiltonian $\hat{h}$ is determined uniquely by the nondegenerate tensor ω_ρ. Due to the Jacobi identity the form ω is closed. By definition, a symplectic manifold is a smooth manifold equipped with a closed, nondegenerate, antisymmetric, second-rank covariant tensor [13]. Thus, the manifold of idempotent densities is a symplectic manifold.

The right-hand side of equation (1.4) has a geometrical interpretation too. The energy functional $\mathcal{E}$ at the idempotent density ρ is the expectation of the Hamiltonian $\hat{H}$ in the corresponding determinantal state Φ. The derivative of the energy functional in the direction $\bar{A}$ is the rate of change of the energy along the curve $\rho(\epsilon)$,

$$\begin{aligned}
\mathrm{d}\mathcal{E}(\bar{A})[\rho] &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} \mathcal{E}[\rho(\epsilon)]|_{\epsilon=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}\epsilon} \langle \mathrm{e}^{-\mathrm{i}\epsilon\hat{A}}\Phi | \hat{H} | \mathrm{e}^{-\mathrm{i}\epsilon\hat{A}}\Phi \rangle |_{\epsilon=0}.
\end{aligned} \tag{1.10}$$

But this derivative is the negative of the right-hand side of equation (1.4). Hence the Hartree–Fock Hamiltonian is determined by the equation

$$\omega_\rho(\bar{h}[\rho], \bar{A}) = \mathrm{d}\mathcal{E}(\bar{A})[\rho] \qquad\qquad (1.11)$$

for all directions $\bar{A}$ tangent at ρ to the coadjoint orbit of idempotent densities.

The construction of the Hartree–Fock Hamiltonian generalizes to any Lie algebra model. Since the coadjoint orbits of any Lie algebra are symplectic manifolds, the form ω is nondegenerate on each orbit. Given an energy functional of the density, the fundamental equation (1.11) determines a unique vector field $\bar{h}[\rho]$, which is the mean field Hamiltonian. In particular, the symplectic geometry of the $su(3)$ coadjoint orbits determines the $su(3)$ mean field Hamiltonian from the $su(3)$ energy functional using equation (1.11).

It is interesting to note that classical mechanics, in its contemporary formulation, is expressed in terms of symplectic geometry [14]. Phase spaces are symplectic manifolds. It is the symplectic form that allows the Poisson bracket of any two functions on a phase space to be computed. It is the symplectic form that gives the 'twist' to the gradient of the Hamiltonian and turns it into a Hamiltonian vector field—the tangent at each point to the solution curve of a dynamical problem. Canonical transformations are those that preserve the symplectic form.

Darboux's theorem guarantees that finite-dimensional symplectic manifolds are even dimensional and are locally isomorphic to phase spaces $\mathbb{R}^{2n}$, i.e. in the vicinity of each point on the $2n$-dimensional manifold a complete set of n generalized position and momentum coordinates can be introduced, in which the symplectic form and Poisson bracket take their canonical forms [14]. But these coordinates are complicated expressions, in general, that do not have a clear physical meaning. Mean field theory is expressed in a more direct physical and geometrical way in terms of algebra generators without using canonical coordinates. In some respects the formulation becomes more abstract, but the gain in physical insight offsets the loss of a more elementary theoretical framework.

A symplectic manifold and an energy function defined on it determine a Hamiltonian dynamical system. Thus, different cases of symplectic manifolds lead to many familiar examples [14]: classical mechanics is built on a cotangent bundle, quantum mechanics can be viewed as a Hamiltonian dynamical system on projective Hilbert space and Hartree–Fock mean field theory as a Hamiltonian dynamical system on the space of normalized Slater determinants [1]. Coadjoint orbits arise in symplectic reduction of a classical mechanical system with symmetry [14].

The mathematical set-up for the Hamiltonian formulation of classical mechanics and algebraic mean field theories is the same, yet they are two very distinct physical pictures. The key is the different microscopic interpretations attached to the points of a coadjoint orbit in the two cases. Formally this is achieved by the moment (or momentum) map [6]. For a classical mechanical model, the moment map is between the phase space $\mathbb{R}^{6A}$ of an A particle system and the coadjoint orbits, while for a quantum mechanical mean field model the moment map originates in projective Fock space.

The $su(3)$ coadjoint orbits and their symplectic geometry are reviewed in section 2. A combination of symplectic geometry and the exterior calculus of differential forms enables the explicit computation of the mean field Hamiltonian for any rotational scalar energy. Dynamics on each coadjoint orbit is given by the equation $\mathrm{i}\,\dot{\rho} = [h[\rho], \rho]$. This equation is formally identical to the time-dependent Hartree–Fock equation of motion. This time evolution is a Hamiltonian dynamical system.

Section 3 presents the $su(3)$ mean field approximation in the rotating body-fixed frame. The mean field Hamiltonian is transformed into the Routhian $h_\Omega = h + \mathrm{i}\Omega$ in the principal axis frame. The real antisymmetric matrix Ω is the angular velocity of the principal axis frame. The principal axis densities form a submanifold of a coadjoint orbit consisting of the densities $\tilde{\rho}$ with a diagonal quadrupole moment. Rotating equilibrium solutions are zeros of the Routhian vector field, $[h_\Omega[\tilde{\rho}], \tilde{\rho}] = 0$. This equation must be solved self-consistently for the equilibrium

principal axis density $\tilde{\rho}$. Analytical solutions, which coincide with the rotational bands found in prior work [12], are obtained in section 4 for many interesting special cases.

2. Symplectic geometry

2.1. Preliminaries

The Lie algebra $su(3)$ is the space of Hermitian traceless 3×3 matrices

$$su(3) = \{Z \in M_3(\mathbb{C}) | Z^\dagger = Z, \text{ tr } Z = 0\}. \tag{2.1}$$

The Lie algebra $so(3)$ of the rotation group consists of the antisymmetric matrices. Suppose σ is a unitary, but not necessarily irreducible, representation of $su(3)$ on some Hilbert space $\mathcal{H}$: $[\sigma(Z), \sigma(W)] = \sigma([Z, W])$ for matrices $Z, W \in su(3)$. The representation may correspond to any physical realization of $su(3)$ dynamical symmetry, for example the Elliott oscillator-based theory [4], the interacting boson $su(3)$ limit [5], pseudo-$su(3)$ symmetry in medium-mass isotopes [15, 16] or cluster model $su(3)$ symmetry [17, 18]. The quantum vector angular momentum operator $\hat{L}$ on $\mathcal{H}$ is the representation of the antisymmetric matrices, and the quantum $su(3)$ quadrupole operator $\hat{\mathcal{Q}}^{(2)}$ on $\mathcal{H}$ is the representation of the traceless symmetric matrices,

$$
\begin{aligned}
\hat{L}_{ij} &= \varepsilon_{ijk}\hat{L}_k = \sigma[-\mathrm{i}(E_{ij} - E_{ji})] \\
\hat{\mathcal{Q}}^{(2)}_{ij} &= \sigma[(E_{ij} + E_{ji})/2 - (1/3)\delta_{ij}Id]
\end{aligned}
\tag{2.2}
$$

where Id denotes the 3×3 identity matrix and E_{ij} is the 3×3 matrix whose entries vanish except for the intersection of row i with column j where the matrix entry is one.

For each normalized state vector $\Psi \in \mathcal{H}$ the expectations of the operators

$$
\begin{aligned}
q_{jk} &= \langle\Psi|\hat{Q}^{(2)}_{jk}|\Psi\rangle \\
l_{jk} &= \langle\Psi|\hat{L}_{jk}|\Psi\rangle
\end{aligned}
\tag{2.3}
$$

define a real symmetric traceless matrix q and a real antisymmetric matrix l. The 'density' matrix corresponding to Ψ is defined as the Hermitian traceless matrix $\rho = q - \frac{1}{2}\mathrm{i}l$. In terms of it, the expectation of a general element of the $su(3)$ operator algebra is

$$\langle\rho, Z\rangle \equiv \text{tr}(\rho Z) = \langle\Psi|\sigma(Z)|\Psi\rangle \tag{2.4}$$

for all $Z \in su(3)$. In fact each traceless Hermitian density matrix ρ defines a real-valued linear functional on the matrix Lie algebra $su(3)$, namely, $\langle\rho, Z\rangle \equiv \text{tr}(\rho Z)$ for all $Z \in su(3)$. The set of all such linear functionals ρ is called the dual space of $su(3)$ and is denoted by $su(3)^*$. The dimension of the dual space equals the dimension of the algebra, $\dim su(3)^* = \dim su(3) = 8$.

The mapping from the Hilbert space to the dual space is called the moment map $M : \mathcal{H} \longrightarrow su(3)^*$, where the density corresponding to the vector Ψ is $\rho = M(\Psi)$ [6, 14]. When Ψ_{HW} is a highest-weight vector for an irreducible representation of $su(3)$, the corresponding density $M(\Psi_{HW})$ is the diagonal matrix ϱ of equation (1.1), where λ, μ are non-negative integers that label the $su(3)$ irrep.

The group $SU(3)$ is related by exponentiation to the algebra $su(3)$, $\exp: su(3) \longrightarrow SU(3)$. When $Z \in su(3)$, $\exp(\mathrm{i}\epsilon Z) \in SU(3)$ is a curve through the group identity. Because $SU(3)$ is simply connected, the algebra representation lifts to a unique group representation, also denoted by σ, that satisfies $\sigma[\exp(\mathrm{i}Z)] = \exp[\mathrm{i}\sigma(Z)]$.

The group $SU(3)$ transforms a normalized vector Ψ from the representation space $\mathcal{H}$ into $\sigma(g)\Psi$. The corresponding density $\rho = M(\Psi)$ transforms into $M(\sigma(g)\Psi) = g\rho g^{-1} \equiv \text{Ad}_g^*\rho$ under the group action [12]. Although it may be difficult to compute the transformed state $\sigma(g)\Psi$ explicitly, the transformed density is just a product of three 3×3 matrices that is

independent of the representation σ. The simplicity of the coadjoint action $\mathrm{Ad}^*_g \rho$ is a principal reason for the tractability of $su(3)$ mean field theory.

2.2. Coadjoint orbits

The model densities in the $su(3)$ mean field approximation are restricted to a coadjoint orbit $\mathcal{O}_\varrho$ in the dual space. The orbit representative ϱ is given by equation (1.1).

The coadjoint orbit is a homogeneous space; i.e., $\mathcal{O}_\varrho$ is diffeomorphic to the coset space $SU(3)/SU(3)_\varrho$, where $SU(3)_\varrho$ denotes the isotropy subgroup at ϱ. The isotropy subgroup consists of the coadjoint transformations that fix ϱ,

$$SU(3)_\varrho = \{h \in SU(3) | h\varrho = \varrho h\}. \tag{2.5}$$

The diffeomorphism $\mathcal{O}_\varrho \simeq SU(3)/SU(3)_\varrho$ is easy to see. Consider the map $\varphi : SU(3) \longrightarrow \mathcal{O}_\varrho$ defined by $g \longmapsto \varphi(g) = \mathrm{Ad}^*_g \varrho$. The map is onto, but it is not one to one. Two different group elements $g_1 \neq g_2$ have the same image under φ, $\varphi(g_1) = \varphi(g_2)$, if and only if $g_2^{-1} g_1$ is an element of the isotropy subgroup at ϱ, $g_2^{-1} g_1 \in SU(3)_\varrho$, which, by definition, means that the two elements belong to the same coset $g_1 SU(3)_\varrho = g_2 SU(3)_\varrho$. Thus the dimension of $\mathcal{O}_\varrho$ is generally less than the dimension of the group, $\dim \mathcal{O}_\varrho = \dim SU(3) - \dim SU(3)_\varrho$.

For the typical diagonal orbit representative, equation (1.1), the isotropy subgroup is the torus $U(1) \times U(1)$, and the coadjoint orbit $\mathcal{O}_\varrho \cong SU(3)/[U(1) \times U(1)]$. The dimension of the generic orbit space is $\dim SU(3) - \dim SU(3)_\varrho = 6$. In the special case of two equal eigenvalues, $\lambda = 0$ or $\mu = 0$, the isotropy subgroup is $U(2)$ and the orbit's dimension equals four.

The orbit representatives ϱ of equation (1.1) are a convenient, but essentially arbitrary choice. When ρ is any point on the coadjoint orbit $\mathcal{O}_\varrho$, the coadjoint orbit through it is the same, $\mathcal{O}_\rho = \mathcal{O}_\varrho$. The isotropy subgroup at $\rho = \mathrm{Ad}^*_g \varrho$ is different from the isotropy subgroup at ϱ, but the two isotropy subgroups are isomorphic. The group isomorphism is the adjoint group transformation, $\mathrm{AD}_g : SU(3)_\varrho \to SU(3)_\rho$, $\mathrm{AD}_g h = ghg^{-1}$.

There are various adjoint group transformations acting on different, but related, domains; for example, AD_g acts on the Lie group, Ad^*_g is a linear transformation acting on the dual space to the Lie algebra, Ad_g is a linear transformation of the Lie algebra [19]. In the special case of a semisimple matrix Lie group like $SU(3)$, every adjoint transformation simplifies to matrix conjugation. For non-semisimple algebras the coadjoint action is not matrix conjugation. Although it may seem pedantic for $su(3)$, the distinctions among the various adjoint maps are essential for future applications.

Each element Z of the $su(3)$ Lie algebra determines a tangent vector field $\bar{Z}$ to the coadjoint orbits. 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 $\mathrm{Ad}^*_{\zeta(\epsilon)} \rho = \exp(-\mathrm{i}\epsilon Z) \rho \exp(\mathrm{i}\epsilon Z)$ lies in the coadjoint orbit through ρ. The tangent to this curve is denoted by $\bar{Z}$.

The Lie algebra of the isotropy subgroup $SU(3)_\rho$ is

$$su(3)_\rho = \{Z \in su(3) | [Z, \rho] = 0\}. \tag{2.6}$$

If Z is an element of the Lie algebra $su(3)_\rho$ of the isotropy subgroup at ρ, then $\bar{Z}$ is a zero-tangent vector at ρ because the curve $\exp(-\mathrm{i}\epsilon Z) \rho \exp(\mathrm{i}\epsilon Z)$ is a fixed point ρ. For example, at each point ρ, $Z = \rho$ is a null tangent vector, $\bar{\rho} = 0$. When the difference between two Lie algebra elements is an element of the isotropy subalgebra at ρ, the corresponding tangent vectors are equal:

$$\bar{Z} = \bar{W} \qquad \text{if and only if} \quad Z - W \in su(3)_\rho. \tag{2.7}$$

Therefore, by definition, the tangent space to the coadjoint orbit at ρ can be identified with the vector space $su(3)$ modulo the isotropy subalgebra at ρ, $su(3)/su(3)_\rho$.

2.3. Symplectic form

For two tangent vectors, $\bar{Z}$ and $\bar{W}$, to the coadjoint orbit at ρ, define the symplectic form by [3,8]

$$\omega_\rho(\bar{Z}, \bar{W}) = -\mathrm{i}\langle\rho, [Z, W]\rangle. \tag{2.8}$$

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 $Z - Z' \in su(3)_\rho$ and $W - W' \in su(3)_\rho$. The form ω is a second-rank covariant tensor on each coadjoint orbit. It is also nondegenerate; i.e., $\omega_\rho(\bar{Z}, \bar{W}) = 0$ for all W in the $su(3)$ Lie algebra if and only if $\bar{Z}$ is a null tangent vector at ρ or $Z \in su(3)_\rho$. Since an antisymmetric form can only be nondegenerate on an even-dimensional vector space, each coadjoint orbit is even dimensional. In fact each coadjoint orbit is a symplectic manifold because the form ω is closed [8]. Canonical coordinates can be introduced for each coadjoint orbit, but it is not always convenient to work with them as discussed in the introduction.

A one-form at ρ is, by definition, a real-valued linear functional of the tangent space $su(3)/su(3)_\rho$. For any one-form α, the symplectic form determines a tangent vector, denoted by $\alpha^\sharp$, from the condition

$$\omega_\rho(\alpha^\sharp, \bar{W}) = \alpha(\bar{W}) \qquad \text{for all tangents } \bar{W} \text{ at } \rho. \tag{2.9}$$

The 'sharp' notation indicates that the components of the tangent vector $\alpha^\sharp$ are given by raising the indices of the one-form α via the tensor ω. Equation (2.9) determines uniquely the vector $\alpha^\sharp$ because the symplectic form is nondegenerate.

Suppose f is any smooth function on the coadjoint orbit $\mathcal{O}_\rho$. The differential $\mathrm{d}f$ is a one-form at ρ. Given any tangent vector $\bar{W}$ at ρ, the derivative of f in the direction of $\bar{W}$ is a linear function of $\bar{W}$,

$$\mathrm{d}f(\bar{W}) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} f(\exp(-\mathrm{i}\epsilon W)\rho \exp(\mathrm{i}\epsilon W))|_{\epsilon=0}. \tag{2.10}$$

The vector $\mathrm{d}f^\sharp$ at ρ is determined uniquely by equation (2.9). Hence, each function f defines a vector field $\mathrm{d}f^\sharp$ on each coadjoint orbit satisfying

$$\omega_\rho(\mathrm{d}f^\sharp, \bar{W}) = \mathrm{d}f(\bar{W}) \tag{2.11}$$

for all directions $\bar{W}$ tangent to the coadjoint orbit at ρ. The vector field $\mathrm{d}f^\sharp$ is called the Hamiltonian vector field associated with the smooth function f. Since each tangent vector can be expressed as a Lie algebra element, there exists a Lie algebra element Z_f such that $\mathrm{d}f^\sharp = \bar{Z}_f$. Two Lie algebra elements Z_f and Z'_f that define the same Hamiltonian vector field $\mathrm{d}f^\sharp$ differ by an element of the isotropy subalgebra $su(3)_\rho$. 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. Note that the vector field $\mathrm{d}f^\sharp$ is called a 'Hamiltonian' vector field for any smooth function f, which is not necessarily the energy function.

For each Lie algebra element Z there is an elementary function f_Z on the dual space given by $f_Z(\rho) = \langle\rho, Z\rangle$. The value of the function f_Z at ρ is the expectation of the physical observable corresponding to Z when the system's state has the $su(3)$ density ρ.

Proposition. *The Hamiltonian vector field associated with an elementary function f_Z for $Z \in su(3)$ is $\mathrm{d}f_Z^\sharp = \bar{Z}$.*

To prove this calculate the derivative of f_Z in the direction $\bar{W}$,

$$\begin{aligned}
\mathrm{d}f_Z(\bar{W}) &= \frac{\mathrm{d}}{\mathrm{d}\epsilon} f_Z[\mathrm{e}^{-\mathrm{i}\epsilon W}\rho\,\mathrm{e}^{\mathrm{i}\epsilon W}]|_{\epsilon=0} \\
&= \frac{\mathrm{d}}{\mathrm{d}\epsilon}\,\mathrm{tr}\,(\mathrm{e}^{-\mathrm{i}\epsilon W}\rho\,\mathrm{e}^{\mathrm{i}\epsilon W}Z)|_{\epsilon=0} \\
&= -\mathrm{i}\,\mathrm{tr}\,(W\rho Z - \rho WZ) \\
&= \omega_\rho(\bar{Z}, \bar{W}).
\end{aligned} \tag{2.12}$$

By definition of the Hamiltonian vector field,

$$\omega_\rho(\mathrm{d}f_Z^\sharp, \bar{W}) = \omega_\rho(\bar{Z}, \bar{W}). \tag{2.13}$$

Since ω_ρ is nondegenerate, the Hamiltonian vector field $\mathrm{d}f_Z^\sharp = \bar{Z}$.

In particular the Hamiltonian vector fields associated with the angular momentum and Elliott quadrupole moment are

$$\begin{aligned}
\mathrm{d}l_{ij}^\sharp &= -\mathrm{i}(E_{ij} - E_{ji}) \\
\mathrm{d}q_{ij}^\sharp &= (E_{ij} + E_{ji})/2 - (1/3)\delta_{ij}Id.
\end{aligned} \tag{2.14}$$

When $Z = E_{ji} - (1/3)\delta_{ji}Id \in su(3)$, the elementary function $f_Z(\rho) = \rho_{ij}$, and, therefore,

$$\mathrm{d}\rho_{ij}^\sharp = E_{ji} - (1/3)\delta_{ji}Id. \tag{2.15}$$

2.4. Dynamics

Let $\mathcal{E}$ be a smooth energy functional on a coadjoint orbit $\mathcal{O}_\rho$. The mean field Hamiltonian $h[\rho]$ at ρ is an element of the Lie algebra $su(3)$ such that the vector field $\overline{h[\rho]} = \mathrm{d}\mathcal{E}^\sharp$ at ρ satisfies

$$\omega_\rho(\overline{h[\rho]}, \bar{W}) = \mathrm{d}\mathcal{E}(\bar{W}) \tag{2.16}$$

for all $W \in su(3)$. The nondegeneracy of the symplectic form guarantees that there exists a unique solution $\overline{h[\rho]}$ to this equation. Note that the mean field Hamiltonian is a smooth function of the density with values in the Lie algebra.

The time evolution of the $su(3)$ density is determined by a geometrical condition: a solution curve $\rho(t)$ must be an integral curve of the $su(3)$ Hamiltonian vector field $\overline{h[\rho]}$. Thus the tangent to a solution curve is everywhere equal to the Hamiltonian vector field. Pick a time t and set $\rho = \rho(t)$. Let $\gamma_1(\epsilon) = \rho(t + \epsilon)$ denote the solution curve through ρ. By definition, the mean field Hamiltonian $h[\rho]$ is the tangent at ρ to the curve $\gamma_2(\epsilon) = \exp(-\mathrm{i}\epsilon h[\rho])\rho\exp(\mathrm{i}\epsilon h[\rho])$. The integral curve condition requires that the tangents to the curves $\gamma_1(\epsilon)$ and $\gamma_2(\epsilon)$ be equal at $\epsilon = 0$,

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\gamma_1(\epsilon)|_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\gamma_2(\epsilon)|_{\epsilon=0} \qquad \text{or} \qquad \mathrm{i}\dot{\rho} = [h[\rho], \rho]. \tag{2.17}$$

The $su(3)$ mean field dynamical equation is formally identical to the time-dependent Hartree–Fock equation.

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 is expressed

$$\dot{q} = \tfrac{1}{2}[l, \mathrm{Re}\,h] - [q, \mathrm{Im}\,h] \tag{2.18}$$

$$\dot{l} = -2[q, \mathrm{Re}\,h] - [l, \mathrm{Im}\,h]. \tag{2.19}$$

2.5. Integrity basis Hamiltonian vector fields

Any rotational scalar function is a function of the $su(3)$ integrity basis elements which are a complete set of functionally independent rotational scalars. An integrity basis for $su(3)$ consists of the two Casimirs, the squared length of the angular momentum, and the scalars $X_3 = \text{tr}(lql)$ and $X_4 = \text{tr}(lq^2l) + (\vec{l} \cdot \vec{l})(q \cdot q)$ [20]. In this section, the Hamiltonian vector fields for the integrity basis functions are calculated. Using these results, the Hamiltonian vector field associated with the rotational scalar energy function $\mathcal{E}$ can be determined.

The mean field Hamiltonian associated with polynomials of the elementary functions f_Z can be evaluated explicitly using two properties of the mapping $\mathcal{E} \mapsto (d\mathcal{E})^\sharp$: linearity and the Leibniz rule [19]. When $\mathcal{E} = a_1\mathcal{E}_1 + a_2\mathcal{E}_2$ is a linear combination of two functions $\mathcal{E}_1$ and $\mathcal{E}_2$, where a_1, a_2 are real numbers, the mean field Hamiltonian is a linear combination of the vector fields corresponding to $\mathcal{E}_1$ and $\mathcal{E}_2$:

$$(d\mathcal{E})^\sharp = a_1(d\mathcal{E}_1)^\sharp + a_2(d\mathcal{E}_2)^\sharp. \tag{2.20}$$

When $\mathcal{E} = \mathcal{E}_1 \cdot \mathcal{E}_2$ is a product of two functions, $d\mathcal{E} = \mathcal{E}_1 \cdot d\mathcal{E}_2 + \mathcal{E}_2 \cdot d\mathcal{E}_1$, because the exterior derivative d is a derivation. Since ω is bilinear,

$$(d\mathcal{E})^\sharp = \mathcal{E}_1 \cdot (d\mathcal{E}_2)^\sharp + \mathcal{E}_2 \cdot (d\mathcal{E}_1)^\sharp. \tag{2.21}$$

The squared length of the angular momentum is $\vec{l} \cdot \vec{l} = -(1/2)\text{tr}(l^2) = (1/2)\sum l_{ij}^2$. The corresponding Hamiltonian vector field is

$$\begin{aligned} d(\vec{l} \cdot \vec{l})^\sharp &= \sum l_{ij} dl_{ij}^\sharp \\ &= -i\sum l_{ij}(E_{ij} - E_{ji}) \\ &= -i(l - l^T) \\ &= -2il. \end{aligned} \tag{2.22}$$

The Hamiltonian vector field of the scalar quadrupole–quadrupole function $q \cdot q = \text{tr}(q^2) = \sum q_{ij}^2$ is calculated similarly

$$d(q \cdot q)^\sharp = 2q. \tag{2.23}$$

The Hamiltonian vector fields of the rotational scalar functions X_3 and X_4 are

$$dX_3^\sharp = 4(q^2 - \tfrac{1}{3}(q \cdot q)Id) \tag{2.24}$$

$$dX_4^\sharp = l^2q + ql^2 - \tfrac{2}{3}X_3 Id + 2(\vec{l} \cdot \vec{l})q + 2i(lq^2 + q^2l - (q \cdot q)l). \tag{2.25}$$

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

$$\mathcal{C}_r(\rho) = \text{tr}\,\rho^r \qquad \text{for} \quad r = 2, 3. \tag{2.26}$$

These functions on the dual space are invariant with respect to the coadjoint transformation, $\mathcal{C}_r(\text{Ad}_g^*\rho) = \mathcal{C}_r(\rho)$; i.e., the Casimir functions are constant on each coadjoint orbit. The Hamiltonian vector fields associated with the Casimir functions are null,

$$d\mathcal{C}_2^\sharp = 2\,\bar{\rho} = 0 \tag{2.27}$$

$$d\mathcal{C}_3^\sharp = 3\,\overline{(\rho^2 - \tfrac{1}{3}\text{tr}\rho^2)} = 0 \tag{2.28}$$

because any power of ρ is a Hermitian matrix that commutes with ρ and its traceless part is an element of the isotropy subalgebra $su(3)_\rho$.

Recall that each Hamiltonian vector field at a point ρ is represented by a Lie algebra element. But the representation is not unique because any element of the isotropy subalgebra at ρ may be added to it without changing the tangent vector. For example, the Hamiltonian vector field associated with the squared length of the angular momentum can be expressed

equivalently as $d(\vec{l} \cdot \vec{l})^\sharp = -2i\bar{l} - 4\bar{\rho} = -4\bar{q}$. Equation (2.24) was simplified by adding a multiple of $dC_3^\sharp$.

The Casimir functions are constant on each coadjoint orbit and their derivatives vanish in all directions tangent to a coadjoint orbit. In particular the values of the Casimirs at the diagonal density (1.1) are

$$\begin{aligned}
C_2(\varrho) &= \tfrac{2}{3}(\lambda^2 + \lambda\mu + \mu^2) \\
C_3(\varrho) &= \tfrac{1}{9}(2\lambda^3 + 3\lambda^2\mu - 3\lambda\mu^2 - 2\mu^3).
\end{aligned} \tag{2.29}$$

To maintain consistency within density matrix theory, the above values of the Casimir functions should not be replaced with their quantum expectations in hopes of an improved theoretical description [12].

3. Principal axis frame

The rotation group $SO(3)$ is a subgroup of the special unitary group $SU(3)$. A density $\rho = q - \tfrac{1}{2}i\,l$ in $su(3)^*$ is transformed by a rotation $R \in SO(3)$ into the density $\mathrm{Ad}_R^*\rho = R\rho R^\mathrm{T} = RqR^\mathrm{T} - \tfrac{1}{2}i\,RlR^\mathrm{T}$. Since any real symmetric matrix can be diagonalized by a rotation matrix, there is an $R \in SO(3)$ such that the rotated quadrupole moment is diagonal,

$$\tilde{q} = RqR^\mathrm{T} = \mathrm{diag}\,(q_1, q_2, q_3). \tag{3.1}$$

The eigenvalues are unique, up to their order, which we fix to be $q_3 \geqslant q_1 \geqslant q_2$. From a geometrical viewpoint, R rotates the laboratory frame into the body-fixed frame in which, by definition, the system's quadrupole moment $\tilde{q}$ is diagonal. At the same time the laboratory angular momentum l is transformed to $I = R\,l\,R^\mathrm{T}$, which is the system's angular momentum projected onto the body-fixed principal axes.

The angular momentum in the body-fixed frame is a pseudovector $\vec{I}$ with components $I_i = \tfrac{1}{2}\varepsilon_{ijk}I_{jk}$. The rotation of the vector angular momentum $\vec{I} = R\vec{l}$ is equivalent to the matrix transformation $I = RlR^\mathrm{T}$. 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 $\tilde{\rho} = \tilde{q} - \tfrac{1}{2}i\,I$ 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,

$$q_1 + q_2 + q_3 = 0 \tag{3.2}$$

$$\sum_k q_k^2 + \tfrac{1}{2}I^2 = C_2(\varrho) \tag{3.3}$$

$$\sum_k q_k^3 - \tfrac{3}{4}\sum_k q_k I_k^2 = C_3(\varrho). \tag{3.4}$$

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

The transformation from a coadjoint orbit $\mathcal{O}_\varrho$ to the principal axis submanifold $\mathcal{M}_\varrho$ is computed efficiently by exploiting the invariance of various rotational scalars. The three principal moments q_k are solutions to the algebraic system [21],

$$\sum_k q_k = 0$$

$$\sum_k q_k^2 = q \cdot q \tag{3.5}$$

$$\sum_k q_k^3 = \operatorname{tr} q^3 = \sum_{ijk} q_{ij} q_{jk} q_{ki}.$$

Taking the exterior derivative of both sides of this system, sharping the one-forms and applying equation (2.14) results in a linear system for the Hamiltonian vector fields $\mathrm{d}q_k^\sharp$ whose solution is

$$(q_k - q_i)(q_k - q_j)\,\mathrm{d}q_k^\sharp = q_k\,q + q^2 - \tfrac{1}{3}(q \cdot q)Id \tag{3.6}$$

for i, j, k cyclic. The rotational scalars that are quadratic in the angular momentum matrix may be expressed in terms of the body-fixed components [22]

$$\sum_k I_k^2 = \vec{l} \cdot \vec{l}$$

$$\sum_k q_k I_k^2 = X_3 \tag{3.7}$$

$$\sum_k q_k^2 I_k^2 = X_4.$$

Applying a strategy similar to the one yielding equations (3.6), the Hamiltonian vector fields $\mathrm{d}I_k^\sharp$ are calculated to be

$$R(\mathrm{d}I_1^\sharp)R^T = \frac{1}{2}\begin{pmatrix} 0 & \frac{I_2}{q_1-q_2} & \frac{I_3}{q_1-q_3} \\ \frac{I_2}{q_1-q_2} & 0 & -2\mathrm{i} \\ \frac{I_3}{q_1-q_3} & 2\mathrm{i} & 0 \end{pmatrix}$$

$$R(\mathrm{d}I_2^\sharp)R^T = \frac{1}{2}\begin{pmatrix} 0 & \frac{I_1}{q_2-q_1} & 2\mathrm{i} \\ \frac{I_1}{q_2-q_1} & 0 & \frac{I_3}{q_2-q_3} \\ -2\mathrm{i} & \frac{I_3}{q_2-q_3} & 0 \end{pmatrix} \tag{3.8}$$

$$R(\mathrm{d}I_3^\sharp)R^T = \frac{1}{2}\begin{pmatrix} 0 & -2\mathrm{i} & \frac{I_1}{q_3-q_1} \\ 2\mathrm{i} & 0 & \frac{I_2}{q_3-q_2} \\ \frac{I_1}{q_3-q_1} & \frac{I_2}{q_3-q_2} & 0 \end{pmatrix}.$$

3.1. Dynamics in the principal axis frame

The Hamiltonian dynamical system on $\mathcal{O}_\varrho$ reduces to a simpler dynamical system on $\mathcal{M}_\varrho$ when the energy functional $\mathcal{E}$ is a rotational scalar. This reduction is analogous to the simplification of classical rigid rotor theory that results from a transformation to the body-fixed system [23]. Another example is 'cranked' Hartree–Fock theory, in which the Slater determinants are interpreted as nuclear states in the rotating body-fixed frame [24]. In classical mechanics and quantum Hartree–Fock theory, dynamics in the noninertial body-fixed frame is determined by the Routhian instead of the inertial laboratory-frame Hamiltonian. In a parallel construction, the rotational dynamics of $su(3)$ densities simplifies in the principal axis frame, and the $su(3)$ mean field Hamiltonian must be transformed into the $su(3)$ Routhian.

Let $R(t) \in SO(3)$ be the time-dependent transformation that rotates the system into the principal axis frame. Define the time-dependent antisymmetric matrix $\Omega = \dot{R}R^T$ in the Lie algebra $so(3)$ of the rotation group. The pseudo-vector $\vec{\omega}$ corresponding to the matrix Ω is the angular velocity vector. 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 (2.17), is equivalent to the following dynamical equation on $\mathcal{M}_\varrho$:

$$i \frac{d\tilde{\rho}}{dt} = [h_\Omega[\tilde{\rho}], \tilde{\rho}],$$ (3.9)

where $h_\Omega[\tilde{\rho}] = Rh[\rho]R^T + i\Omega$ 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 becomes

$$\frac{d}{dt} I = [\Omega, I] + R\dot{l}R^T$$ (3.10)

$$\frac{d}{dt} \tilde{q} = [\Omega, \tilde{q}] + R\dot{q}R^T$$ (3.11)

where $R\dot{l}R^T$ and $R\dot{q}R^T$ are given by equations (2.18), (2.19). These dynamical equations on the principal axis submanifold differ from the equations on the coadjoint orbit by Coriolis terms, namely, the commutators involving the angular velocity matrix.

When the energy $\mathcal{E}$ is invariant with respect to rotations, its derivative in the direction $Z \in so(3)$ vanishes, $d\mathcal{E}(Z) = 0$. From equation (2.16) the mean field Hamiltonian satisfies $\omega_\rho(h[\rho], Z) = 0$ for all antisymmetric Z. According to the dynamical equation on $\mathcal{O}_\varrho$,

$$\begin{aligned} i \langle \dot{\rho}, Z \rangle &= \text{tr}([h[\rho], \rho] Z) \\ &= \text{tr}(\rho [Z, h[\rho]]) \\ &= 0 \end{aligned}$$ (3.12)

for all $Z \in so(3)$. The time rate of change of each angular momentum component is $\dot{l}_{ij} = \langle \dot{\rho}, (E_{ij} - E_{ji}) \rangle = 0$. Hence, the angular momentum is a conserved quantity for a rotationally invariant energy functional, $\dot{l} = 0$. On the principal axis submanifold, the time rate of change of the body-fixed angular momentum obeys the precession equation

$$\begin{aligned} \dot{I} &= [\Omega, I], \\ \frac{d}{dt} \vec{I} &= -\vec{\omega} \times \vec{I}. \end{aligned}$$ (3.13)

Although the precession equation is formally identical to the Euler equation, that fact does not imply rigid body rotation. The reason is that the moments of inertia are not constant. Indeed the deformation depends on the angular momentum due to the mean field constraint to a coadjoint orbit, equations (3.3), (3.4).

Since $\tilde{q}$ is diagonal, the off-diagonal components of the right side of equation (3.11) must vanish,

$$(q_i - q_j) \Omega_{ij} = (R\dot{q}R^T)_{ij} \qquad \text{for} \quad i \neq j.$$ (3.14)

The body-fixed projection of the time derivative of the quadrupole moment is

$$R\dot{q}R^T = \tfrac{1}{2}[I, R(\text{Re}\, h)R^T] - [\tilde{q}, R(\text{Im}\, h)R^T].$$ (3.15)

The solution of equation (3.14) determines the angular velocity as a function of the angular momentum I and the body-fixed deformation $\tilde{q}$. The vibration of the quadrupole deformation in the principal axis frame is determined by

$$\frac{d}{dt} q_k = (R\dot{q}R^T)_{kk} = \frac{1}{2}[I, R(\text{Re}\, h)R^T]_{kk}.$$ (3.16)

4. Rotating equilibrium solutions

A rotating body is in equilibrium when the principal axis lengths and body-fixed angular momentum components are constant in time. From equation (3.13) the angular momentum must commute with the angular velocity, $[I, \Omega]$, or, equivalently, the vector angular momentum $\vec{I}$ is parallel to the angular velocity $\vec{\omega}$. Unless the angular momentum or angular velocity vanish, they must be proportional, $\Omega = AI$ for some real constant A. The moment of inertia is the reciprocal of A.

As an example, consider the simple energy functional

$$\mathcal{E}[\rho] = A_1 I_1^2 + A_2 I_2^2 + A_3 I_3^2, \tag{4.1}$$

where A_1, A_2, A_3 are real constants. Its Hamiltonian vector field is

$$h[\rho] = 2A_1 I_1 (\mathrm{d}I_1)^\sharp + 2A_2 I_2 (\mathrm{d}I_2)^\sharp + 2A_3 I_3 (\mathrm{d}I_3)^\sharp. \tag{4.2}$$

The body-fixed projection $h[\tilde{\rho}]$ is determined by using equation (3.8). A rotating equilibrium solution $\tilde{\rho}$ self-consistently satisfies $[h_\Omega[\tilde{\rho}], \tilde{\rho}] = 0$, where the cranking mean field Hamiltonian is $h_\Omega[\tilde{\rho}] = h[\tilde{\rho}] + \mathrm{i}\, AI$. The equilibrium density $\tilde{\rho}$ is a point of the submanifold $\mathcal{M}_\varrho$ and must also satisfy equations (3.2)–(3.4).

An important particular solution corresponds to rotation about a principal axis. Suppose $I = I_1$ is the total angular momentum so that $I_2 = I_3 = 0$. The commutator of the cranking Hamiltonian and the body-fixed density simplifies to

$$[h_\Omega[\tilde{\rho}], \tilde{\rho}] = \mathrm{i}\, (A - 2A_1) I_1 (q_2 - q_3) \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{4.3}$$

Excluding spheroidal densities, equation (4.3) is satisfied when $A = 2A_1$, or A_1 is the reciprocal of twice the moment of inertia. The components of the quadrupole moment in the principal axis frame are solutions to equations (3.2)–(3.4) constraining the points to $\mathcal{M}_\varrho$ and are given analytically as follows:

For rotation about the principal 1-*axis, there are three bands of equilibrium solutions that describe rotation about the short, long and medium axis lengths,*

$$q_1 = -\frac{\lambda + 2\mu}{3} \qquad 0 \leqslant I \leqslant I_{\max} = \lambda \qquad \text{short} \tag{4.4}$$

$$q_1 = +\frac{2\lambda + \mu}{3} \qquad 0 \leqslant I \leqslant I_{\max} = \mu \qquad \text{long} \tag{4.5}$$

$$q_1 = -\frac{\lambda - \mu}{3} \qquad 0 \leqslant I \leqslant I_{\max} = \lambda + \mu \qquad \text{middle} \tag{4.6}$$

where the axis lengths perpendicular to the rotation axis are

$$q_{2,3} = -\frac{q_1}{2} \pm \frac{1}{2}\sqrt{I_{\max}^2 - I^2}. \tag{4.7}$$

These solutions were derived recently as critical points of the $su(3)$ energy functional on a coadjoint orbit subject to the additional constraint that the total angular momentum is I [12]. The principal axis rotors are solutions for other $su(3)$ energy functionals, for example $E[\rho] = AI^2 + BX_3 + CX_4$ [12]. They are also familiar from the theory of the cranked anisotropic oscillator [25]. There are many other rotating equilibrium solutions, including tilted triaxial rotors [12].

The equilibrium conditions considered in this paper and its companion paper are mathematically equivalent. Suppose $\tilde{\rho}$ is a critical point of the $su(3)$ energy functional $\mathcal{E}$ on the surface $\mathcal{M}_\varrho$ subject to the constraint that the total angular momentum is I.

According to the Lagrange multiplier theorem, $\tilde{\rho}$ is a critical point of the functional $\mathcal{E}_I = \mathcal{E} - (A/2)(I_1^2 + I_2^2 + I_3^2 - I^2)$ on $\mathcal{M}_\varrho$ for some real multiplier A. The Hamiltonian vector field at $\tilde{\rho}$ associated with the function $\mathcal{E}_I$ is $R(\mathrm{d}\mathcal{E}_I^\sharp)R^{\mathrm{T}} = h[\tilde{\rho}] + \mathrm{i}AI$. Since $\tilde{\rho}$ is a critical point of $\mathcal{E}_I$ on $\mathcal{M}_\varrho$, the Hamiltonian vector field vanishes, $[h[\tilde{\rho}] + \mathrm{i}AI, \tilde{\rho}] = 0$. This condition is identical to equation (3.9) when $\Omega = AI$.

The critical points of the constrained energy functional were investigated thoroughly in prior work [12] and need not be repeated here using the self-consistent mean field Hamiltonian method.

5. Conclusion

This paper uses the symplectic geometry of coadjoint orbits to derive the $su(3)$ mean field Hamiltonian. Viewed geometrically, the mean field Hamiltonian is a vector field tangent to each coadjoint orbit. An equilibrium $su(3)$ density is a zero of the mean field Hamiltonian vector field.

The mean field Hamiltonian determines time-dependent $su(3)$ density dynamics as well as equilibrium configurations. The time evolution equation for the density is a Hamiltonian dynamical system on each coadjoint orbit surface. One of the applications of $su(3)$ mean field dynamics is to the description of normal mode vibrations in the small-amplitude limit [26]. Large-amplitude motion, which can be chaotic, may be investigated using the full equations of motion. These applications are the analogues of the random phase approximation and time-dependent Hartree–Fock from conventional mean field theory.

Note that the $su(3)$ mean field formulation allows for the use of the principal axis frame while in representation theory the body-fixed system is ill defined. As a consequence, the 'K' quantum number, which is a component of the angular momentum along a principal axis, is defined only approximately in $su(3)$ representation theory via angular momentum projection from a highest-weight vector followed by Gram–Schmidt orthogonalization [27]. The physical interpretation of $su(3)$ rotational bands is optimal in mean field theory because the angular momentum projections onto the principal axes are well defined. The rotational dynamics of $su(3)$ densities reduces to an Euler equation in the principal axis frame, equation (3.13). The full dynamics of $su(3)$ mean field theory obeys a Lax equation (3.9).

The energy in group theoretical models of nuclear structure is approximated usually by a rotationally invariant polynomial of the algebra generators. The polynomial's coefficients are chosen to attain a good fit to experimental energy levels and transition rates. In $su(3)$ mean field theory, the generalized Hohenberg–Kohn theorem [11] shows that there *exists* an energy functional whose minimum is the exact $su(3)$ ground state density, but the theorem does not provide a method for the functional's explicit construction. This theorem indicates that the $su(3)$ density method has the potential to be an exact theory, but it does not give a final answer. The energy functional $\mathcal{E}$ used in this paper is the rotor energy, equation (4.1), and its three real coefficients can be fitted to the energy levels and deformations of rotational bands of deformed nuclei. Another natural choice with similar properties is a low-degree polynomial in the $su(3)$ integrity basis [20]. This procedure parallels the application of the original Hohenberg–Kohn theorem in density functional theory [10]. The theorem proves only the existence of an exact energy functional which can replace the simple model functional of Thomas–Fermi theory in atomic physics. The construction of the exact energy functional continues to stimulate the efforts of many researchers in quantum chemistry.

Mean field theory applies to any dynamical symmetry algebra. The model densities are one coadjoint orbit of the dynamical symmetry group in the algebra's dual space. The symplectic

structure on the coadjoint orbit determines the mean field Hamiltonian from a model energy functional. The time development of the density is a Hamiltonian dynamical system on the coadjoint orbit.

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