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Abstract

The Lie algebra gcm(3) is a 15-dimensional semidirect sum that contains the algebra of the general linear group $GL_+(3, R)$. The six-dimensional Abelian ideal of gcm(3) is generated by the mass quadrupole and monopole tensors. The Bohr–Mottelson quantum model of nuclear rotational and vibrational states is a particular irreducible representation of gcm(3). The gcm(3) dual space consists of density matrices which are defined by the expectations of the gcm(3) generators. A coadjoint orbit is a level surface in the dual space of the gcm(3) Casimir, which is the squared length of the conserved Kelvin circulation vector. This paper develops mean field theory on any coadjoint orbit of gcm(3) densities. A Lax pair determines the dynamics of gcm(3) densities on each coadjoint orbit. This Lax equation is equivalent to the Riemann ellipsoid equations of motion.

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1. Introduction

This paper applies the algebraic mean field method to the general collective motion Lie algebra gcm(3) [1–3]. This 15-dimensional algebra is the hidden dynamical symmetry of the quantum Bohr–Mottelson geometrical model of rotational and vibrational states in atomic nuclei [4] and the classical Riemann ellipsoid theory of rotating stars and galaxies [5].

For systems of identical fermions, the two pre-eminent mean field theories are Hartree–Fock and Hartree–Fock–Bogoliubov. These theories have underlying Lie algebraic and geometric structures that play essential roles in their mathematical foundation and physical application [6–8]. Given any Lie algebra of many-particle observables, these structures permit the construction of a dynamical theory of densities as follows. The algebra's dual space consists of densities that are defined by the quantum expectations of the algebra's generators.

The mean field approximation restricts the model densities to a single coadjoint orbit of the corresponding Lie group in the dual space. The canonical symplectic form on the coadjoint orbit determines Hamiltonian dynamics from a model energy function. This paper explicitly implements this general method for gcm(3). In prior work, the algebraic mean field method was applied in the field of nuclear structure physics to the Elliott $su(3)$ model [9–13] and the symplectic $sp(3, R)$ collective model [14–17].

The paper is organized into three sections. Section 1 defines the gcm(3) Lie algebra and GCM(3) Lie group, discusses the physical interpretation of the algebra generators, enumerates the coadjoint orbits in the dual space gcm(3)* and identifies the Casimir function as the squared length of the conserved Kelvin circulation vector. Section 2 derives the mean field Hamiltonian from an energy function $\mathcal{E}$ using the natural symplectic geometry of a coadjoint orbit. The mean field Hamiltonian, a gcm(3)-valued function of the density, determines a finite-dimensional Lax equation which is the equation of motion on each coadjoint orbit. For a rotationally invariant energy function, the dynamics simplifies in the principal axis frame. Such a scalar energy function is adopted that is the sum of the Riemann ellipsoid kinetic energy plus a potential energy which is a pure function of the quadrupole and monopole moments. The angular momentum and Kelvin circulation vectors each obey an Euler precession equation in the principal axis frame. These precession equations plus a differential equation involving the axis lengths of the inertia ellipsoid are equivalent to the Lax dynamical system. The paper's conclusion discusses various aspects of the mean field method for Lie algebra models of nuclear structure.

The general collective motion Lie algebra gcm(3) is a 15-dimensional Lie subalgebra of $M_6(R)$,

$$\mathrm{gcm}(3) = \left\{ S = \begin{pmatrix} X & -U \\ 0 & -{}^T X \end{pmatrix} \,\middle|\, X, U \in M_3(R), {}^T U = U \right\}, \tag{1}$$

where $M_n(\mathrm{R})$ denotes the set of real $n \times n$ matrices and a left superscript ${}^T X$ indicates matrix transposition of X. A representation of gcm(3) provides the algebra's physical interpretation in quantum mechanical many-body physics. Let $(\hat{x}_{\alpha j}, \hat{p}_{\alpha j})$, $1 \leqslant j \leqslant 3$, denote the dimensionless Cartesian components of the position and momentum Hermitian operators for particle α in a finite system of particles. They obey the canonical commutation relation, $[\hat{x}_{\alpha j}, \hat{p}_{\beta k}] = \mathrm{i}\delta_{\alpha\beta}\delta_{jk}$. The set of Hermitian one-body operators,

$$\hat{Q}_{jk} = \sum_\alpha \hat{x}_{\alpha j}\hat{x}_{\alpha k}, \qquad \hat{N}_{jk} = \sum_\alpha \left(\hat{x}_{\alpha j}\hat{p}_{\alpha k} - \frac{\mathrm{i}}{2}\delta_{jk} \right), \tag{2}$$

close under commutation to form a Lie algebra. For A identical fermions (bosons) these one-body operators act on the Hilbert space $\mathcal{H}$ that is the antisymmetrized (symmetrized) tensor product of A-copies of the single-particle space. For each S in gcm(3), define the operator

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

When S is a matrix in gcm(3), the operator $\sigma(S)$ is a skew-adjoint one-body operator on $\mathcal{H}$. This set of operators is a reducible representation of gcm(3), $[\sigma(S_1), \sigma(S_2)] = \sigma([S_1, S_2])$.

The general collective motion group GCM(3) is a connected Lie matrix group given by exponentiation of gcm(3),

$$\mathrm{GCM}(3) = \left\{ g = \begin{pmatrix} x & -x \cdot U \\ 0 & {}^T x^{-1} \end{pmatrix} \,\middle|\, x \in GL_+(3, R), U \in M_3(R), {}^T U = U \right\}. \tag{4}$$

The connected general linear group $\mathrm{GL}_+(3, R)$ consists of the 3×3 real matrices with positive determinant; it is a subgroup of GCM(3) given by all $g = \mathrm{diag}(x, {}^T x^{-1}) \in \mathrm{GCM}(3)$ for

$x \in \mathrm{GL}_+(3, R)$. The set of matrices in GCM(3) with $x = \mathrm{Id}$, the identity matrix, and U any symmetric matrix is an Abelian normal subgroup isomorphic to the additive group R^6. The group GCM(3) is a semidirect product of R^6 and $\mathrm{GL}_+(3, R)$. The representation σ lifts to a unitary reducible representation of the group GCM(3) on $\mathcal{H}$. Mackey inducing constructs all the irreducible unitary representations of GCM(3) [18].

I choose to embed the dual space gcm(3)* as a 15-dimensional connected submanifold in the space $M_6(R)$:

$$\mathrm{gcm}(3)^* = \left\{ \rho = \begin{pmatrix} {}^T n & t \\ -q & -n \end{pmatrix} \middle| \, n, q, t \in M_3(R), {}^T q = q, t = {}^T n q^{-1} n \right\}. \tag{5}$$

The nondegenerate pairing between the dual space element $\rho \in \mathrm{gcm}(3)^*$ and a Lie algebra element $S \in \mathrm{gcm}(3)$ is the real number

$$\langle \rho, S \rangle \equiv \tfrac{1}{2} \operatorname{tr}(\rho \cdot S) = \operatorname{tr}({}^T n \cdot X) + \tfrac{1}{2} \operatorname{tr}(q \cdot U). \tag{6}$$

The matrix Lie group GCM(3) acts on its matrix Lie algebra gcm(3) by the adjoint action, $\mathrm{Ad}_g(S) = gSg^{-1}$ for all $g \in \mathrm{GCM}(3)$ and $S \in \mathrm{gcm}(3)$. The group GCM(3) then acts on the dual space gcm(3)* by the coadjoint action that satisfies the defining equation, $\langle \mathrm{Ad}^*_g(\rho), S \rangle = \langle \rho, \mathrm{Ad}_{g^{-1}}(S) \rangle$ for all $g \in \mathrm{GCM}(3)$, $\rho \in \mathrm{gcm}(3)^*$ and $S \in \mathrm{gcm}(3)$, or

$$\operatorname{tr}(\mathrm{Ad}^*_g(\rho) \cdot S) = \operatorname{tr}(\rho \cdot g^{-1} S g) = \operatorname{tr}(g \rho g^{-1} \cdot S), \qquad \text{for all } S \in \mathrm{gcm}(3). \tag{7}$$

The coadjoint action will be matrix conjugation, $\mathrm{Ad}^*_g(\rho) = g\rho g^{-1}$, provided $g\rho g^{-1}$ is in the dual space for all $\rho \in \mathrm{gcm}(3)^*$ and $g \in \mathrm{GCM}(3)$. As direct calculation shows, $g\rho g^{-1}$ is indeed a matrix in the dual space,

$$g \rho g^{-1} = \begin{pmatrix} {}^T n' & t' \\ -q' & -n' \end{pmatrix} \in \mathrm{gcm}(3)^*, \tag{8}$$

where $n' = {}^T x^{-1} \cdot (n + qU) \cdot {}^T x$, $q' = {}^T x^{-1} \cdot q \cdot x^{-1}$ is symmetric, and $t' = {}^T n' \cdot (q')^{-1} \cdot n'$. In this calculation, I used the inverse to g in GCM(3),

$$g^{-1} = \begin{pmatrix} x & -x \cdot U \\ 0 & {}^T x^{-1} \end{pmatrix}^{-1} = \begin{pmatrix} x^{-1} & U \cdot {}^T x \\ 0 & {}^T x \end{pmatrix}. \tag{9}$$

It is surprising that the coadjoint action simplifies to matrix conjugation because gcm(3) is not a semisimple matrix Lie algebra. (The nondegenerate Killing form of a semisimple Lie algebra identifies the dual space with the algebra, and the coadjoint action with the adjoint action.) Although the matrix t that is part of the definition of the dual element ρ in equation (5) plays a passive role in the pairing $\langle \rho, S \rangle$, its inclusion achieves the desired simplification of the coadjoint action.

Corresponding to any normalized wavefunction $\Psi \in \mathcal{H}$ is a dual element ρ where the real matrix $n = (n_{jk})$ and the real symmetric matrix $q = (q_{jk})$ are the expectations of the Hermitian operators $\hat{N}_{jk}$ and $\hat{Q}_{jk}$,

$$n_{jk} = \langle \Psi | \hat{N}_{jk} | \Psi \rangle, \qquad q_{jk} = \langle \Psi | \hat{Q}_{jk} | \Psi \rangle. \tag{10}$$

The quantum mechanical expectation of the gcm(3) representation $\sigma(S)$ equals half the trace of the product of this density matrix times the Lie algebra element S,

$$\langle \rho, S \rangle = \tfrac{1}{2} \operatorname{tr}(\rho \cdot S) = -\mathrm{i} \langle \Psi | \sigma(S) | \Psi \rangle. \tag{11}$$

Not every dual element is associated with a quantum mechanical state. Those that do are called density matrices. For example, a density matrix ρ must have q positive-definite. In the typical situation, many distinct quantum state vectors yield the same gcm(3) density matrix.

The matrix $q = (q_{ij})$ of a gcm(3) density is the monopole–quadrupole tensor or inertia tensor. The trace of this tensor, which is the expectation of the monopole operator, determines the nuclear radius. The traceless part, namely $q_{ij} - (1/3)\delta_{ij}\,\mathrm{tr}\,q$, which is the expectation of the quadrupole operator, determines the nuclear deformation. The inertia ellipsoid is the surface in Cartesian space (x^1, x^2, x^3) satisfying the equation $\sum_{ij} q^{-1}_{ij} x^i x^j = 1$ (recall that q is positive-definite). This ellipsoidal surface gives a useful visualization of the size and deformation of a quantum system of discrete particles.

The action of the group element $x \in \mathrm{GL}_+(3, R)$ on three-dimensional Cartesian space induces a transformation of the inertia ellipsoid with tensor q into another inertia ellipsoid with tensor ${}^T xqx$. When $x \in SO(3)$, the rotation group, the inertia ellipsoid is rotated into another ellipsoid with the same intrinsic deformation and size. The generators of a rotation are the angular momenta, and the antisymmetric part $l = n - {}^T n$ of the matrix $n = (n_{ij})$ of a gcm(3) density provides the expectations of the angular momentum. The expectations of the components of the angular momentum pseudovector $\vec{l}$ are given by $l_{ij} = \varepsilon_{ijk} l_k$.

Suppose the many-body Hamiltonian $\hat{H}$ on $\mathcal{H}$ is the sum of the kinetic energy Laplacian and any potential energy multiplication operator that is a pure function of the position coordinates. The commutator of the monopole–quadrupole operator $\hat{Q}_{ij}$ with the Hamiltonian is $\mathrm{i}[\hat{Q}_{ij}, \hat{H}] = \hat{N}_{ij} + \hat{N}_{ji}$. Adopting the Heisenberg picture, the time rate of change of $\hat{Q}_{ij}$ is the operator $(\hat{N}_{ij} + \hat{N}_{ji})$, and, therefore, the symmetric matrix $(n + {}^T n)$ measures the system's monopole–quadrupole vibrational momentum. In particular, $\mathrm{tr}(n)$ determines the rate of monopole breathing mode oscillations, and the traceless matrix $(n + {}^T n - (2/3)\,\mathrm{tr}(n)\,\mathrm{Id})$ determines the rate of the quadrupole deformation vibrations.

1.1. Coadjoint orbits

The coadjoint orbit $\mathcal{O}_\rho$ consists of the density ρ and all transformed densities $\mathrm{Ad}^*_g \rho$ as g ranges over the entire group GCM(3). An orbit $\mathcal{O}_\rho$ is a smooth connected surface contained in the dual space gcm(3)*.

Each coadjoint orbit of density matrices contains a matrix with the following special form:

$$\varrho = \begin{pmatrix} -|C|(E_{12} - E_{21})/2 & |C|^2(E_{11} + E_{22})/4 \\ -\mathrm{Id} & -|C|(E_{12} - E_{21})/2 \end{pmatrix}, \tag{12}$$

for $|C| \geqslant 0$. E_{ij} denotes the elementary matrix whose only nonzero entry is one at the intersection of row i and column j and $\mathrm{Id} = E_{11} + E_{22} + E_{33}$ is the identity matrix. To achieve the special form ϱ starting with a general density matrix ρ, first transform q in ρ to the identity matrix using a pure $\mathrm{GL}_+(3, \mathrm{R})$ group element x, ${}^T x^{-1} q x^{-1} = \mathrm{Id}$. This transformation is possible for density matrices that have q positive-definite. Next make an R^6 transformation U to remove the symmetric part of the matrix n, cf equation (8). Finally the antisymmetric matrix n is a pseudovector that can be rotated so that it is aligned with the z-axis, i.e., $n = |C|(E_{12} - E_{21})/2$ where $|C|$ is a nonnegative real number.

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

$$\mathcal{O}_\varrho = \{\rho = \mathrm{Ad}^*_g \varrho = g\varrho g^{-1} \in \mathrm{gcm}(3)^* \mid g \in \mathrm{GCM}(3)\}. \tag{13}$$

The space of densities in gcm(3)* is a disjoint union of the coadjoint orbits $\mathcal{O}_\varrho$ as ϱ ranges over the orbit representatives (12) with $|C|$ a nonnegative real number. When $|C|$ is positive, the coadjoint orbit is in general position, and $\mathcal{O}_\varrho$ is a 14-dimensional surface contained in the dual space. When $|C| = 0$, the singular coadjoint orbit is 12-dimensional.

1.2. Casimir invariant

A Casimir invariant is a real-valued function on the dual space that is invariant with respect to the coadjoint action. Casimir functions, therefore, are constant on each coadjoint orbit. The gcm(3) algebra has one independent Casimir invariant,

$$\mathcal{C}_2(\rho) = -\tfrac{1}{2}\,\mathrm{tr}\rho^2 = \mathrm{tr}(tq - n^2) = \mathrm{tr}({}^T nq^{-1}nq - n^2). \tag{14}$$

This function is trivially constant on each coadjoint orbit, $\mathcal{C}_2(\mathrm{Ad}^*_g\rho) = \mathcal{C}_2(\rho)$; its value at the orbit representative (12) is

$$\mathcal{C}_2(\varrho) = |C|^2. \tag{15}$$

The trace of any power of ρ is a Casimir invariant, but these are not independent of $\mathcal{C}_2$. The traces of powers of ρ are the coefficients of the secular equation for ρ, and, hence, the eigenvalues of ρ are constant on a coadjoint orbit. Since $\rho \in \mathrm{gcm}(3)^*$ is a matrix in the Lie algebra $sp(3, R)$ of the real symplectic group, its eigenvalues occur in pairs, $\pm\lambda$, and the multiplicity of the zero eigenvalue is even [19]. But, the kernel of ρ is at least three-dimensional because of the following observation: when v is any column vector in R^3 and ρ is any density matrix,

$$\rho\begin{pmatrix} -q^{-1}nv \\ v \end{pmatrix} = \begin{pmatrix} {}^T n & t \\ -q & -n \end{pmatrix}\begin{pmatrix} -q^{-1}nv \\ v \end{pmatrix} = 0. \tag{16}$$

Since the kernel of ρ cannot have an odd dimension, it must be at least four-dimensional and the nonzero eigenvalues of ρ are $\pm\mathrm{i}|C|$. Thus, the quadratic Casimir $\mathcal{C}_2$ exhausts the independent Casimir functions.

For any density matrix ρ, define the matrix $c = q^{-1/2}\cdot n\cdot q^{1/2} - q^{1/2}\cdot {}^T n\cdot q^{-1/2}$. The pseudovector $\vec{c}$ corresponding to this antisymmetric matrix is the Kelvin circulation. The gcm(3) Casimir is the squared length of the Kelvin circulation vector, $\mathcal{C}_2(\rho) = -(1/2)\,\mathrm{tr}(c^2) = \vec{c}\cdot\vec{c} = |C|^2$.

Rapidly rotating nuclei make a shape transition from oblate spheroids to triaxial ellipsoids at some critical angular momentum I_{cr} that depends on the isotope [20]. In self-gravitating systems this transition is the classical Jacobi bifurcation [5]. A recent experimental analysis of the giant dipole resonance in the nucleus ^{46}Ti [21] indicates that the Kelvin circulation remains constant after the shape transition and that the circulation of the triaxial ellipsoids equals the critical angular momentum, $|C| = I_{\mathrm{cr}} \approx 29\hbar$ [22].

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

An important mathematical theorem in representation theory is that the coadjoint orbits of any Lie group are symplectic manifolds [23–25]. In many-body physics, the symplectic geometry of a coadjoint orbit determines the mean field Hamiltonian from the energy function of a group theoretical model.

Each element S of the gcm(3) Lie algebra defines a tangent vector field $\overline{S}$ to each coadjoint orbit. Consider the curve $\zeta(\epsilon) = \exp(\epsilon S)$ in the group GCM(3). Given any point ρ in the dual space, the curve $\epsilon \mapsto \mathrm{Ad}^*_{\zeta(\epsilon)^{-1}}\rho = \exp(-\epsilon S)\rho\exp(\epsilon S)$ lies in the coadjoint orbit through ρ. The tangent to this curve at ρ is denoted by $\overline{S}[\rho]$.

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

$$\mathcal{A}_\rho = \{S \in \mathrm{gcm}(3) \mid [S, \rho] = 0\}. \tag{17}$$

When S is an element of the annihilator at ρ, $\overline{S}[\rho]$ 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

Table 1. Hamiltonian vector fields in gcm(3).

	Hamiltonian vector field $S_f[\rho]$	
Function f	X	U
$\lambda(S)$	X	U
q_{ij}	0	$E_{ij}+E_{ji}$
n_{ij}	E_{ij}	0
$\mathcal{C}_2$	0	0
$\mathrm{tr}(q)$	0	2Id
$\mathrm{tr}(q^2)$	0	4q
$\mathrm{tr}(q^3)$	0	$6\mathrm{q}^2$
$\mathrm{tr}(q^4)$	0	$8\mathrm{q}^3$
$(q^{-1})_{ij}$	0	$-\sum_{nm}(q^{-1})_{in}(E_{nm}+E_{mn})(q^{-1})_{mj}$
$\mathrm{tr}({}^T n\cdot q^{-1}\cdot n)$	$2q^{-1}n$	$-2q^{-1}\cdot n\cdot {}^T n\cdot q^{-1}$

element of the annihilator at ρ, the corresponding tangent vectors are equal: $\overline{S}[\rho]=\overline{S'}[\rho]$ if and only if $S-S'\in\mathcal{A}_\rho$. Therefore, the tangent space to the coadjoint orbit at ρ can be identified with the vector space gcm(3) modulo the annihilator $\mathcal{A}_\rho$.

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

$$\omega_\rho(\overline{S}[\rho],\overline{T}[\rho])=-\langle\rho,[S,T]\rangle. \tag{18}$$

This antisymmetric bilinear form is well defined on the tangent space to the coadjoint orbit at ρ since, $\langle\rho,[S,T]\rangle=\langle\rho,[S',T']\rangle$ when $S-S'\in\mathcal{A}_\rho$ and $T-T'\in\mathcal{A}_\rho$. The form ω is nondegenerate, i.e., $\omega_\rho(\overline{S}[\rho],\overline{T}[\rho])=0$ for all T in the gcm(3) Lie algebra if and only if $\overline{S}[\rho]$ 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 $\overline{T}[\rho]$ is defined by

$$\mathrm{df}(\overline{T})(\rho)=\frac{\mathrm{d}}{\mathrm{d}\epsilon}f(\exp(-\epsilon T)\rho\exp(\epsilon T))|_{\epsilon=0}. \tag{19}$$

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

$$\omega_\rho(\overline{S}_f[\rho],\overline{T}[\rho])=\mathrm{df}(\overline{T})(\rho), \tag{20}$$

for all directions $\overline{T}[\rho]$ tangent to the coadjoint orbit at ρ. The solution $\overline{S}_f[\rho]$ to this equation is unique because the symplectic form is nondegenerate. The vector field $\overline{S}_f$ is called the Hamiltonian vector field associated with the smooth function f. There exists a Lie algebra element $S_f[\rho]$ whose corresponding tangent vector is $\overline{S}_f[\rho]$. The assignment of the Lie algebra element $S_f[\rho]$ 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 $\overline{S}_f[\rho]$ 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 S there is an elementary function $\lambda(S)$ on the dual space defined by $\lambda(S)(\rho)=\langle\rho,S\rangle$. The value of the function $\lambda(S)$ at ρ is the expectation of the physical observable corresponding to S when the system's state has the gcm(3) density ρ. It is easily shown that the Hamiltonian vector field associated with $\lambda(S)$ is S. The Hamiltonian vector fields associated with various smooth functions are provided in table 1.

In this table, the functions n_{ij} and q_{ij} are the 'coordinate functions' that map ρ into the i,j real entries of the matrices n and q, respectively. Using the results for these coordinate

functions and properties of the exterior derivative, the Hamiltonian vector field corresponding to other functions in table 1 may be determined.

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

A geometrical condition determines the time evolution of a gcm(3) density matrix: a solution $\rho(t)$ must be an integral curve of the gcm(3) Hamiltonian vector field $\overline{h}[\rho]$ or

$$\dot{\rho} = [\rho, h[\rho]]. \tag{21}$$

Equation (21) is a finite-dimensional Lax equation [27, 28]. It is formally the same as the time-dependent Hartree–Fock equation [29].

Dynamics may be expressed equivalently using the Poisson bracket. The Poisson bracket on $\mathcal{O}_\varrho$ is defined from the symplectic form. The bracket of two smooth real-valued functions f, g on $\mathcal{O}_\varrho$ is

$$\{f, g\}(\rho) \equiv \omega_\rho(\overline{S}_f[\rho], \overline{S}_g[\rho]). \tag{22}$$

When f is any smooth function on a coadjoint orbit, its time rate of change along a solution curve is

$$\dot{f} = \{f, \mathcal{E}\}. \tag{23}$$

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

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\lambda(S) = \langle\dot{\rho}, S\rangle &= \frac{1}{2}\operatorname{tr}([\rho, h[\rho]]S) \\ &= \omega_\rho(\overline{S}, \overline{h}[\rho]) = \{\lambda(S), \mathcal{E}\}(\rho).\end{aligned} \tag{24}$$

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

2.2. Rotation group SO(3)

The rotation group $SO(3)$ is a subgroup of $\mathrm{GL}_+(3, \mathrm{R}) \subset \mathrm{GCM}(3)$ consisting of all block diagonal matrices $\tau(R) = \operatorname{diag}(R, R)$ for $R \in SO(3)$. A density ρ in gcm(3)* is transformed by a rotation $R \in SO(3)$ into the density $\tau(R) \cdot \rho \cdot \tau(R)^{-1}$. In terms of the matrix entries of ρ, a rotation R makes the following transformations: $n \mapsto R \cdot n \cdot {}^TR$, $q \mapsto R \cdot q \cdot {}^TR$ and $t \mapsto R \cdot t \cdot {}^TR$.

Any real symmetric matrix can be diagonalized by a rotation matrix. Hence, there is an $R \in SO(3)$ that diagonalizes the positive-definite inertia tensor,

$$\tilde{q} = R \cdot q \cdot {}^TR = \operatorname{diag}\bigl(a_1^2, a_2^2, a_3^2\bigr), \tag{25}$$

where a_1, a_2, a_3 are real positive numbers. The inertia ellipsoid corresponding to the diagonal matrix $\tilde{q}$ is defined by $(x^1/a_1)^2 + (x^2/a_2)^2 + (x^3/a_3)^2 = 1$. From a geometrical viewpoint, R rotates the laboratory frame into the principal axis frame in which, by definition, the system's inertia tensor $\tilde{q}$ is diagonal. The quantity a_k is the half-length of the kth principal axis of the inertia ellipsoid.

Let $\mathcal{M}_\varrho$ denote the surface of all principal axis densities contained in the coadjoint orbit $\mathcal{O}_\varrho$. The points $\tilde{\rho}$ of $\mathcal{M}_\varrho$ have a diagonal inertia tensor, $\tilde{q}$, and

$$\tilde{\rho} = \begin{pmatrix} {}^T\tilde{n} & \tilde{t} \\ -\tilde{q} & -\tilde{n} \end{pmatrix} \tag{26}$$

satisfies an algebraic equation for the gcm(3) Casimir

$$\mathrm{tr}({}^T\tilde{n}\tilde{q}^{-1}\tilde{n}\tilde{q} - \tilde{n}^2) = |C|^2. \tag{27}$$

The circulation in the principal axis frame is denoted by the antisymmetric matrix $C = R \cdot c \cdot {}^T R = A^{-1} \cdot \tilde{n} \cdot A - A \cdot {}^T\tilde{n} \cdot A^{-1}$, where the diagonal matrix $A = \mathrm{diag}(a_1, a_2, a_3)$. The squared length of the corresponding pseudovector $\vec{C}$ equals the gcm(3) Casimir, $\vec{C} \cdot \vec{C} = |C|^2$. The principal axis manifold $\mathcal{M}_\varrho$ is 11-dimensional when $|C| \neq 0$.

When the energy function is a rotational scalar, transformation of the dynamical system to the principal axis frame simplifies the analysis. Let $R(t) \in SO(3)$ be a smooth time-dependent rotation that transforms a solution curve of the dynamical system (21) into the submanifold of principal axis densities. Define the time-dependent matrix $\Omega(t) = \dot{R} \cdot {}^T R$ in the Lie algebra $so(3)$ of the rotation group. The pseudovector $\vec{\omega}$ corresponding to the antisymmetric matrix Ω is the angular velocity. Let $\tilde{\rho}(t) = \tau(R) \cdot \rho(t) \cdot \tau(R)^{-1} \in \mathcal{M}_\varrho$ denote the density in the principal axis frame. The Hamiltonian dynamical system on the coadjoint orbit, equation (21), is equivalent to the following dynamical equation on $\mathcal{M}_\varrho$:

$$\frac{\mathrm{d}\tilde{\rho}}{\mathrm{d}t} = [\tilde{\rho}, h_\Omega[\tilde{\rho}]], \tag{28}$$

where $h_\Omega[\tilde{\rho}] = \tau(R) \cdot h[\rho] \cdot \tau(R)^{-1} - \mathrm{diag}(\Omega, \Omega)$ is the gcm(3) Routhian. When the energy function is a rotational scalar, the Hamiltonian vector field is invariant under rotations, $h[\tilde{\rho}] = \tau(R) \cdot h[\rho] \cdot \tau(R)^{-1}$.

2.3. Energy function

The energy function $\mathcal{E}(\rho)$ is a real-valued function defined on the dual space gcm(3)*. It is the sum of kinetic and potential energies. This function is assumed to be invariant under rotations, $\mathcal{E}(\tau(R) \cdot \rho \cdot \tau(R)^{-1}) = \mathcal{E}(\rho)$ for all $R \in SO(3)$. As a consequence, the angular momentum vector $\vec{l}$ is constant along each solution curve,

$$\dot{l}_{ij} = \{l_{ij}, \mathcal{E}\}(\rho) = -\mathrm{d}\mathcal{E}(\overline{T})(\rho) = -\frac{\mathrm{d}}{\mathrm{d}\theta}\mathcal{E}(\tau(R(-\theta)) \cdot \rho \cdot \tau(R(\theta)))|_{\theta=0} = 0, \tag{29}$$

where $l_{ij} = n_{ij} - n_{ji} = \lambda(T)(\rho)$ is a component of the angular momentum vector for $T = \mathrm{diag}(E_{ij} - E_{ji}, E_{ij} - E_{ji}) \in \mathrm{gcm}(3)$, and $R(\theta) = \exp(\theta(E_{ij} - E_{ji}))$ is a rotation in the i–j plane through an angle θ.

The energy function is a sum of kinetic and potential energies. To respect time-reversal symmetry, the kinetic energy must be of even degree in n. The kinetic energy formula must also have the correct dimensional unit. A quadratic polynomial in n, which has the correct dimensional unit and which is a rotational scalar, is the Riemann ellipsoid kinetic energy,

$$T(\rho) = \tfrac{1}{2}\,\mathrm{tr}({}^T n \cdot q^{-1} \cdot n). \tag{30}$$

The Riemann kinetic energy also enjoys a correct scaling property. When $x = \mathrm{diag}(b, b, b)$, $b > 0$ is a scaling transformation in $\mathrm{GL}_+(3, R)$, $n \mapsto x^{-1} \cdot n \cdot x$, $q \mapsto x^{-1} \cdot q \cdot x^{-1}$, and the Riemann kinetic energy is transformed from T to $b^2 T$, which agrees with the scaling of the exact quantum kinetic energy. The Hamiltonian vector field corresponding to the Riemann ellipsoid kinetic energy is given in table 1.

The potential energy function $V(q)$ is assumed to be a pure function of the quadrupole–monopole tensor q, i.e., a function that depends only on the size and deformation of the system. It is rotationally invariant, $V(q) = V(R \cdot q \cdot {}^T R)$. Such a scalar potential may be regarded as a function of the three scalar quantities, $u_k = \mathrm{tr}(q^k)$, for $k = 1, 2, 3$. The exterior derivative of the potential energy function is

$$\mathrm{d}V = \frac{\partial V}{\partial u_1}\,\mathrm{d}u_1 + \frac{\partial V}{\partial u_2}\,\mathrm{d}u_2 + \frac{\partial V}{\partial u_3}\,\mathrm{d}u_3. \tag{31}$$

Hence, according to the table, the Hamiltonian vector field corresponding to the potential energy has $X = 0$ and

$$U = 2\frac{\partial V}{\partial u_1}\,\mathrm{Id} + 4\frac{\partial V}{\partial u_2}q + 6\frac{\partial V}{\partial u_3}q^2. \tag{32}$$

In the principal axis frame, U is rotated to

$$\tilde{U} = R \cdot U \cdot {}^T R = 2\frac{\partial V}{\partial u_1}\,\mathrm{Id} + 4\frac{\partial V}{\partial u_2}\tilde{q} + 6\frac{\partial V}{\partial u_3}\tilde{q}^2, \tag{33}$$

which is a diagonal matrix.

Another convenient way to regard a rotationally invariant function of q is as a function of the eigenvalues of q. The derivative of $V(a_1, a_2, a_3)$ with respect to the semi-axis lengths a_k simplifies to

$$\begin{aligned}\frac{\partial V}{\partial a_k} &= \frac{\partial V}{\partial u_1}\frac{\partial u_1}{\partial a_k} + \frac{\partial V}{\partial u_2}\frac{\partial u_2}{\partial a_k} + \frac{\partial V}{\partial u_3}\frac{\partial u_3}{\partial a_k} \\ &= a_k\left(2\frac{\partial V}{\partial u_1} + 4\frac{\partial V}{\partial u_2}a_k^2 + 6\frac{\partial V}{\partial u_3}a_k^4\right) \\ &= a_k\tilde{U}_{kk}.\end{aligned} \tag{34}$$

Define the entries of a diagonal matrix by $\tilde{W}_{kk} = -a_k\partial V/\partial a_k$ in terms of which $\tilde{U} = -\tilde{q}^{-1}\tilde{W}$, a product of two diagonal matrices.

Thus, the Hamiltonian vector field in the rotating principal axis frame for the scalar energy function $\mathcal{E} = T(\rho) + V(q)$ is

$$h_\Omega[\tilde{\rho}] = \begin{pmatrix} \tilde{q}^{-1}\cdot\tilde{n} - \Omega & \tilde{q}^{-1}\cdot\tilde{n}\cdot{}^T\tilde{n}\cdot\tilde{q}^{-1} + \tilde{W}\cdot\tilde{q}^{-1} \\ 0 & -{}^T(\tilde{q}^{-1}\cdot\tilde{n}) - \Omega \end{pmatrix}. \tag{35}$$

The equations of motion equation (28) in the principal axis frame for this energy are

$$\frac{\mathrm{d}\tilde{q}}{\mathrm{d}t} = \tilde{n} + {}^T\tilde{n} + [\Omega, \tilde{q}] \tag{36}$$

$$\frac{\mathrm{d}\tilde{n}}{\mathrm{d}t} = \tilde{t} + \tilde{W} + [\Omega, \tilde{n}], \tag{37}$$

where $\tilde{t} = {}^T\tilde{n}\cdot\tilde{q}^{-1}\cdot\tilde{n}$. The commutators involving the angular velocity Ω are Coriolis terms. This dynamical system is the Riemann ellipsoid equations of motion [5]. This set of 15 coupled ordinary differential equations should be solved with proscribed initial conditions for the 15 unknown functions, $\tilde{q}(t), \tilde{n}(t), \Omega(t)$.

2.4. Precession equations for I and C

Since $\tilde{q}$ is diagonal, equation (36) determines the angular velocity in terms of off-diagonal entries of the symmetric matrix $(\tilde{n} + {}^T\tilde{n})$,

$$\left(a_i^2 - a_j^2\right)\Omega_{ij} = \tilde{n}_{ij} + \tilde{n}_{ji}, \qquad \text{for} \quad i \neq j. \tag{38}$$

The six differential equations for the off-diagonal components of n may be expressed equivalently as two precession equations for the angular momentum and circulation vectors. The angular momentum in the rotating frame, $I(t) = \tilde{n} - {}^T\tilde{n} = R(t)\cdot I\cdot {}^T R(t)$, is not constant. From equation (37), this angular momentum obeys the Euler precession equation,

$$\frac{\mathrm{d}}{\mathrm{d}t}I = [\Omega, I], \qquad \text{or, equivalently,} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\vec{I} = -\vec{\omega}\times\vec{I}, \tag{39}$$

where the components of the pseudovector $\vec{I}$ are related to the entries of the antisymmetric matrix I by $I_{ij} = \varepsilon_{ijk} I_k$. Define the antisymmetric matrix

$$\Lambda = \tfrac{1}{2}(A \cdot \Omega \cdot A^{-1} + A^{-1} \cdot \Omega \cdot A - A^{-1} \cdot I \cdot A^{-1}), \tag{40}$$

and let $\vec{\lambda}$ denote the corresponding pseudovector. The circulation in the rotating frame also obeys a precession equation,

$$\frac{\mathrm{d}}{\mathrm{d}t} C = [\Lambda, C], \qquad \text{or, equivalently,} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\vec{C} = -\vec{\lambda} \times \vec{C}, \tag{41}$$

as can be verified from equations (36) and (37). The vector $\vec{\lambda}$ is called the vortex velocity. The velocities Ω and Λ may be expressed as functions of the angular momentum and Kelvin circulation vectors,

$$\Omega_{ij} = \frac{\left(a_i^2 + a_j^2\right) I_{ij} - 2 a_i a_j C_{ij}}{\left(a_i^2 - a_j^2\right)^2}, \qquad \Lambda_{ij} = \frac{2 a_i a_j I_{ij} - \left(a_i^2 + a_j^2\right) C_{ij}}{\left(a_i^2 - a_j^2\right)^2}. \tag{42}$$

The precession equations (39) and (41) for I and C demonstrate explicitly that the squared lengths of the angular momentum vector and the Kelvin circulation vector are constant on solution curves. The total energy $\mathcal{E}$ is also conserved.

The diagonal components of $\tilde{n}$ determine, according to equation (36), the vibrational rate of the semi-axis lengths,

$$a_k \frac{\mathrm{d}a_k}{\mathrm{d}t} = \tilde{n}_{kk}, \qquad \text{for} \quad k = 1, 2, 3. \tag{43}$$

Using this identity, the diagonal parts of equation (37) determines three second-order differential equations for the axis lengths a_k,

$$\frac{\mathrm{d}^2 a_j}{\mathrm{d}t^2} = \frac{1}{2} \sum_{i \neq j} \left(\frac{(I_{ij} + C_{ij})^2}{(a_i + a_j)^3} - \frac{(I_{ij} - C_{ij})^2}{(a_i - a_j)^3} \right) - \frac{\partial V}{\partial a_j}, \qquad \text{for} \quad j = 1, 2, 3. \tag{44}$$

Hence, the Lax equation (28) is equivalent to the system, equations (36) and (37), and to the system, equations (39), (41) and (44), for $I(t), C(t), a_k(t)$. To make further progress in solving this system, a specific choice for the potential energy function $V(a_1, a_2, a_3)$ is necessary.

When $\mathrm{d}\tilde{\rho}/\mathrm{d}t = 0$, the rotating system is in equilibrium, and, hence, the right-hand sides of equations (36) and (37) are zero. Thus, an equilibrium solution has constant axis lengths a_k, a constant vibrational momentum tensor $\tilde{n}$, and constant angular momentum $\tilde{I}$ and circulation $\tilde{C}$. The angular velocity $\vec{\omega}$, respectively, vortex velocity $\vec{\lambda}$, is aligned or anti-aligned with the angular momentum $\vec{I}$, respectively, Kelvin circulation $\vec{C}$. This alignment is only possible when these vectors are all aligned with one principal axis (a S-type ellipsoid) or all lie in one principal plane. This restriction is known as Riemann's theorem [5]. Given $\vec{I}$ and $\vec{C}$, the three axis lengths a_k are solved for by requiring that the right-hand side of equation (44) vanishes. When the sum of an attractive surface tension term and a Coulomb repulsion term approximates the atomic nuclear potential, many equilibrium solutions are known explicitly [18, 20, 30].

2.5. S-type ellipsoids

An S-type ellipsoid is a special solution for the important case of rotation about one principal axis, say the 3-axis. When $\vec{I}, \vec{\omega}, \vec{C}$ and $\vec{\lambda}$ are all aligned with one principal axis, the precession equations (39) and (41) are satisfied trivially with the angular momentum $\vec{I}$ and Kelvin

circulation $\vec{C}$ vectors constant in time. The remaining equations for the axis length vibrations, equation (44), simplify to

$$\frac{\mathrm{d}^2 a_j}{\mathrm{d}t^2} = -\frac{\partial V_{\mathrm{eff}}}{\partial a_j}, \qquad \text{for} \quad j = 1, 2, 3, \tag{45}$$

where the effective potential $V_{\mathrm{eff}}(a_1, a_2, a_3) = T + V$ is the sum of the kinetic energy $T(a_1, a_2, a_3)$ and the potential energy $V(a_1, a_2, a_3)$ with

$$T(a_1, a_2, a_3) = \frac{1}{4}\left\{ \frac{(I+C)^2}{(a_1+a_2)^2} + \frac{(I-C)^2}{(a_1-a_2)^2} \right\}. \tag{46}$$

An equilibrium S-type ellipsoid is attained when $V_{\mathrm{eff}}(a_1, a_2, a_3)$ is minimized.

2.6. GCM(3) group transformation

Another way to set up the equations of motion is to determine the time-dependent matrix $g(t)$ in the group GCM(3) that transforms the coadjoint orbit representative ϱ of equation (12) to $\rho(t) = \mathrm{Ad}^*_{g(t)}\varrho$. From the Lax equation (21), the group transformation $g(t)$ satisfies the matrix differential equation,

$$\frac{\mathrm{d}g}{\mathrm{d}t} = -h[g\varrho g^{-1}] \cdot g. \tag{47}$$

When the group element g is written as equation (4), the density $\rho = g\varrho g^{-1}$ of equation (5) has entries $n = {}^T x^{-1}(|C|(E_{12}-E_{21})/2+U)^T x$ and $q = {}^T x^{-1} x^{-1}$. The $\mathrm{GL}_+(3, R)$ matrix x can be expressed as the product of a rotation, a diagonal matrix with positive real numbers as entries, and another rotation, $x = {}^T R \cdot A \cdot S$ with $R, S \in SO(3)$, $A = \mathrm{diag}(a_1, a_2, a_3)$, $a_k > 0$. Using this special form for x, the monopole–quadrupole tensor is $q = {}^T R \cdot A^2 \cdot R$. The orthogonal matrix R rotates the inertia tensor into its principal axis value $\tilde{q} = A^2$, and the entries of the diagonal matrix A are the half-lengths of the principal axes of the inertia ellipsoid. Thus, these matrices R and A are the same as those defined by equation (25). The vibrational momentum is $n = {}^T R \cdot \tilde{n} \cdot R$ with $\tilde{n} = A \cdot ((|C|/2)S \cdot (E_{12} - E_{21}) \cdot {}^T S + U^S) \cdot A^{-1}$ and $U^S = S \cdot U \cdot {}^T S$ is a real symmetric matrix.

The circulation in the principal axis frame is

$$\begin{aligned} C &= A^{-1} \cdot \tilde{n} \cdot A - A \cdot {}^T\tilde{n} \cdot A^{-1} \\ &= S \cdot |C|(E_{12} - E_{21}) \cdot {}^T S, \end{aligned} \tag{48}$$

and, therefore, the rotation matrix S aligns the circulation vector in the principal axis frame with the 3-axis. Define the vortex velocity matrix $\Lambda = \dot{S} \cdot {}^T S$; the vortex velocity $\vec{\lambda}$ is the pseudovector corresponding to this antisymmetric matrix. The circulation obeys the precession equation (41), and it will be shown shortly below that this Λ is the same as that given in equation (40).

By multiplying both sides of equation (47) on the left by $\tau(R)$, the dynamical equation in the laboratory frame simplifies to an equation in the rotating principal axis frame,

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} A^{-1} \cdot S & -A^{-1} \cdot U^S \cdot S \\ 0 & A \cdot S \end{pmatrix} = -h_\Omega[\tilde{\rho}]\begin{pmatrix} A^{-1} \cdot S & -A^{-1} \cdot U^S \cdot S \\ 0 & A \cdot S \end{pmatrix}. \tag{49}$$

This equation may be simplified further by right multiplication with $\tau(S)^{-1}$:

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} A^{-1} & -A^{-1} \cdot U^S \\ 0 & A \end{pmatrix} = \begin{pmatrix} -{}^T F & G \\ 0 & F \end{pmatrix}\begin{pmatrix} A^{-1} & -A^{-1} \cdot U^S \\ 0 & A \end{pmatrix}, \tag{50}$$

$$F = A^{-1} \cdot (-C/2 + U^S) \cdot A^{-1} + \Omega - A \cdot \Lambda \cdot A^{-1}$$
$$G = A^{-1} \cdot ((C/2 + U^S) \cdot A^{-2} \cdot (C/2 - U^S) + [U^S, \Lambda] - \tilde{W}) \cdot A^{-1}. \tag{51}$$

Since A is diagonal, F must be likewise diagonal. The antisymmetric part of the diagonal matrix AFA vanishes and determines the circulation,

$$C = 2A \cdot \Omega \cdot A - (A^2 \cdot \Lambda + \Lambda \cdot A^2). \tag{52}$$

The off-diagonal entries of the symmetric part of AFA also vanish and this determines the off-diagonal entries of the symmetric matrix U^S,

$$U^S_{ij} = \tfrac{1}{2}\big(a_i^2 - a_j^2\big)\Lambda_{ij}, \qquad \text{for} \quad i \neq j. \tag{53}$$

These formulae for C and U^S imply an expression for the angular momentum $I = \tilde{n} - {}^T\tilde{n}$,

$$I = (A^2 \cdot \Omega + \Omega \cdot A^2) - 2A \cdot \Lambda \cdot A, \tag{54}$$

which agrees with the prior definition of Λ in (40). In equation (50), the matrix F simplifies to a diagonal one with entries, $F_{ii} = U^S_{ii}/a_i^2$, and the dynamical equation involving F is

$$a_i \frac{\mathrm{d}a_i}{\mathrm{d}t} = U^S_{ii}. \tag{55}$$

Finally, the time rate of change of U^S according to equation (50) is

$$\frac{\mathrm{d}U^S}{\mathrm{d}t} = -A \cdot G \cdot A = (U^S + C/2) \cdot A^{-2} \cdot (U^S - C/2) + [\Lambda, U^S] + \tilde{W}. \tag{56}$$

This matrix equation is equivalent to equations (39) and (44) for the precession of the angular momentum vector and the vibration of the axis lengths.

3. Conclusion

This paper demonstrates the simplicity and power of the algebraic mean field method in the case of gcm(3). Starting from the definition of the gcm(3) Lie algebra of observables and following a well-defined construction, I derive the Lax equation that determines Hamiltonian mean field dynamics of gcm(3) densities on GCM(3) coadjoint orbits. I also show that the Lax equation is equivalent to the Riemann ellipsoid system of equations.

All the irreducible unitary representations of GCM(3) are produced via the method of geometric quantization [31]. This quantization technique applies to integral coadjoint orbits which are special orbits that satisfy a kind of Bohr–Sommerfeld quantization rule [23–25]. For gcm(3) the integral orbits are those for which the Kelvin circulation $|C|$ equals a nonnegative integer multiple of $\hbar$.

Kirillov's metatheorem asserts that all the properties of a unitary irreducible representation of a Lie group are encoded in the symplectic geometry of its integral coadjoint orbits. This sweeping metatheorem is unproven, but it motivates an important research programme in Lie representation theory that has achieved significant results [23, 32]. For algebraic mean field theory the metatheorem indicates that quantum properties of a group theoretic model may be inferred from an investigation of integral coadjoint orbits. For example, the decomposition of unitary discrete series representations of $Sp(3, R)$ into irreducible representations of GCM(3) [33] is given correctly by the range of the gcm(3) Casimir function on integral coadjoint orbits of $Sp(3, R)$ [16]. Algebraic mean field theory, although a semiclassical approximation, replicates many exact quantum results using a simpler mathematical framework than representation theory. When necessary, the quantum representations may be recovered by geometric quantization of the integral coadjoint orbits.

When Ψ is a vector in the space of a representation π of a Lie group G, the states in the set $\mathcal{C}(\Psi) = \{\pi(g)\Psi \mid g \in G\}$ are called coherent states [34–37]. If ϱ is the density corresponding to Ψ, then $\mathrm{Ad}^*_g\varrho$ is the density corresponding to the coherent state $\pi(g)\Psi$:

$$\mathcal{C}(\Psi) \to \mathcal{O}_\varrho, \qquad \pi(g)\Psi \mapsto \mathrm{Ad}^*_g\varrho, \tag{57}$$

where $\mathcal{O}_\varrho$ denotes the coadjoint orbit contained in the dual space of the group's Lie algebra. If the group G is semisimple, the representation π is an irreducible highest weight representation, and Ψ is a highest weight vector, then the mapping, equation (57), is a diffeomorphism and $\mathcal{O}_\varrho$ is an integral coadjoint orbit. In this favourable, case the space of coherent states is a symplectic manifold, and the properties of π may be determined by quantizing its coherent states, a method that is closely related to the geometric quantization construction for an integral coadjoint orbit [37]. But GCM(3) is not semisimple and the mapping, equation (57), is generally many-to-one. An exception is the $|C| = 0$ irreducible representation of GCM(3) that extends to an irreducible highest weight representation of the simple metaplectic group $Mp(3, R)$. The space of coherent states associated with such a highest weight representation of $Mp(3, R)$ is diffeomorphic to the symplectic manifold $Mp(3, R)/U(3) \cong \mathrm{GCM}(3)/SO(3) \cong \mathcal{O}_\varrho$, where ϱ is the density (12) with $|C| = 0$.

The coadjoint orbit used in a particular physical application is not limited to the class of integral orbits which correspond to irreducible representations. The freedom in choosing an orbit is an essential advantage to mean field theory. When one or more physically significant degrees of freedom are not part of the Lie algebra of observables, the quantum Hamiltonian operator is not an approximate function of the algebra generators, and its eigenstates are not vectors contained in one irreducible representation space. Thus, the dynamical symmetry is broken and no irreducible representation space adequately models the system. Nevertheless a mean field theory using one nonintegral coadjoint orbit may make a viable model. A typical example is collective rotational bands in deformed nuclei. Excitation energies and deformations of states forming a rotational band may be described accurately in many isotopes if the algebra contains the angular momentum and a quadrupole operator, e.g., $su(3)$, rot(3), or gcm(3). However, pairing and spin–orbit forces strongly break the symmetry of the ground state of the band, and the ground-state wavefunction is mixed among many irreducible representation spaces. In this scenario, the coadjoint orbit adopted for mean field theory should be the orbit that contains the density of the ground state. The mean field approximation applies to the band members when the energies of the excited states are given accurately by a function of the collective observables in the algebra.

A generalization of the Hohenberg–Kohn theorem of density functional theory shows that there *exists* an energy function on the dual space of any Lie algebra of observables whose global minimum is the density of the exact ground-state wavefunction [38, 39]. But, like the original Hohenberg–Kohn proof, 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 knowledge of the existence of the exact energy function in traditional Hohenberg–Kohn density functional theory stimulates the efforts of many researchers, especially in quantum chemistry, to find it. The energy function in group theoretical models is approximated usually by a rotationally invariant low-degree polynomial of the algebra generators, cf section 2.3. The polynomial's coefficients are chosen to attain a good fit to experimental energy levels.

When the dimension of the algebra or the dimension of the representation space is large, representation theory may become intractable, and the mean field approximation is the only useful method available to create an algebraic physical model. In the case of the noncompact algebra gcm(3), the irreducible representations are infinite-dimensional, while the dimension

of a coadjoint orbit is either 14 or 12. The gcm(3) mean field theory only requires matrix operations with 6×6 real matrices. For a matrix Lie algebra, calculations in the mean field approximation involve just matrix operations.

Any dynamical symmetry algebra $\mathfrak{g}$ determines a mean field theory and the general procedure for its construction is clear. The model densities are the points of one coadjoint orbit $\mathcal{O}_\varrho$ of the dynamical symmetry group in the algebra's 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. The final form of the mean field theory simplifies when the algebra has a faithful matrix representation, as in equation (1) for gcm(3). When the coadjoint action is matrix conjugation, a Lax equation, such as equation (21), determines the dynamics. In future work the mean field theories associated with dynamical symmetry algebras of the interacting boson model will be investigated, e.g., $\mathfrak{g} = u(6), u(5), so(6), so(5)$ [40].

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