DETECTING THE MOMENTS OF INERTIA OF A MOLECULE VIA ITS ROTATIONAL SPECTRUM, II

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Abstract. Let G be one of the three-dimensional compact simple Lie groups SU(2) or SO(3). The Laplace-Beltrami spectrum is shown to mutually distinguish isometry classes of left-invaraint metrics on G. Consequently, the rotational spectrum of a molecule determines its moments of inertia.

1. Introduction

Riemannian homogeneous spaces are not, in general, determined by their Laplace spectrum. For example, Schueth demonstrated that the classical Lie groups $\mathrm{SO}(n \geq 8)$, $\mathrm{SU}(n \geq 6)$ and $\mathrm{Sp}(n \geq 8)$ each admit continuous one-paramter families of isospectral left-invariant metrics [Sc]. In fact, the Lie groups $\mathrm{SO}(n \geq 11)$, SO(9), $\mathrm{SU}(n \geq 8)$, and $\mathrm{Sp}(n \geq 4)$ each admit continuous multi-dimensional families of isospectral left-invariant metrics [Pr]. Although the isospectral deformations produced in [Sc, Pr] can be arranged to occur arbitrarily close to a bi-invariant metric, it is interesting to note that a bi-invariant metric on a compact Lie group is spectrally isolated within the space of all left-invariant metrics [GSS]; consequently, there are no paths of isospectral left-invariant metrics passing through a bi-invariant metric.

The construction method used in [Sc, Pr] exploits the fact that the Lie groups in question have rank at least two. We demonstrate that there are no non-trivial isospectralities among the left-invariant metrics on a compact Lie group of rank one.

Theorem 1.1. *Let G be either* SU(2) *or* SO(3)*. If g_1 and g_2 are isospectral left-invariant metrics on G, then g_1 and g_2 are isometric. Specifically, the first four heat invariants mutually distinguish isometry classes of left-invariant metrics on G.*

As spectral geometry has its origins in spectroscopy and quantum mechanics, we note that Theroem 1.1 has the following application to physical chemistry, which we will explain in Section 7.

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Theorem 1.2 (Physical Chemistry Application of Theorem 1.1)**.** *The rotational spectrum of a molecule determines its moments of inertia.*

Riemannian homogeneous manifolds (M, g) and $(\widehat{M}, \hat{g})$ have *identical* curvature tensors R and $\widehat{R}$ if for each $p \in M$, $\hat{p} \in \widehat{M}$ there is an isometry $F : (T_pM, g_p) \to (T_{\hat{p}}\widehat{M}, \hat{g}_{\hat{p}})$ such that $F^*\widehat{R}_{\hat{p}} = R_p$. In dimension 2 it is clear that homogeneous manifolds with identical curvature tensors are locally isometric. In contrast, continuous families of non-isometric left-invariant metrics on SU(2) (resp. SO(3), $\mathrm{SL}(2,\mathbb{R})$) with identical curvature tensor are exhibited in [La, ScWo1, ScWo2]. The methods employed in proving Theorem 1.1 allow us to show that these ambiguities can be resolved by considering the volume.

Theorem 1.3. *Let G be either* SU(2) *or* SO(3)*. Left-invariant metrics on G with identical volume and curvature tensors are isometric.*

The first three heat invariants of a left-invariant metric g on SU(2) or SO(3) are $a_0 = V$, $a_1 = \frac{1}{6}VS$, and $a_2 = \frac{1}{360}V(2(|R|^2 - |\rho|^2) + 5S^2)$, where V, S, R, and ρ denote the volume, scalar curvature, curvature tensor, and Ricci tensor of g, respectively. Although volume and the curvature tensor determine $\{a_0, a_1, a_2\}$, these heat invariants need not determine the isometry class of g. Examples presented in Section 6 illustrate this fact. Nevertheless, $\{a_0, a_1, a_2\}$ nearly specify isometry classes.

Theorem 1.4. *Let G be* SU(2) *or* SO(3) *and let g be a left-invariant metric on G.*

1. *If g is scalar flat, then the first three heat invariants determine the isometry class of g among left-invariant metrics.*
2. *There is at most one additional isometry class of left-invariant metrics on G having the same first three heat invariants as g.*

To the best of our knowledge there are no known examples of isospectral compact homogeneous 3-manifolds. This contrasts with the case of *locally* homogeneous 3-manifolds [Vi, R, DoRo]. Theorem 1.1 and the non-existence of isospectralities amongst flat 3-tori [Schi] motivates the following problem.

Problem. *Does the Laplace spectrum mutually distinguish compact homogeneous 3-manifolds?*

We conclude with a brief outline. *Heat invariants* are a family of spectral invariants obtained by integrating universal polynomials in the components of the curvature tensor over the manifold. They are computable at a point in a homogeneous manifold. Section 2 reviews this material and introduces the *modified heat invariants* for a homogenous manifold. These determine and are determined by the ordinary heat invariants. Section 3 reviews a parameterization of the isometry classes of left-invariant metrics on SU(2) and SO(3) in terms of points (x, y, z) from a convex subset $\mathcal{M}$ of $\mathbb{R}^3$ and expresses the modified heat invariants (implicitly) as functions on $\mathcal{M}$. A preliminary analysis of the modified heat invariants as (implicit) functions on $\mathcal{M}$ is carried out in Section 4. The main theorems are proven in Section 5, followed by an example in Section 6, and the application to Physical Chemistry in Section 7.

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2. **Heat invariants**

The Laplace-Beltrami operator of a closed and connected Riemannian n-manifold (M, g) is the (essentially) self-adjoint operator $\Delta_g \equiv -\operatorname{div} \circ \operatorname{grad}_g$ on $L^2(M, \nu_g)$. The sequence $\lambda_0 = 0 < \lambda_1 \leq \lambda_2 \leq \cdots \nearrow \infty$ of eigenvalues of Δ_g, repeated according to multiplicity, is the *spectrum* of (M, g) and we will say that two manifolds are *isospectral* when their spectra agree.

The heat semi-group $\{e^{-t\Delta}\}_{t>0}$ is a family of self-adjoint operators on $L^2(M, \nu_g)$ defined by $e^{-t\Delta}\phi \equiv e^{-t\lambda}\phi$ for each $t > 0$ and λ-eigenfunction ϕ, and extended linearly to all of $L^2(M, \nu_g)$. The trace of these operators, $Z_{(M,g)}(t) \equiv \operatorname{Tr}(e^{-t\Delta})$, admits an asymptotic expansion

$$Z_{(M,g)}(t) \sim (4\pi t)^{-n/2} \sum_{m=0}^{\infty} a_m(M, g) t^m,$$

as t approaches 0 from above [MiPl].

The coefficients $\{a_m(M, g)\}_{m=0}^{\infty}$ in this expression are the *heat invariants* of (M, g). Isospectral manifolds clearly have equal heat invariants. There are universal polynomials in the components of the curvature tensor and its covariant derivatives, $u_m(M, g)$, such that $a_m(M, g) = \int_M u_m(M, g)\, d\nu_g$ [Be, p. 145] or [Sa2, Chp. VI.5]. Explicit formulae for the heat invariants are known in few cases (cf. [Po]).

Let ∇, $R = (R^i_{jkl})$, $\rho = (\rho_{jl} = R^i_{jil})$, $S = (g^{jl}\rho_{jl})$, and ν_g denote the Levi-Civita connection, Riemannian curvature tensor, Ricci curvature tensor, scalar curvature, and Riemannian density, respectively. We follow the sign convention for the curvature tensor in [Ta] and [Sa1]; namely, for smooth vector fields $X, Y, Z \in \chi(M)$

$$R(X, Y)Z = \nabla_{[X,Y]}Z - [\nabla_X, \nabla_Y]Z. \tag{2.1}$$

The first four heat invariants are given by ([Ta]):

$$a_0(g) = \operatorname{vol}(M, g) = \int_M 1\, d\nu_g, \tag{2.2}$$

$$a_1(g) = \frac{1}{6} \int_M S\, d\nu_g, \tag{2.3}$$

$$a_2(g) = \frac{1}{360}\int_M 2(|R|^2 - |\rho|^2) + 5S^2\, d\nu_g, \tag{2.4}$$

and

$$a_3(g) = \frac{1}{6!}\int_M \bar{A} - \frac{1}{9}|\nabla R|^2 - \frac{26}{63}|\nabla\rho|^2 - \frac{142}{63}|\nabla S|^2 + \frac{2}{3}S(|R|^2 - |\rho|^2) + \frac{5}{9}S^3\, d\nu_g, \tag{2.5}$$

where $\bar{A}$ is defined by

$$\bar{A} = \frac{8}{21}(R, R, R) - \frac{8}{63}(\rho; R, R) + \frac{20}{63}(\rho;\rho;R) - \frac{4}{7}(\rho\rho\rho),$$

and where for tensor fields $P = (P_{ijkl})$, $Q = (Q_{ijkl})$, $T = (T_{ijkl})$, $U = (U_{ij})$, $V = (V_{ij})$, and $W = (W_{ij})$ on (M, g), we have the following products

$$\begin{aligned}
(P, Q) &= P_{ijkl}Q^{ijkl},\\
|P|^2 &= (P, P),\\
(P, Q, T) &= P^{ij}_{kl}Q^{kl}_{rs}T^{rs}_{ij},\\
(U; Q, T) &= U^{rs}Q_{rjkl}T^{jkl}_{s},\\
(U; V; T) &= U^{ij}V^{jl}T_{ijkl},\\
(UVW) &= U^i_jV^j_kW^k_i.
\end{aligned}$$

Specialization to three-manifolds. Assume that (M, g) is three-dimensional. At each point $p \in M$ there is a local orthonormal framing $\{e_1, e_2, e_3\}$ of TM that diagonalizes the Ricci curvature tensor. With respect to this framing,

$$R(e_i, e_j)e_k = 0 \tag{2.6}$$

whenever i, j, and k are distinct. For $i \neq j$, let $K_{ij} = g(R(e_i, e_j)e_i, e_j)$ denote the *principal curvatures* and $\Gamma^k_{ij} = g(\nabla_{e_i}e_j, e_k)$ the Christoffel symbols. Routine calculations yield the following expressions derived with respect to a local framing satisfying (2.6):

$$S = 2\{K_{12} + K_{13} + K_{23}\}, \tag{2.7}$$

$$|R|^2 = 4\{(K_{12})^2 + (K_{13})^2 + (K_{23})^2\}, \tag{2.8}$$

$$|\rho|^2 = (K_{12} + K_{13})^2 + (K_{12} + K_{23})^2 + (K_{13} + K_{23})^2. \tag{2.9}$$

With the additional hypothesis that

$$[e_i, e_j] \perp e_i, e_j, \tag{2.10}$$

maintained in the cases of interest, we obtain:

$$|\nabla R|^2 = 8\{(\Gamma_{12}^3 K_{13} + \Gamma_{13}^2 K_{12})^2 + (\Gamma_{21}^3 K_{23} + \Gamma_{23}^1 K_{12})^2 + (\Gamma_{31}^2 K_{23} + \Gamma_{32}^1 K_{13})^2\}, \tag{2.11}$$

$$|\nabla \rho|^2 = \frac{1}{4}|\nabla R|^2, \tag{2.12}$$

$$(R, R, R) = 8\{(K_{12})^3 + (K_{13})^3 + (K_{23})^3\}, \tag{2.13}$$

$$(\rho; R, R) = 2\{(K_{12} + K_{13})[(K_{12})^2 + (K_{13})^2] + (K_{12} + K_{23})[(K_{12})^2 + (K_{23})^2] + (K_{13} + K_{23})[(K_{13})^2 + (K_{23})^2]\}, \tag{2.14}$$

$$(\rho; \rho; R) = 2\{K_{12}(K_{12} + K_{13})(K_{12} + K_{23}) + K_{13}(K_{12} + K_{13})(K_{13} + K_{23}) + K_{23}(K_{12} + K_{23})(K_{13} + K_{23})\}, \tag{2.15}$$

$$(\rho\rho\rho) = (K_{12} + K_{13})^3 + (K_{12} + K_{23})^3 + (K_{13} + K_{23})^3. \tag{2.16}$$

Specialization to locally homogeneous manifolds. Assume that (M, g) is a closed locally homogeneous Riemannian manifold. Then S, $|R|$ and $|\rho|$ $|\nabla R|^2$, $|\nabla\rho|^2$, $|\nabla S|^2$, and $\bar{A}$ are constant functions on M. It follows that $\{a_0, a_1, a_2, a_3\}$ determine and are determined by $\{\text{vol}(M, g), S, |R|^2 - |\rho|^2, \Theta\}$ where

$$\Theta = \bar{A} - \frac{1}{9}|\nabla R|^2 - \frac{26}{63}|\nabla\rho|^2.$$

Consider the following *modified heat invariants* of a closed locally homogeneous space (M, g). For $\omega > 0$, define

$$V(g, \omega) = (\frac{\text{vol}(g)}{\omega})^2, \tag{2.17}$$

$$\tilde{a}_0(g; \omega) = 64V(g, \omega)^2, \tag{2.18}$$

$$\tilde{a}_1(g; \omega) = 2SV(g, \omega), \tag{2.19}$$

$$\tilde{a}_2(g; \omega) = 8V(g, \omega)^2(|R|^2 - |\rho|^2), \tag{2.20}$$

and

$$\tilde{a}_3(g; \omega) = \frac{63\Theta(4V(g, \omega))^3}{16}. \tag{2.21}$$

For each $j \in \{0, 1, 2, 3\}$ and $\omega > 0$, the collection of modified heat invariants $\tilde{a}_0(g, \omega), \dots \tilde{a}_j(g, \omega)$ determine and are determined by the ordinary heat invariants $a_0(g), \dots a_j(g, \omega)$.

3. Isometry classes of left-invariant metrics on SU(2)

Let G be a compact Lie group endowed with a fixed bi-invariant metric g_0 induced by an Ad-invariant inner product $\langle\cdot,\cdot\rangle_0$ on the Lie algebra $\mathfrak{g}$. Let g be an arbitrary left-invariant metric on G induced by an inner product $\langle\cdot,\cdot\rangle$ on $\mathfrak{g}$. Define a positive self-adjoint isomorphism $\Omega : (\mathfrak{g}, \langle\cdot,\cdot\rangle_0) \to (\mathfrak{g}, \langle\cdot,\cdot\rangle_0)$ by $\langle X, Y\rangle = \langle \Omega(X), Y\rangle_0$, for each $X, Y \in \mathfrak{g}$.

Let $\{u_1, \ldots, u_n\} \subset \mathfrak{g}$ be an $\langle\cdot,\cdot\rangle_0$-orthonormal basis consisting of eigenvectors of Ω with corresponding positive eigenvalues $\mu_1^2, \mu_2^2, \ldots, \mu_n^2 > 0$. The vectors $\{u_1, \ldots, u_n\}$ are referred to as *eigenvectors of the metric g* (with respect to the background metric g_0) and the corresponding eigenvalues are referred to as the *eigenvalues of the metric g* (with respect to the background metric g_0). Isometry classes of left-invariant metrics on SO(3) are classified by the multi-set of their eigenvalues [BFSTW].

Proposition 3.1 ([BFSTW])**.** *Two left-invariant metrics on* SO(3) *have the same multi-set of eigenvalues (with respect to a background bi-invariant metric g_0) if and only if they are isometric.*

The following corollary is immediate since the two-fold covering map $\pi : \mathrm{SU}(2) \to \mathrm{SO}(3) = \mathrm{SU}(2)/Z(\mathrm{SU}(2))$ induces a bijection between isometry classes of left-invariant metrics on SU(2) and SO(3).

Corollary 3.2. *Two left-invariant metrics on* SU(2) *have the same multi-set of eigenvalues (with respect to a background bi-invariant metric g_0) if and only if they are isometric.*

Let $G = \mathrm{SU}(2)$. Its Cartan-Killing form, $B(x, y) = \mathrm{trace}(\mathrm{ad}(x)\,\mathrm{ad}(y))$ for $x, y \in \mathfrak{su}(2)$, is symmetric and negative-definite. For each $c > 0$, the inner-product $-cB$ induces a bi-invariant metric on SU(2). Let $\{u_1, u_2, u_3\}$ be a $-cB$ orthonormal basis of $\mathfrak{su}(2)$.

Define structure constants α_{ijk} by $[u_i, u_j] = \sum_{k=1}^{3} \alpha_{ijk} u_k$. Use the fact that $B([u_i, u_j], u_k) = B(u_i, [u_j, u_k])$ to deduce $\alpha_{ijk} = \alpha_{jki} = \alpha_{kij}$ for any $i, j, k \in \{1, 2, 3\}$. Therefore, there is a nonzero δ such that the only nonzero structure constants are $\alpha_{123} = \alpha_{231} = \alpha_{312} = \delta$. After possibly replacing u_1 with $-u_1$ we may assume that $\delta > 0$. Calculate $-cB(u_i, u_i) = 2c\delta^2$ so that $2c\delta^2 = 1$. Summarizing, after possibly replacing u_1 with $-u_1$ in a $-cB$ orthonormal basis of $\mathfrak{su}(2)$,

$$[u_1, u_2] = \frac{1}{\sqrt{2c}} u_3 \quad [u_2, u_3] = \frac{1}{\sqrt{2c}} u_1 \quad [u_3, u_1] = \frac{1}{\sqrt{2c}} u_2. \tag{3.1}$$

The bi-invariant metric on SU(2) induced from $-cB$ is isometric to the round three-sphere of radius $\sqrt{8c}$, constant sectional curvatures $\frac{1}{8c}$, and volume $32\sqrt{2}\pi^2 c^{3/2}$.

Convention. *In the remainder of this paper, g_0 denotes the bi-invariant metric on* SU(2) *defined by $g_0 = -\frac{1}{2}B$, making $(\mathrm{SU}(2), g_0)$ isometric to the round 3-sphere with radius 2, constant sectional curvatures $\frac{1}{4}$, and volume $16\pi^2$.*

Let g denote a left-invariant metric on SU(2) with eigenvectors $\{u_1, u_2, u_3\}$ and corresponding eigenvalues $\mu_1^2, \mu_2^2, \mu_3^2 > 0$. Set

$$x = \mu_3^2, \quad y = \mu_2^2, \quad z = \mu_1^2. \tag{3.2}$$

Letting the symmetric group on three elements, S_3, act on ordered triples in the usual way, Corollary 3.2 implies that isometry classes of left-invariant metrics can be identified with $\mathcal{M} = \mathbb{R}_+^3/S_3$, where $\mathbb{R}_+$ is the set of positive real numbers.

Given an isometry class $[g] \in \mathcal{M}$, its *standard representation* is the ordered triple $(x, y, z) \in \mathbb{R}_+^3$, where $x \geq y \geq z > 0$, so that $\mathcal{M}$ is in bijective correspondence with the set $\{(x, y, z) \in \mathbb{R}^3 \,|\, x \geq y \geq z > 0\}$. Under this parametrization the isometry classes of the constant curvature metrics are given by $[(r, r, r)]$, with $r > 0$; in particular, the isometry class of g_0 corresponds to $[(1, 1, 1)]$.

Following Section 2 (see p. 5), let $\omega = \mathrm{vol}(g_0)$ and define the positive function $V : \mathcal{M} \to \mathbb{R}^+$ by

$$[(x, y, z)] \mapsto \left(\frac{\mathrm{vol}([(x, y, z)])}{\mathrm{vol}([(1, 1, 1)])}\right)^2 = \left(\frac{\mathrm{vol}([(x, y, z)])}{\mathrm{vol}([g_0])}\right)^2 = \left(\frac{\mathrm{vol}([(x, y, z)])}{16\pi^2}\right)^2$$

for $[(x, y, z)] \in \mathcal{M}$. Verify that V is the elementary symmetric polynomial of degree three in the variables x, y, z:

$$V([(x, y, z)]) = xyz = (\mu_1\mu_2\mu_3)^2. \tag{3.3}$$

The following scaled eigenvectors of the metric g form a g-orthonormal basis of $\mathfrak{su}(2)$:

$$\{e_1 = \frac{u_1}{\mu_1}, e_2 = \frac{u_2}{\mu_2}, e_3 = \frac{u_3}{\mu_3}\}.$$

After possibly replacing u_1 with $-u_1$ the Lie bracket structure of $\mathfrak{su}(2)$ is given by (3.1) with $c = \frac{1}{2}$:

$$[u_1, u_2] = u_3, \quad [u_2, u_3] = u_1, \quad [u_3, u_1] = u_2. \tag{3.4}$$

Letting α_{ijk} denote the structure constants $\alpha_{ijk} = g([e_i, e_j], e_k)$ of the basis $\{e_1, e_2, e_3\}$ with respect to the metric g, the *nonzero* structure constants are (3.5)

$$\alpha_{123} = -\alpha_{213} = \frac{\mu_3}{\mu_1\mu_2}, \quad \alpha_{231} = -\alpha_{321} = \frac{\mu_1}{\mu_2\mu_3}, \quad \alpha_{312} = -\alpha_{132} = \frac{\mu_2}{\mu_1\mu_3}.$$

Let ∇ denote the Levi-Civita connection for the metric g. The Christoffel symbols $\Gamma_{ij}^k = g(\nabla_{e_i} e_j, e_k)$ for the metric g are determined by substituting the expressions from (3.5) into Koszul's formula

$$2\Gamma_{ij}^k = \alpha_{ijk} - \alpha_{jki} + \alpha_{kij}.$$

The *nonzero* Christoffel symbols are given by

$$\Gamma_{12}^3 = -\Gamma_{13}^2 = \frac{\mu_2^2 + \mu_3^2 - \mu_1^2}{2\mu_1\mu_2\mu_3} = \frac{y + z - x}{2\sqrt{V}} \tag{3.6}$$

$$\Gamma_{23}^1 = -\Gamma_{21}^3 = \frac{\mu_1^2 + \mu_3^2 - \mu_2^2}{2\mu_1\mu_2\mu_3} = \frac{x+z-y}{2\sqrt{V}} \tag{3.7}$$

$$\Gamma_{31}^2 = -\Gamma_{32}^1 = \frac{\mu_1^2 + \mu_2^2 - \mu_3^2}{2\mu_1\mu_2\mu_3} = \frac{x+y-z}{2\sqrt{V}}. \tag{3.8}$$

Use (2.1) and (3.6)-(3.8) to deduce

$$R(e_i, e_j)e_k = 0 \tag{3.9}$$

whenever i, j, and k are all distinct. Use (2.1) and (3.6)-(3.8) to calculate the principal curvatures $K_{ij} \equiv K_{ij}(x, y, z) = g(R(e_i, e_j)e_i, e_j)$:

$$K_{12} = \frac{A}{4V}, \qquad K_{13} = \frac{B}{4V}, \qquad K_{23} = \frac{C}{4V}, \tag{3.10}$$

where

$$A \equiv A(x, y, z) = x^2 + y^2 - 3z^2 + 2(xz + yz - xy), \tag{3.11}$$

$$B \equiv B(x, y, z) = x^2 + z^2 - 3y^2 + 2(xy + yz - xz), \tag{3.12}$$

$$C \equiv C(x, y, z) = y^2 + z^2 - 3x^2 + 2(xy + xz - yz). \tag{3.13}$$

Introduce new variables

$$a = \frac{A+B}{2}, \quad b = \frac{A+C}{2}, \quad c = \frac{B+C}{2}. \tag{3.14}$$

Then

$$A = a + b - c, \quad B = a + c - b, \quad C = b + c - a. \tag{3.15}$$

Use (3.11)-(3.14) to derive

$$a \equiv a(x, y, z) = (x + y - z)(x - y + z), \tag{3.16}$$

$$b \equiv b(x, y, z) = (x + y - z)(-x + y + z), \tag{3.17}$$

$$c \equiv c(x, y, z) = (x - y + z)(-x + y + z). \tag{3.18}$$

For $[g] \in \mathcal{M}$ with standard representation (x, y, z) the inequalities $x \geq y \geq z > 0$ imply that $(x + y - z) > 0$ and $(x - y + z) > 0$. Use (3.16)-(3.18) to deduce

$$a > 0 \text{ and } bc \geq 0, \tag{3.19}$$

with equality if and only if $b = c = 0$ (equivalently, $x = y + z$).

We conclude this section by noting that it will be advantageous for us to partition $\mathcal{M}$ into two disjoint subsets.

Definition 3.3. An isometry class of left-invariant metrics $[g] \in \mathcal{M}$ is said to be of *Type I* if its standard representation (x, y, z) satisfies $x \neq y + z$; otherwise, it is said to be of *Type II*. Equivalently, $[g] \in \mathcal{M}$ is of Type I if its standard representation satisfies $b(x, y, z) \cdot c(x, y, z) > 0$; otherwise, it is of Type II.

4. Preliminary analysis of the $\tilde{a}_i$ as functions on $\mathcal{M}$

This section derives expressions for the modified heat invariants in terms of the variable a, b and c.

Section 3 parameterizes isometry classes of left-invariant metrics on SU(2) by points in the convex set $\mathcal{M} \simeq \{(x, y, z) \in \mathbb{R}^3 : x \geq y \geq z > 0\}$. The modified heat invariants $\tilde{a}_i(g, \omega)$, with g a left-invariant metric on SU(2) and $\omega = \mathrm{vol}(g_0) = 16\pi^2$, descend to well-defined functions $\tilde{a}_i([(x, y, z)], \omega)$ on $\mathcal{M}$

In this section, all variables are implicitly functions of isometry classes $[(x, y, z)] \in \mathcal{M}$. Let $\tilde{a}_i := \tilde{a}_i([(x, y, z)], \omega)$ and $V := V([(x, y, z)])$ throughout. By (3.4) and (3.9), the g-orthonormal frame e_1, e_2, e_3 satisfies condition (2.6). Therefore, (2.7)-(2.9) are valid in this frame, a fact used in the remainder of the paper. Let

$$P_1(x_1, x_2, x_3) = x_1 + x_2 + x_3$$
$$P_2(x_1, x_2, x_3) = x_1x_2 + x_1x_3 + x_2x_3$$
$$P_3(x_1, x_2, x_3) = x_1x_2x_3$$

denote the elementary homogeneous polynomials in the variables x_1, x_2, x_3.

Lemma 4.1. *The modified heat invariants $\tilde{a}_1$ and $\tilde{a}_2$ satisfy*

$$\tilde{a}_1 = P_1(a, b, c) \qquad \tilde{a}_2 = 4P_1^2(a, b, c) - 12P_2(a, b, c).$$

Proof. Compute using (2.7), (2.8), (2.9), (2.19), (2.20), (3.9), (3.10), and (3.15). □

Lemma 4.2. *An isometry class with modified heat invariants $\tilde{a}_1$ and $\tilde{a}_2$ is of Type II if and only if $\tilde{a}_2 = 4\tilde{a}_1^2$.*

Proof. An isometry class is of Type II if and only if $b = c = 0$. If $b = c = 0$, then $P_2(a, b, c) = ab + ac + bc = 0$. Lemma 4.1 then implies $\tilde{a}_2 = 4\tilde{a}_1^2$. Conversely, if $\tilde{a}_2 = 4\tilde{a}_1^2$, Lemma 4.1 implies that $P_2(a, b, c) = ab+ac+bc = 0$. Substituting (3.16)-(3.18) and simplifying yields $(x - y - z)(x + y - z)(x - y + z)(x + y + z) = 0$, whence $x = y + z$. □

Specialization to Type I isometry classes. In this subsection, $[(x, y, z)] \in \mathcal{M}$ denotes a Type I isometry class of metrics.

Lemma 4.3. *If $[(x, y, z)] \in \mathcal{M}$ is a Type I isometry class of metrics, then*

$$x^2 = \frac{a(b+c)^2}{4bc} \qquad y^2 = \frac{b(a+c)^2}{4ac} \qquad z^2 = \frac{c(a+b)^2}{4ab}.$$

$$xy = \frac{(b+c)(a+c)}{4c} \qquad xz = \frac{(a+b)(b+c)}{4b} \qquad yz = \frac{(a+b)(a+c)}{4a}.$$

Proof. As $[(x, y, z)]$ is of Type I, $abc > 0$. Substitute expressions (3.16) - (3.18) for a, b, c in terms of x, y, z into the above formulae and simplfy. □

Corollary 4.4. *If $[(x,y,z)] \in \mathcal{M}$ is a Type I isometry class of metrics, then*

$$4V(\Gamma_{12}^3)^2 = \frac{bc}{a} = 4V(\Gamma_{13}^2)^2,$$
$$4V(\Gamma_{23}^1)^2 = \frac{ac}{b} = 4V(\Gamma_{21}^3)^2,$$
$$4V(\Gamma_{31}^2)^2 = \frac{ab}{c} = 4V(\Gamma_{32}^1)^2.$$

Proof. Use (3.6)-(3.8) to derive expressions for $4V(\Gamma_{ij}^k)^2$ in terms of x^2, y^2, z^2, xy, xz, and yz; substitute the expressions for these monomials as rational functions of a, b, and c in Lemma 4.3, and then simplify. □

Corollary 4.5. *If $[(x,y,z)] \in \mathcal{M}$ is a Type I isometry class of metrics, then*

$$\tilde{a}_0 = \big(\frac{P_3^2 - 2P_1P_2P_3 + P_1^2P_2^2}{P_3}\big)(a,b,c).$$

Proof. Compute using (2.18), (3.3) and Lemma 4.3. □

Corollary 4.6. *If $[(x,y,z)] \in \mathcal{M}$ is a Type I isometry class of metrics, then*

$$\tilde{a}_3 = \big(\frac{-135P_3^2 + 44P_1^3P_3 - 198P_1P_2P_3 - 27P_1^2P_2^2 + 108P_2^3}{P_3}\big)(a,b,c).$$

Proof. Use (2.11)-(2.16), (2.20), (3.10), and the symmetry $\Gamma_{ij}^k = -\Gamma_{ik}^j$, to derive

$$\begin{aligned} 4\tilde{a}_3 &= 32[A^3 + B^3 + C^3] + 30[ABC] \\ &\quad -21[A^2(B+C) + B^2(A+C) + C^2(A+B)] \\ &\quad -27(4V)[(\Gamma_{12}^3)^2(A-B)^2 + (\Gamma_{21}^3)^2(A-C)^2 + (\Gamma_{31}^2)^2(B-C)^2]. \end{aligned} \tag{4.1}$$

Use Corollary 4.4 and (4.1) to derive

$$\begin{aligned} 4\tilde{a}_3 &= 32[A^3 + B^3 + C^3] + 30[ABC] \\ &\quad -21[A^2(B+C) + B^2(A+C) + C^2(A+B)] \\ &\quad -27[\tfrac{bc}{a}(A-B)^2 + \tfrac{ac}{b}(A-C)^2 + \tfrac{ab}{c}(B-C)^2]. \end{aligned} \tag{4.2}$$

Use (3.15) and (4.2) to obtain the desired expression for $\tilde{a}_3$ after simplification. □

Specialization to Type II isometry classes. In this subsection, $[(x,y,z)] \in \mathcal{M}$ denotes a Type II isometry class of metrics so that its standard representation (x,y,z) satisfies $x = y + z$. Use (3.16)-(3.18) and Lemma 4.1 to derive

$$\tilde{a}_1 = a = 4yz > 0, \quad b = c = 0. \tag{4.3}$$

Use (3.3) and (4.3) to derive

$$V = xyz = \frac{\tilde{a}_1 x}{4} = \frac{ax}{4}. \tag{4.4}$$

5. Proofs of Theorems 1.1, 1.3, and 1.4

We will use the following well-known lemma.

Lemma 5.1. *Values of the elementary symmetric polynomials $P_i(x_1,\dots,x_n)$, $i=1,\dots,n$, in complex variables $x_1,\dots,x_n$ uniquely specify the multi-set $\{x_1,\dots,x_n\}$.*

Proof. The lemma is a consequence of the fundamental theorem of algebra and the factorization $\Pi_{i=1}^n(x+x_1)=\Sigma_{i=0}^n P_{n-i}(x_1,\dots,x_n)x^i$. □

Remark 5.1. The two fold covering $\pi:\mathrm{SU}(2)\to\mathrm{SO}(3)$ induces a bijection between isometry classes of left-invariant metrics on SO(3) and SU(2) preserving the properties of having identical volumes, curvature tensors, and (modified) heat invariants.

Proof of Theorem 1.3. By Remark 5.1, it suffices to prove the Theorem when $G=\mathrm{SU}(2)$.

Given an isometry class $[g]\in\mathcal{M}$ the curvature tensor determines and is determined by the multi-set $\{K_{12},K_{13},K_{23}\}$ of principal curvatures. By (3.10) and (3.14), isometry classes of metrics $[g]$ and $[g']$ with identical curvature tensors and volumes have the same associated multi-set $\{a,b,c\}$ and $\{a',b',c'\}$. Lemma 4.1 implies that $\tilde a_i([g])=\tilde a_i([g'])$ for $i=1,2$ and Lemma 4.2 implies that the classes $[g]$ and $[g']$ have the same type.

Case I: Suppose $g=(x,y,z),g'=(x',y',z')\in\mathcal{M}$ are both of Type I. By the preceding discussion the multisets $\{a,b,c\}$ and $\{a',b',c'\}$ are identical. By Lemma 4.3 the multi sets $\{x,y,z\}$ ad $\{x',y',z'\}$ are identical, showing that the isometry classes agree.

Case II: Suppose $g=(x,y,z),g'=(x',y',z')\in\mathcal{M}$ are both of Type II.

As noted above, the corresponding multisets $\{a,b,c\}=\{a,0,0\}$ and $\{a',b',c'\}=\{a',0,0\}$ agree. From (4.4), $x=\frac{4V}{a}=x'$. Therefore $P_1(y,z)=x=x'=P_1(y',z')$. From (4.3), $4P_2(y,z)=a=4P_2(y',z')$. Lemma 5.1 implies that the multi-sets $\{x,y,z\}$ and $\{x',y',z'\}$ agree, concluding the proof. □

Proof of Theorem 1.4. By Remark 5.1, it suffices to prove the Theorem when $G=\mathrm{SU}(2)$.

Proof of (1): Let $[g]$ be an isometry class with zero scalar curvature. Assume that $[g']$ is an isometry class with $a_i([g])=a_i([g'])$ for $i=0,1,2$. Then $\tilde a_i([g])=\tilde a_i([g])$ for $i=0,1,2$ and $\tilde a_1=2SV=0$. By (4.3) both classes are Type I. By Lemma 4.1, $P_1(a,b,c)=P_1(a',b',c')=0$ and $P_2(a,b,c)=P_2(a',b',c')=-\tilde a_2/12$. By Lemma 4.5, $P_3(a,b,c)=P_3(a',b',c')=\tilde a_0$. The multi-sets $\{a,b,c\}$ and $\{a',b',c'\}$ coincide by Lemma 5.1. The isometry classes $[g]=[g']$ by Lemma 4.3.

Proof of (2): Let $[g]$ and $[g']$ be isometry classes with $a_i([g]) = a_i([g'])$ for $i = 0, 1, 2$. Then $\tilde{a}_i([g]) = \tilde{a}_i([g])$ for $i = 0, 1, 2$. By (4.3), the classes $[g]$ and $[g']$ have the same type. Lemma 4.1 implies that $P_i(a, b, c) = P_i(a, b, c)$ for $i = 1, 2$.

If $[g]$ and $[g']$ are both of Type I, then Lemma 4.5, shows that $P_3(a, b, c)$ and $P_3(a', b', c')$ are both roots of the quadratic polynomial

$$p(x) = x^2 - (2P_1P_2 - \tilde{a}_0)x + P_1^2P_2^2.$$

The Theorem now follows from Lemma 5.1 and Lemma 4.3.

If $[g]$ and $[g']$ are both of Type II, then Case II in the proof of Theorem 1.3 proves that $[g] = [g']$. □

Proof of Theorem 1.1. By Remark 5.1, it suffices to prove the Theorem when $G = \mathrm{SU}(2)$.

Assume that $[g]$ and $[g']$ are isometry classes with $a_i() = a_i()$ for $i = 0, 1, 2, 3$. Then $\tilde{a}_i([g]) = \tilde{a}_i([g])$ for $i = 0, 1, 2, 3$. By Lemma 4.2, the classes $[g]$ and $[g']$ are of the same type.

If $[g]$ and $[g']$ are both of Type I, then Lemma 4.1 implies that $P_i(a, b, c) = P_i(a', b', c')$ for $i = 1, 2$. Solving for P_3^2 in the formula for $\tilde{a}_0$ in Corollary 4.5 and then substituting into the expression for $\tilde{a}_3$ in Corollary 4.6 expresses P_3 as a rational function in P_1, P_2, $\tilde{a}_0$, and $\tilde{a}_3$. Therefore $P_3(a, b, c) = P_3(a', b', c')$. The multisets $\{a, b, c\}$ and $\{a', b', c'\}$ coincide by Lemma 5.1 and the isometry classes $[g] = [g']$ by Lemma 4.3.

If $[g]$ and $[g']$ are both of Type II, then Case II in the proof of Theorem 1.3 proves that $[g] = [g']$. □

6. Left-invariant metrics with equal a_0, a_1, and a_2

In this section, we demonstrate that the heat invariants a_0, a_1, a_2 do not in general determine the isometry class of a left-invariant metric on SU(2) (or on SO(3)). Equivalently, the first three modified heat invariants $\tilde{a}_0$, $\tilde{a}_1$, and $\tilde{a}_2$ do not determine the isometry class of a left-invariant metric on SU(2).

Lemma 6.1. *If $L, K \in \mathbb{R}$ satisfy $\Delta(L, K) := -4L^3 + L^2 + 18KL - 27K^2 - 4K \geq 0$, then the multi-set $\{a, b, c\}$ of solutions to the system*

$$P_1(a, b, c) = 1$$
$$P_2(a, b, c) = L$$
$$P_3(a, b, c) = K$$

is a multi-set of real (nonzero when $K \neq 0$) numbers.

Proof. If a, b, and c are solutions to the above system, then a, b, c are roots of the polynomial $p(x) = (x - a)(x - b)(x - c) = x^3 - x^2 + Lx - K$. The polynomial $p(x)$ has three real roots when its discriminant $\Delta = \Delta(L, K) \geq 0$. □

Let $L = -100$, $K_1 = 150 - 50\sqrt{5}$, $K_2 = 150 + 50\sqrt{5}$ and verify that

$$\Delta(L, K_1) \approx 3901700,$$

$$\Delta(L, K_2) \approx 1687099.$$

By Lemma 6.1, there exist distinct multi-sets $\{a_1, b_1, c_1\}$ and $\{a_2, b_2, c_2\}$ of nozero real numbers that solve the systems $P_1 = 1, P_2 = -100$, and $P_3 = K_i$ for $i = 1, 2$, respectively. Note that since $a_i b_i c_i = K_i > 0$ and $a_i b_i + a_i c_i + b_i c_i = -100$, we have (up to reordering), $a_i > 0$ and $b_i, c_i < 0$.

These two multi-sets determine isometry classes of metrics on SU(2) via Lemma 4.3 and these isometry classes are distinct by (3.16)-(3.18). Lemma 4.1 implies that $\tilde{a}_1 = 1$ and $\tilde{a}_2 = -1196$ for both classes. Finally, use Corollary 4.5 to calculate that $\tilde{a}_0 = 500$ for both classes.

7. An application to physical chemistry

Consider a rigid three-dimensional body $\mathbf{W}$ with center of mass at the origin. The *moment of inertia tensor* of $\mathbf{W}$ is a positive, self-adjoint linear isomorphism $\mathbb{I} : (\mathbb{R}^3, \langle\cdot,\cdot\rangle) \to (\mathbb{R}^3, \langle\cdot,\cdot\rangle)$ with respect to the Euclidean inner product $\langle\cdot,\cdot\rangle$. The *moment of inertia* of $\mathbf{W}$ about an axis $\mathbb{R}\mathbf{v}$, where $\mathbf{v} \in S^2$, is the scalar $\langle\mathbb{I}(\mathbf{v}), \mathbf{v}\rangle$ and measures the resistance of $\mathbf{W}$ to rotation about the axis $\mathbb{R}\mathbf{v}$.

The moment of inertia tensor has an orthonormal eigenbasis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$, with corresponding eigenvalues $0 < I_1 \le I_2 \le I_3$. The numbers I_1, I_2, and I_3 are the *principal moments of inertia* of the body and the vectors $\mathbf{e}_1, \mathbf{e}_2$ and $\mathbf{e}_3$ are the *principal axes*. A body is *spherical* when all principal moments of inertia are equal (e.g., the molecule methane), *symmetric* when exactly two of the principal moments of inertia are equal (e.g., benzene and chloromethane), and *asymmetric* otherwise (e.g., water).

The principal moments of inertia $0 < I_1 \le I_2 \le I_3$ determine a left-invariant metric $g_{(I_1,I_2,I_3)}$ on SO(3) as follows. Let $B(\cdot,\cdot)$ denote the Killing form on the Lie algebra $\mathfrak{so}(3)$ and let $\Theta_1, \Theta_2, \Theta_3$ denote the usual orthonormal basis of $\mathfrak{so}(3)$ with respect to the inner product $-B$. The triple $0 < I_1 \le I_2 \le I_3$ determines a self-adjoint map $\mathbb{I}_{I_1,I_2,I_3} : (\mathfrak{so}(3), -B) \to (\mathfrak{so}(3), -B)$ defined by $\Theta_j \mapsto \frac{1}{I_j}\Theta_j$, for $j = 1, 2, 3$. Then $g_{(I_1,I_2,I_3)}$ is the left-invariant metric on SO(3) induced by the inner product $\langle A, B\rangle = -B(\mathbb{I}_{I_1,I_2,I_3}(A), B)$ on $\mathfrak{so}(3)$. For example, the metric $g_{(1,1,1)}$ is the unique (up to scaling) bi-invariant metric on SO(3). Letting $\mathcal{I} = \{(I_1, I_2, I_3) : 0 < I_1 \le I_2 \le I_3\}$ and letting $\mathcal{M}_{\text{left}}(\text{SO}(3))$ denote the space of isometry classes of left-invariant metrics on SO(3), Proposition 3.1 implies that the map $\mathcal{I} \to \mathcal{M}_{\text{left}}(\text{SO}(3))$ defined by $(I_1, I_2, I_3) \mapsto g_{(I_1,I_2,I_3)}$ is a bijection.

Classical mechanics implies that the geodesics in SO(3) with respect to the left-invariant metric $g_{(I_1,I_2,I_3)}$ describe free rotations of $\mathbf{W}$ about its center of mass (cf. [GuSt, Section 28]). When $\mathbf{W}$ is a molecule, Schrödinger's equation implies that the eigenvalues associated to the Laplacian of $g_{(I_1,I_2,I_3)}$

describe the rotational spectrum (or energy levels) of the molecule. Specializing Theorem 1.1 to the class of left-invaraint metrics on SO(3) yields Theorem 1.2 from the introduction:

Theorem 1.2: *The rotational spectrum of a molecule determines its moments of inertia.*

Theorem 1.2 improves [Su, Corollary 1.4], where the second author establishes this result for spherical and symmetric molecules via wave-trace techniques.

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