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Orbit Recovery for Band-Limited Functions*

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Abstract. We study the third moment for functions on arbitrary compact Lie groups. We use techniques of representation theory to generalize the notion of band-limited functions in classical Fourier theory to functions on the compact groups $\mathrm{SU}(n), \mathrm{SO}(n), \mathrm{Sp}(n)$. We then prove that for generic band-limited functions the third moment or its Fourier equivalent, the bispectrum, determines the function up to translation by a single unitary matrix. Moreover, if $G = \mathrm{SU}(n)$ or $G = \mathrm{SO}(2n+1)$, we prove that the third moment determines the G-orbit of a band-limited function. As a corollary, we obtain a large class of finite-dimensional representations of these groups for which the third moment determines the orbit of a generic vector. When $G = \mathrm{SO}(3)$ this gives a result relevant to cryo-EM, which was our original motivation for studying this problem.

Key words. orbit recovery, bispectrum

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1. Introduction.

Let G be a compact Lie group. The purpose of this paper is to construct a class of finite-dimensional representations V of G for which the third moment can determine the orbit of a generic vector $f \in V$. As we explain, this work is motivated by several applications, including multi-reference alignment (MRA), cryo-EM, and machine learning.

In its basic form, the MRA problem seeks to recover a signal $f \in V$ from noisy group translates of the signal

$$y_i = g_i \cdot f + \epsilon_i,$$

where the g_i are randomly selected from a uniform distribution on G and the ϵ_i are taken from a Gaussian distribution $\mathcal{N}(0, \sigma^2 I)$ which is independent of the group element g_i. Without prior knowledge of the group elements, there is no way to distinguish f from $g \cdot f$ for any $g \in G$. Thus the MRA problem is one of orbit recovery. The MRA problem has been extensively studied in recent years, beginning with action of $\mathbb{Z}_N$ on $\mathbb{R}^N$ by cyclic shifts [3, 25, 8, 1, 5]. Other models include the dihedral group [10] and the rotation group $\mathrm{SO}(2)$ acting on band-limited functions on $\mathbb{R}^2$ [4, 24, 19]. The case where $G = \mathrm{SO}(3)$ is particularly important because of its connection to cryo-EM, a leading technique in molecular imaging. There, the measured

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data can be modeled as $y_i = T(g \cdot f) + \epsilon$, where f is the Coulomb potential of an unknown molecular structure and T is a tomographic projection [6].

In the low-noise regime, the products $g_i g_j^{-1}$ can be estimated using the method of synchronization and then the signal can be approximated by averaging [26]. However, in the high-noise regime, as is the case for cryo-EM measurements of small molecules, there is no way to accurately estimate the relation between the unknown group elements [7, Proposition 2.1]. One common approach to this problem is to use the *method of moments.* In this case, it can be shown [25] that the moments of the unknown signal can be accurately approximated by the computing of the corresponding moments of the experimental data. Thus, a crucial aspect of the MRA problem is understanding how to recover a signal $f \in V$ from its moments which are, by definition, G-invariant tensors in the signal.

In machine learning, it is desirable to build neural networks whose architecture reflects the intrinsic structure of the data. When the data has natural symmetries under a group G, then we want to build the network from *G-equivariant functions.* (Recall that if $\mathbb{V}$ and $\mathbb{W}$ are sets with a G action, then a function $f\colon \mathbb{V} \to \mathbb{W}$ is G-equivariant if $f(gv) = gf(v)$ for all $g \in G$.) The basic model of an equivariant neural network [14, 22] is a sequence of maps

$$\mathbb{R}^{n_0} \xrightarrow{A_1} \mathbb{R}^{n_1} \xrightarrow{\sigma_{b_1}} \mathbb{R}^{n_2} \dots \xrightarrow{\sigma_{b_{k-1}}} \mathbb{R}^{n_{k-1}} \xrightarrow{A_k} \mathbb{R}^{n_k},$$

where each $\mathbb{R}^{n_i}$ is a representation of G, the A_i are G-equivariant linear transformations, and the σ_{b_i} are nonlinear maps.

One difficulty with this model is that there may be relatively few G-equivariant linear maps of representations $A_i\colon \mathbb{R}^n \to \mathbb{R}^m$, so an equivariant neural network built this way may not be sufficiently expressive. Two common and mathematically related ideas are to use equivariant linear maps on tensors $(\mathbb{R}^n)^{\otimes k} \to (\mathbb{R}^m)^{\otimes \ell}$ or invariant polynomials of degree ℓ from $\mathbb{R}^n \to \mathbb{R}^m$ [21, 15, 12].

In both MRA and machine learning, the use of tensors is theoretically desirable, but the cost of computing tensors grows exponentially in the degree. In addition, in MRA the sample complexity (the minimum number of observations required for accurate approximation) grows as σ^{2d}, where d is the number of moments used and σ^2 is the variance of the noise. For this reason, we wish to identify representations for which moments of low-degree separate generic orbits. Previous work of Bendory and the first author demonstrated that neither the first nor the second moment carries enough information to separate orbits in all but the simplest representations [9]. Thus, an important problem is to understand and classify representations of compact groups for which the third moment can separate orbits. Previous work [2] showed that for any finite group the generic orbit in the regular representation can be recovered from the third moment using Jennrich's algorithm. More generally it is proved in [27] that if G is a positive-dimensional compact group, then the G-orbit of a function with nonsingular Fourier coefficients in the infinite-dimensional representation $L^2(G)$ can recovered from its third moment.

In this paper, we show that if G is one of the classical groups $\mathrm{SU}(n), \mathrm{SO}(n), \mathrm{Sp}(n)$, then it is possible to use representation theory to define the notion of *band-limited function* which generalizes the notion of band-limited function in Fourier theory as well as previous definitions for $G = \mathrm{SO}(3)$. Our main result can be stated as follows.

Theorem 1.1 (informal).

(i) *If G is one of the classical groups, then the generic band-limited function can be recovered up to translation by a single unitary matrix from its third moment.*

(ii) *The orbit of any generic band-limited function in $L^2(\mathrm{SU}(n))$ or real-valued band-limited function in $L^2(\mathrm{SO}(2n+1))$ can be recovered from its third moment.*

Remark 1.2. As is the case in Fourier theory, for any band level, the vector space of band-limited functions is finite dimensional. When we say that the orbits of generic band-limited functions can recovered from their third moments, we mean that the set of orbits which cannot be recovered is contained in a proper real algebraic subset of this finite-dimensional vector space. A precise sufficient condition in terms of the nonsingularity of Fourier coefficients is given in Theorem 4.1.

We note that our result gives a large class of finite-dimensional representations for which the third moment separates generic orbits.

The proof of Theorem 1.1 uses representation theory to generalize the well-known frequency marching result that states that a band-limited function on S^1 can be recovered from its bispectrum. A short discussion of potential algorithms using generalized frequency marching is given in section 5.2. When $G = \mathrm{SO}(3)$, Kakarala [20] showed that the SO(3)-orbit of a band-limited real-valued function can be recovered up to reflection from the bispectrum, and our result eliminates the reflection ambiguity. Indeed, the idea of using techniques of representation theory to study the orbit recovery problem was motivated by Kakarala's earlier work for SO(3).

In section 5.3, we focus on the group SO(3), since results for this group have the most potential applications. In particular, we compare our work with recent work of Liu and Moitra [23] for recovering band-limited functions in $L^2(S^2)$. We also prove (Corollary 5.1) that if we consider the finite-dimensional approximation of $L^2(\mathbb{R}^3)$ as band-limited functions on R spherical shells, where the number of shells exceeds the band limit, then the SO(3) orbit of a generic function can be recovered from the third moment. This is a standard assumption in the cryo-EM literature [4], and our result affirms many cases of a conjecture made in [2].

2. Moments of representations of compact groups.

Let V be a unitary representation of a compact group G. The dth moment of V is the function $m_d\colon V \to \underbrace{V \otimes \cdots \otimes V}_{d-1 \text{ times}} \otimes V^*$ defined by the formula

$$f \mapsto m_d(f)\colon = \int_G \overbrace{g \cdot f \otimes \cdots \otimes g \cdot f}^{d-1 \text{ times}} \otimes \overline{g \cdot f}\, dg. \tag{2.1}$$

Note that the formula of (2.1) is invariant under translation by G, so for any $f \in V$, $m_d(f)$ is a G-invariant element of the tensor $V^{d-1} \otimes V^*$ or, equivalently, a G-invariant element of $\mathrm{Hom}(V, V^d)$.

If V is a real representation, then the dth moment is an element of $\mathrm{Sym}^d V$ and the collection of moments form a set of generators for the invariant ring $\mathbb{R}[V]^G$.

When V is identified with a space of functions $D \to \mathbb{C}$, where D is a domain on which G acts (for example, we can take $D = G$ and consider V as a subspace of $L^2(G)$), then $m_d(f)$ is viewed as a function $D^d \to \mathbb{C}$ defined by the formula

$$m_d(f)(x_1,\dots,x_d) = \int_G (g\cdot f)(x_1)\dots(g\cdot f)(x_{d-1})\overline{(g\cdot f)(x_d)}\,dg, \tag{2.2}$$

where $g\cdot f\colon D\to\mathbb{C}$ is the function $(g\cdot f)(x) = f(g^{-1}x)$.

2.1. Moments and the decomposition into irreducibles. A general finite-dimensional representation of a compact group can be decomposed as $V = \oplus_{\ell=1}^{L} V_\ell^{R_\ell}$, where the V_ℓ are distinct nonisomorphic irreducible representations of G of dimension N_ℓ. An element $f\in V$ has a unique G-invariant decomposition as a sum

$$f = \sum_{\ell=1}^{L}\sum_{i=1}^{R_\ell} f_\ell[i], \tag{2.3}$$

where $f_\ell[i]$ is in the ith copy of the irreducible representation V_ℓ. For fixed ℓ, the vectors $f_\ell[1],\dots,f_\ell[R_\ell]$ determine an $N_\ell\times R_\ell$ matrix $A_\ell(f)$ which we sometimes refer to as the *coefficient matrix of* f *in* V_ℓ.

The dth moment is a map $m_d\colon V\to (V^{\otimes(d-1)}\otimes V^*)^G$, which takes a vector $f\in V$ to the invariant part of the tensor $f\otimes f\otimes\cdots\otimes\overline{f}$. Identifying $V^{\otimes(d-1)}\otimes V^* = \mathrm{Hom}(V, V^{\otimes d-1})$, the dth moment decomposes according to the decomposition of V into irreducibles as a function

$$m_d[V_{i_1},\dots,V_{i_d}]\colon V\to \oplus_{i_1,\dots,i_d}\mathrm{Hom}(W_{i_d}, W_{i_1}\otimes\cdots\otimes W_{i_{d-1}}))^G,$$

where $W_\ell = V_\ell^{R_\ell}$. By Schur's lemma, $m_d[V_{i_1},\dots,V_{i_d}]$ is nonzero if and only if the irreducible representation V_{i_d} is a summand in the tensor product $W_{i_1}\otimes\cdots\otimes W_{i_{d-1}}$.

The map $m_d[V_{i_1},\dots,V_{i_d}]$ can be described explicitly as follows: If $f = \sum_{\ell=1}^{L} A_\ell(f)$, where $A_\ell(f) = (f_\ell[1],\dots,f_\ell[R_L])\in W_\ell$, let $B_{i_d}(f)$ be the projection of

$$A_{i_1}(f)\otimes\cdots\otimes A_{i_{d-1}}(f)\in W_{i_1}\otimes\cdots\otimes W_{i_{d-1}}$$

to the isotypic component T_{i_d} of $W_{i_1}\otimes\cdots\otimes W_{i_{d-1}}$ corresponding to the irreducible representation V_{i_d}. Then $m_d[V_{i_1},\dots,V_{i_d}](f)$ is the element of $\mathrm{Hom}(W_{i_d}, T_{i_d})$ represented by the matrix $A_{i_d}(f)B_{i_d}(f)^*$.

In the case when $d=2$, there is a simple description of the information determined by the second moment.

Proposition 2.1 (see [9, Theorem 2.3]). *Let V be a finite-dimensional representation of G. The second moment $m_2(f)$ determines, for each irreducible V_ℓ appearing in V, the product $A_\ell(f)A_\ell(f)^*$. In particular, the second moment determines $A_\ell(f)$ up to translation by an element of $U(V_\ell)$ or, if $A_\ell(f)$ is real, an element of $O(V_\ell)$.*

The next result proves that if V contains a copy of the trivial representation, then the third moment determines the first and second moments.

Proposition 2.2. *If the coefficient matrix, $A_0(f)$, of the trivial representation is nonzero, then $m_1(f)$ and $m_2(f)$ are determined from $m_3(f)$.*

Proof. Since the trivial representation V_0 is one dimensional, the coefficient matrix $A_0(f) = (f_0[1], \ldots, f_0[R_0])$ is just a row vector of length R_0, where R_0 is the multiplicity. The first moment is simply the projection of $V \to V^G = V_0^{R_0}$ so $m_1(f) = A_0(f)$. On the other hand, consider the component $m_3[V_0, V_0, V_0]$ of the third moment which is a G-invariant map $V \to W_0 \otimes W_0 \otimes W_0^*$. Since G acts trivially on W_0, the entire tensor product $W_0 \otimes W_0$ is the V_0 isotypic component. Thus, $m_3(f)[V_0, V_0, V_0] = A_0(f)(A_0(f) \otimes A_0(f))^*$, where we view $A_0(f) \otimes A_0(f)$ as a matrix of size $1 \times R_0^2$. Among the entries of this matrix are the products $f_0[j]\overline{f_0[j]f_0[j]} = \overline{f_0[j]}|f_0[j]|^2$. Writing $f_0[j] = r_j e^{i\theta}$ for $r_j > 0$, we see that $f_0[j]$ is determined by $\overline{f_0[j]}|f_0[j]|^2$.

In particular, if $f_0[i] \neq 0$ is known, $m_2(f)$ is determined by $\frac{1}{|A_0(f)|}\int_G A_0[f] \otimes g \cdot f \otimes \overline{g \cdot f}$, which is a sum of components of $m_3(f)$. ∎

The following bootstrap result is a generalization of [2, Proposition 4.15].

Proposition 2.3. *Let V be a representation of G with $V = V_1^{R_1} \oplus \cdots \oplus V_L^{R_L}$, where $V_1, \ldots, V_L$ are distinct irreducibles. Assume that for every $1 \le k \le L$, the generic vector f in the representation $V_1^{R_1} \oplus \widehat{V_k^{R_k}} \oplus \cdots \oplus V_L^{R_L}$ has a trivial stabilizer. (Here the notation $\widehat{V_k^{R_k}}$ means that the summand is omitted.)*

If the orbit of a generic vector $f \in V$ is determined from the dth moment $m_d(f)$ and $W \supset V$ is another representation with the same irreducible components, then the orbit of a generic vector $h \in W$ is determined by its the dth moment $m_d(h)$.

Example 2.4. The hypothesis that W has the same irreducible components as V is necessary. Consider the case where $G = S^1$ and $V = V_0 \oplus V_1$, $W = V_0 \oplus V_1 \oplus V_3$, where the V_n is the one-dimensional representation of S^1, where S^1 acts with weight n; i.e., $e^{i\theta} \cdot v = e^{ni\theta}v$. If $v = (v_0, v_1) \in V$, then the third moment determines v_0 and $|v_1|^2$, which determine the vector v up to multiplication by an element S^1. On the other hand, the third moment of $w = (w_0, w_1, w_3) \in W$ determines $w_0, |w_1|^2, |w_3|^2$, which is not sufficient to determine the vector w up to multiplication by an element of S^1.

Proof. By induction on the multiplicities, we may reduce to the case that

$$W = V_1^{R_1} \oplus \cdots \oplus V_\ell^{R_\ell+1} \oplus \cdots \oplus V_L^{R_L},$$

i.e., all multiplicities of irreducibles in W are the same as in V, except for the multiplicity of V_ℓ, which is R_ℓ in V and $R_\ell + 1$ in W. By reordering the irreducibles, we assume that $\ell = 1$.

Suppose $h \in W$ has coefficient matrices $B_1, B_2, \ldots, B_L$, where $B_1 = (f_1[1], \ldots, f_1[R_1+1])$. For each $j = 1, \ldots, R_1+1$, consider the G-invariant projection $\pi_j \colon W \to V$ which sends h to the vector f_j with coefficient matrices $B_1^j, B_2, \ldots, B_L$, where $B_1^j = (f_1[1], \ldots, \widehat{f_1[j]}, \ldots, f_1[R_1+1])$ By assumption, the G-orbit of f_j is determined from $m_2(f_j) = m_2(\pi_j h))$. In particular, if h' is another vector in W with $m_d(h) = m_d(h')$ and coefficient matrices $B'_1, \ldots, B'_L$, then there exists $g_1, \ldots, g_{R_1+1} \in G$ such that $g_j(B_1^j, \ldots, B_L) = (B_1'^j, \ldots, B'_L)$. To show that g_j's are all equal, note that for any j_1, j_2 the vector in the representation $V_2^{R_2} \oplus \cdots \oplus V_L^{R_L}$ with coefficient matrices $B_2, \ldots, B_L$ is fixed by $g_{j_1}g_{j_2}^{-1}$ so by assumption on the representation we can conclude that $g_{j_1} = g_{j_2}$. Thus, there exists $g \in G$ such that for every j, $g(B_1^j, B_2, \ldots, B_L) = (B_1'^j, B'_2, \ldots, B_L)$. Since every row vector in B_1 (resp., B'_1) is in some matrix B_1^j (resp., $B_1'^j$) it follows that $g(B_1, \ldots, B_L) = (B'_1, \ldots, B'_L)$. In other words, $h' = gh$ for some $g \in G$. ∎

2.2. The Fourier transform on compact groups. If G is a compact group and $f \in L^2(G)$, then the *Fourier transform* (see [27] as well as [18, Chapter 8]) of f is a matrix-valued function $F(f)$ defined on the set representations of G by the formula

$$F(f)(V) = \int_G f(g) D_V(g)^* \, dg \in \mathrm{End}(V), \tag{2.4}$$

where $D_V(g)$ is the unitary linear transformation $V \to V$ defined by $v \mapsto gv$.

The matrix $F(f)(V)$ is called the *Fourier coefficient* of V. Later, we will implicitly choose a basis for each irreducible representation so we can view the Fourier coefficient as a matrix. As is the case for the classical Fourier transform, a function $f \in L^2(G)$ is uniquely determined by its Fourier coefficients $F(f)(V)$, where V runs through all irreducible representations of G [18, Theorem 31.5].

Conversely, if V is a representation of G and $T \in \mathrm{End}(V)$ is an endomorphism, then the inverse Fourier transform of T is the function

$$f_T(g) = \frac{1}{\dim V} \mathrm{Tr}(T D_v(g)^*). \tag{2.5}$$

2.3. The regular representation and higher-order spectra. Here we take $V = L^2(G)$ to be the regular representation. In this case,

$$m_d(f)(g_1, \ldots, g_d) = \int_G f(g^{-1}g_1) f(g^{-1}g_2) \ldots f(g^{-1}g_{d-1}) \overline{f(g^{-1}g_d)} \, dg.$$

Applying the change of variables $g = g^{-1}g_d$, we can rewrite

$$m_d(f)(g_1, \ldots, g_d) = m_d(f)(g_d^{-1}g_1, \ldots, g_d^{-1}g_{d-1}, 1).$$

Hence, after replacing g with g^{-1}, we may view the dth moment of the regular representation as the function on G^{d-1}:

$$m_d(f)(g_1, \ldots, g_{d-1}) = \int_G f^*(g) f(gg_1) \ldots f(gg_{d-1}) \, dg, \tag{2.6}$$

where $f^*(g) = \overline{f(g)}$.

The $(d-1)$*st higher-spectrum* $a_d(f)$ is defined as the Fourier transform of the function $m_d(f) \in L^2(G^{d-1})$. Since every irreducible representation of G^{d-1} is of the form $V_1 \otimes \cdots \otimes V_{d-1}$, we have that

$$\begin{aligned} a_d(f)(V_1 \otimes \cdots \otimes V_{d-1}) = \int_{G^{d-1}} &\left(\int_G f^*(g) f(gg_1) \ldots f(gg_{d-1}) \, dg \right) \\ &\times D_{V_1}(g_1)^* \otimes \cdots \otimes D_{V_{d-1}}(g_{d-1}^*) \, dg_1 \ldots dg_{d-1}. \end{aligned} \tag{2.7}$$

Using the change of coordinates where we replace g_i with gg_i and reversing the order of integration, the right-hand side of (2.7) becomes

$$\begin{aligned} &\int_G \int_{G^{d-1}} f(g_1) \ldots f(g_{d-1}) \\ &\quad \times [D_{V_1}(g_1)^* \otimes \cdots \otimes D_{V_{d-1}}(g_{d-1})^*)] \, dg_1 \ldots d_{g_{d-1}} [D_{V_1}(g) \otimes \cdots \otimes D_{V_{d-1}}(g)] f^*(g) \, dg \\ &= [F(f)(V_1) \otimes \cdots \otimes F(f)(V_{d-1})] \int_G f^*(g) [D_{V_1}(g) \otimes \cdots \otimes D_{V_{d-1}}(g)] \, dg \\ &= [F(f)(V_1) \otimes \cdots \otimes F(f)(V_{d-1})][F(f)(V_1 \otimes \cdots \otimes V_{d-1})]^*, \end{aligned} \tag{2.8}$$

where the product is taken in the ring $\mathrm{End}(V_1 \otimes \cdots \otimes V_{d-1})$. Since the $(d-1)$st higher spectrum is the Fourier transform of the dth moment and the Fourier transform is invertible, the $(d-1)$st higher spectrum carries the same information as the dth moment.

2.4. The bispectrum. When $d=3$, the third moment $m_d(f)$ carries the same information as the bispectrum $a_2(f)$ whose value on a tensor $V \otimes W$ is

$$a_2(f)(V \otimes W) = [F(f)(V) \otimes F(f)(W)][F(f)(V \otimes W)]^*. \tag{2.9}$$

For every pair of irreducible representations V, W, we choose an isomorphism

$$V \otimes W \simeq V_1 \oplus \cdots \oplus V_r$$

with the V_i not necessarily distinct irreducibles. It follows that there are unitary matrices $C_{V,W}$ such that for all $f \in L^2(G)$

$$F(f)(V \otimes W) = C_{V,W}\,(F(f)(V_1) \oplus \cdots \oplus F(f)(V_r))\,C^*_{V,W},$$

where we identify $F(f)(V \otimes W)$ as a matrix with respect to a pre-chosen basis for $V \otimes W$. Thus, we can rewrite the bispectrum as

$$a_2(f)(V \otimes W) = [F(f)(V) \otimes F(f)(W)]C_{V,W}[F(f)(V_1)^* \oplus \cdots \oplus F(f)(V_r)^*]C^*_{V,W}. \tag{2.10}$$

Lemma 2.5. *Let V and W be irreducible representations of G, and let V_i be any irreducible appearing as a summand in $V \otimes W$. If $f \in L^2(G)$ is chosen such that the Fourier coefficients $F(f)(V)$ and $F(f)(W)$ are invertible, then the Fourier coefficient $F(f)(V_i)$ is determined by $F(f)(V)$, $F(f)(W)$ and the coefficient $a_2(f)(V \otimes W)$ of the bispectrum.*

Proof. Since

$$a_2(f)(V \otimes W) = [F(f)((V) \otimes F(f)(W)][F(f)(V \otimes W)]^*$$

and $F(f)(V) \otimes F(f)(W)$ is invertible by hypothesis, we obtain

$$F(f)(V \otimes W)^* = [F(f)(V) \otimes F(f)(W)]^{-1} a_2(f)(V \otimes W).$$

Using the decomposition

$$F(f)(V_1 \otimes V_2) = C_{V,W}[F(f)(V_1) \oplus \cdots \oplus F(f)(V_r)]C^*_{V,W},$$

where $V_1, \ldots, V_r$ are irreducible, yields the lemma. ∎

Remark 2.6. The value of Lemma 2.5 is that it shows that if V, W are irreducibles and V_i is an irreducible summand appearing in $V \otimes W$, then $F(f)(V_i)$ is determined from $F(f)(V)$, $F(f)(W)$ and the bispectrum coefficient $a_2(f)(V \otimes W)$. We will use this observation repeatedly.

Proposition 2.7 (see [27, Theorem 5]). *If the Fourier coefficients of $f \in L^2(G)$ are all nonsingular, then f is uniquely determined by its bispectrum.*

Proof of sketch. We first observe that for every irreducible representation V, $a_2(f)(V\otimes\mathbf{1}) = F(f)(V)F(f)(V)^*$, where $\mathbf{1}$ denotes the trivial representation. Hence, we know the matrices $F(f)(V)$ up to multiplication by some unknown unitary matrix $u(V)\in U(V)$. In particular, if h is a function with the same bispectrum as f, then $F(h)(V) = F(f)(V)u(V)$ for all irreducible representations V. The goal is to show that these unitary matrices are all of the form $D_V(g)$ for a fixed $g\in G$.

Since we know that the function h whose Fourier coefficient $F(h)(V) = F(f)(V)u(V)$ has the same bispectrum as f, we see that

$$\begin{aligned}(2.11)\qquad &[F(f)(V)\otimes F(f)(W)][(F(f)(V\otimes W))]^* \\ &= [F(f)(V)u(V)\otimes F(f)(W)u(W)][F(f)(V\otimes W)u(V\otimes W))]^*.\end{aligned}$$

Since we assume that Fourier coefficients are all invertible, we can conclude that $u(V)\otimes u(W) = u(V\otimes W)$. Moreover, if $A\colon V\to W$ is an intertwining operator between representations, i.e., a G-invariant element of $\operatorname{Hom}(V,W)$, then $Au(V) = u(W)A$.

These facts imply that $u(V) = D_V(g)$ for some fixed element $g \in G$ by Tannaka–Krein duality [18, Theorem 30.43]. ■

3. Banding functions for simple compact Lie groups.

The goal of this section is to introduce the notion of band-limited functions on compact Lie groups, generalizing the usual notion of band-limited functions on S^1. We refer the reader to Appendix B for some of the basic terminology in the theory of compact Lie groups.

For functions on S^1, the notion of band limiting is well understood. We say that $f\in L^2(S^1)$ is b-band-limited if the Fourier coefficient $f_n = \int_{S^1} e^{in\theta} f(\theta)\, d\theta = 0$ for $|n| > b$, where the functions $\{e^{in\theta}\}_{n\in\mathbb{Z}}$ form an orthonormal basis for $L^2(S^1)$. For functions on S^2, there is also a corresponding notion of banding using the fact that any $f \in L^2(S^2)$ can be expanded in terms of spherical harmonics $\{Y_\ell^m(\phi,\theta)\}$, where $\ell \in \mathbb{N}$ and for each ℓ, m ranges from $-\ell$ to ℓ. In this context, we say that $f = \sum_{\ell,m} a_{\ell,m} Y_\ell^m$ is L-band-limited if $a_{\ell,m} = 0$ for all $\ell > L$ and all $m \in [-\ell, \ell]$. Band-limited functions on S^2 can be understood in terms of the representation theory of SO(3) as follows. The space of functions $L^2(S^2)$ decomposes as a representation of SO(3) into an infinite sum of irreducibles $\oplus_{\ell\geq 0} V_\ell$, where V_ℓ is the $(2\ell+1)$-dimensional irreducible representation of SO(3) spanned by the functions $\{Y_\ell^m\}_{m=-\ell,\dots,\ell}$. With this notation, any $f \in V_\ell$ has *band* ℓ and the space of L-band-limited functions is the finite-dimensional representation $\oplus_{\ell=0}^L V_\ell$.

Using the theory of highest-weight vectors, we show that the irreducible representations of a large class of Lie groups, including the classical groups $\mathrm{SU}(n), \mathrm{SO}(2n), \mathrm{Sp}(n)$, can be banded. However, for groups of rank more than one, there will be more than one representation with a given band b. Nevertheless, every irreducible representation of a given band b appears as a summand in the tensor product of irreducible representations of lower band. As a consequence, we can use a generalized frequency marching argument to show (Proposition 3.5) that if suitable Fourier coefficients are invertible, then the Fourier coefficients of irreducible representations of band $b > 1$ can be recovered from the bispectrum and the Fourier coefficients of the irreducible representations of band one. For the classical groups $\mathrm{SU}(n), \mathrm{SO}(n), \mathrm{Sp}(2n)$, we can go further and prove in Theorem 3.7 that the Fourier coefficients of the irreducible representations of band one can be ordered in such a way that they are determined from the bispectrum and the Fourier coefficient of a single representation which we call the *defining representation.* The defining representation corresponds to the smallest realization of the particular group as a group of unitary matrices. For $\mathrm{SU}(n)$ and $\mathrm{SO}(n)$, it is an n-dimensional representation, while for $\mathrm{Sp}(2n)$ it is a $2n$-dimensional representation.

3.0.1. Fundamental representations and banding for simply connected groups. We begin with the case that G is simply connected, which is true for $G = \mathrm{SU}(n)$ or $G = \mathrm{Sp}(n)$. Any compact Lie group is the maximal compact subgroup of a corresponding complex algebraic group $G_{\mathbb{C}}$ [13, Propositions 8.3, 8.6]. When G is simply connected, the representations of G correspond to the representations of $\mathfrak{g}$, where $\mathfrak{g}$ is the Lie algebra of $G_{\mathbb{C}}$ [17, Theorem 3.7]. Since $\mathfrak{g}$ is a semi-simple Lie algebra, any representation decomposes into a sum of irreducible representations. Each irreducible representation decomposes as a sum of *weight spaces.* These are the common eigenspaces for the action of the Cartan subalgebra $\mathfrak{h}$, which is the maximal abelian Lie subalgebra of $\mathfrak{g}$. The dimension of $\mathfrak{h}$ is called the *rank* of $\mathfrak{g}$. The eigenvalues for the action of $\mathfrak{h}$ on all representations of $\mathfrak{g}$ generate a lattice in $\mathfrak{h}^*$ called the weight lattice Λ_W. The eigenvalues for the action of $\mathfrak{g}$ on itself are called *roots*, and they generate the root lattice Λ_R in $\mathfrak{h}^*$. The root lattice Λ_R has finite index in the weight lattice Λ_W, and Λ_R is the dual lattice to Λ_W with respect to a natural inner product on $\mathfrak{h}^*$. The set of roots Φ of $\mathfrak{g}$ can be divided (by choice of a hyperplane in $\mathfrak{h}^*$) into positive and negative roots. The *positive simple roots* form the basis for the root lattice characterized by the property that any positive root is a nonnegative integral linear combination of the positive simple roots. A weight vector $\lambda \in \Lambda_W$ is *dominant* if its inner product with every positive simple root is nonnegative. Any dominant weight vector is a nonnegative integral linear span of the *fundamental weights* $\omega_1, \ldots, \omega_n$, where n is the rank of the Lie algebra $\mathfrak{g}$.

Irreducible representations of a semi-simple Lie algebra are determined by their *highest weight vectors,* which is the unique dominant weight of the irreducible representation which maximizes the sum of the inner products with the fundamental weights. Moreover, any dominant weight $\lambda = a_1\omega_1 + \cdots + a_n\omega_n$ with $a_i \in \mathbb{N}$ is the highest weight vector for a unique irreducible representation V_λ [16, p. 205].

Definition 3.1. *When G is simply connected, we define the* band *of the representation V_λ with the highest weight vector $\lambda = a_1\omega_1 + \cdots + \omega_n$ to be $b = a_1 + \cdots + a_n$.*

3.0.2. Type A_{n-1}: the group $\mathrm{SU}(n)$. The compact group $\mathrm{SU}(n)$ is a compact form of the algebraic group $\mathrm{SL}(n,\mathbb{C})$, and because $\mathrm{SU}(n)$ is simply connected, representations of $\mathrm{SU}(n)$ bijectively correspond to representations of the complex Lie algebra $\mathfrak{sl}_n$, which has type A_{n-1} for $n \geq 2$. The Lie algebra $\mathfrak{sl}_n$ is the vector space of traceless $n \times n$ complex matrices, and the Cartan subalgebra $\mathfrak{h}$ is the subspace of diagonal traceless matrices.

The weight lattice is the lattice spanned by vectors $L_1, \ldots, L_{n-1}, L_n$ with $L_1 + \cdots + L_n = 0$, where L_i is the function on $\mathfrak{h}$ which reads the ith entry along the diagonal. In this case, the positive simple roots are

$$L_1 - L_2, \ldots, L_{n-1} - L_n$$

and the fundamental weights are [16, p. 216]

$$\omega_i = \sum_{j \leq i} L_j$$

for $i < n$. The irreducible representation corresponding to ω_1 is the n-dimensional defining representation V, i.e., the representation $\mathrm{SU}(n) \subset U(n)$. The other representations of band one (i.e., those associated to the fundamental representations) are the exterior powers $V_k = \wedge^k V$ for $i = 1, \ldots, n-1$. (Note that $\wedge^n V$ is the trivial representation which is consistent with the fact that $L_1 + \cdots + L_n = 0$.)

Example 3.2 (The groups SU(2) and SU(3)). The group SU(2) has rank one, and there is a single representation of each band, namely the representation $V_n = \mathrm{sym}^n V_1$, where V_1 is the two-dimensional defining representation and $V_n = \mathrm{sym}^n V_1$ can be identified with the vector space of homogeneous binary forms of degree n.

By contrast, group SU(3) has two irreducible representations of band one: the defining representation V_1 and $\wedge^2 V_1 \simeq V_1^*$. The irreducible representations of band b can be indexed by pairs of nonnegative integers (n_1, n_2) with $n_1 + n_2 = b$. Hence, there are $b+1$ irreducible representations of each band. The dimension of the irreducible representation Γ_{n_1,n_2} with the highest weight vector $n_1\omega_1 + n_2\omega_2$ is $\frac{(n_1+1)(n_2+1)(n_1+n_2+2)}{2}$ [16, formula (15.17), p. 224]. For example, the three representations of band two $\Gamma_{2,0}, \Gamma_{1,1}, \Gamma_{0,2}$ have dimensions $6, 8, 6$, respectively. Explicitly, $\Gamma_{2,0} = \mathrm{Sym}^2 V_1$, $\Gamma_{0,2} = \mathrm{Sym}^2 V_1^*$, and $\Gamma_{1,1}$ is the kernel of the pairing $V_1 \otimes V_1^* \to \mathbb{C}$ defined by $v \otimes f \mapsto f(v)$.

3.0.3. Type C_n: the group $\mathrm{Sp}(n)$. The compact symplectic group $\mathrm{Sp}(n)$ is the intersection of the complex symplectic group $\mathrm{Sp}(2n, \mathbb{C})$ with the unitary group $U(2n, \mathbb{C})$. Since this group is simply connected, the irreducible representations of $\mathrm{Sp}(2n)$ are the same as the irreducible representations of the complex Lie algebra $\mathfrak{sp}_{2n}$ which has type C_n in the classification of Lie algebras. In this case, the weight lattice is freely generated by vectors $L_1, \ldots, L_n$. The positive simple roots are

$$L_1 - L_2, \ldots, L_{n-1} - L_n, 2L_n$$

and the fundamental weights are

$$\omega_i = \sum_{j \leq i} L_j$$

for $i \leq n$ [16, section 17.1]. There are n irreducible representations of band one, and the irreducible representation V_k with the highest weight vector ω_k is the kernel of the contraction map $\wedge^k V \to \wedge^{k-2} V$ [16, Theorem 17.5].

3.1. The nonsimply connected groups $\mathrm{SO}(n)$. As discussed in [16, section 23.1], a general simple Lie group G has a finite abelian fundamental group, so it is a quotient $\tilde{G}/Z$, where $\tilde{G}$ is simply connected and Z is a finite abelian group. Any irreducible representation of G is an irreducible representation of $\tilde{G}$, but not every irreducible representation of $\tilde{G}$ descends to an irreducible representation of G. The set of weights of representations of G forms a sublattice of the set of weights of representations of the universal cover $\tilde{G}$ of finite index. In this case, there need not be an analogue of fundamental weights. That is, we cannot guarantee that the weight lattice of G has a basis $\omega_1,\dots,\omega_n$ such that every highest weight vector can be written as a nonnegative integral linear combination of the ω_i. For the group $\mathrm{SO}(2n+1)$, it is possible to find such weights, and thus we can define the band of an irreducible representation as above. For the group $\mathrm{SO}(2n)$, the weight lattice does not have a fundamental system of weights. Despite this, we are still able to define the band of an irreducible representation, as we see below.

3.1.1. Type B_n: the group $\mathrm{SO}(2n+1,\mathbb{R})$. The compact group $\mathrm{SO}(2n+1,\mathbb{R})$ is a compact form of the complex group $\mathrm{SO}(2n+1,\mathbb{C})$ with Lie algebra $\mathfrak{so}_{2n+1}$ which has type B_n. The root system of type B_n has weight space generated by $L_1,\dots,L_n$. The positive simple roots are [16, section 19.4]

$$\alpha_1 = L_1 - L_2,\dots,\alpha_{n-1} = L_{n-1} - L_n, \alpha_n = L_n$$

and the fundamental weights are

$$\omega_i = \sum_{j\le i} L_j$$

for $i<n$ and $\omega_n = \frac{1}{2}\sum_{j=1}^{n} L_j$.

Note that because $\mathrm{SO}(2n+1)$ is not simply connected not every irreducible representation of $\mathfrak{so}_{2n+1}$ gives rise to an irreducible representation of $\mathrm{SO}(2n+1)$. The representations of the Lie algebra $\mathfrak{so}_{2n+1}$ are in bijective correspondence with the representations of the simply connected spin group $\mathrm{Spin}(2n+1)$, and the irreducible representations of $\mathrm{SO}(2n+1)$ are exactly the representations with the highest weight vectors $a_1\omega_1+\cdots+a_{n-1}\omega_{n-1}+a_n\omega_n$, where a_n is required to be even [16, Proposition 23.13(iii)]. In particular, we can take the vectors $\omega_k = L_1+\cdots+L_k$ for $k<n$ and $\omega_n' = 2\omega_n = L_1+\cdots+L_n$ to be a set of fundamental weights for the Lie group $\mathrm{SO}(2n+1)$.

The representations $V_1,\dots,V_n$ associated to the fundamental weights are the exterior powers $V_1 = \wedge^1 V,\dots,V_n=\wedge^n V$, where V is the defining representation of $\mathrm{SO}(2n+1)$. Note that V has dimension $2n+1$ [16, Theorem 19.14].

Example 3.3. The group $\mathrm{SU}(2)$ is the universal cover of $\mathrm{SO}(3)$. Since these groups have rank one, the weights are integers. For $\mathrm{SU}(2)$, the fundamental weight is $\omega=1$, while for $\mathrm{SO}(3)$ the fundamental weight is $\omega=2$. As a result, the irreducible $\mathrm{SO}(3)$ representation of band b, which has dimension $2b+1$, is the same as the irreducible representation of $\mathrm{SU}(2)$ of band $2b$. Note that the weight lattice for $\mathrm{SO}(3)$ has index 2 in the weight lattice for $\mathrm{SU}(2)$, corresponding to the fact that $\mathrm{SU}(2)\to\mathrm{SO}(3)$ is a 2-to-1 cover.

3.2. Type D_n: the group $\mathrm{SO}(2n,\mathbb{R})$. The group $\mathrm{SO}(2n,\mathbb{R})$ is the compact form of $\mathrm{SO}(2n,\mathbb{C})$ whose Lie algebra $\mathfrak{so}_{2n}$ has type D_n. Its weight space is generated by $L_1,\dots,L_n$. The positive simple roots are

$$\alpha_1 = L_1 - L_2,\dots,\alpha_{n-1} = L_{n-1} - L_n, \alpha_n = L_{n-1} + L_n$$

and the fundamental weights are [16, section 19.2]

$$\omega_i = \sum_{j\le i} L_j$$

for $i < n-1$,

$$\omega_{n-1} = \frac{1}{2}\sum_{j=1}^{n} L_j, \quad \text{and} \quad \omega_n = \frac{1}{2}(L_1 + \cdots + L_{n-1} - L_n).$$

Once again, $\mathrm{SO}(2n)$ is not simply connected so not every irreducible representation of $\mathfrak{so}_{2n}$ gives rise to a representation of the Lie group $\mathrm{SO}(2n)$. The irreducible representations of $\mathrm{SO}(2n)$ are precisely those with the highest weight vector $\sum_{i=1}^{n} a_i\omega_i$, where $a_{n-1} + a_n$ is even [16, Proposition 23.13(iii)]. In this case, every highest weight vector can be expressed nonuniquely as a nonnegative linear combination of the weights $\omega_1, \ldots, \omega_{n-2}$ and

$$\begin{aligned} \omega'_{n-1} &= \omega_{n-1} + \omega_n = L_1 + \cdots + L_{n-1}, \\ \omega'_n &= 2\omega_{n-1} = L_1 + \cdots + L_n, \\ \omega'_{n+1} &= 2\omega_n = L_1 + \cdots + L_{n-1} - L_n. \end{aligned}$$

If λ is a highest weight vector for an irreducible representation of $\mathrm{SO}(2n)$ and we write

$$\lambda = b_1\omega_1 + \cdots + b_{n-2}\omega_{n-2} + b_{n-1}\omega'_{n-1} + b_n\omega'_n + b_{n+1}\omega'_{n+1},$$

then, although the nonnegative integers b_i are not unique, the sum $\sum_{i=1} b_i$ is independent of the choice of b_i's. For example, the weight $2L_1 + \cdots + 2L_{n-1}$ has band two since it can be expressed as $2\omega'_{n-1}$ or as $\omega'_n + \omega'_{n+1}$. Hence, we can define the band of λ to be $\sum_{i=1}^{n} b_i$. In particular, the $n+1$ irreducible representations with the highest weights $\omega_1, \ldots, \omega_{n-2}, \omega'_{n-1}, \omega'_n$ all have band one.

By [16, Remark on p. 289], if $k \leq n-2$, then the representation V_k with the highest weight vector ω_k is the exterior product $\wedge^k V$. Likewise, the representation V_{n-1} with the highest weight ω'_{n-1} is the exterior power $\wedge^{n-1}V$. Finally, the exterior power $\wedge^n V$ is the sum of the representations V_n and V_{n+1} which have the highest weights ω'_n and ω'_{n+1}, respectively.

Example 3.4 (irreducible representations of SO(4)). The group SO(4) has rank two, and there are three representations of band one. The defining representation V_1 has dimension four, and the two additional representations of band one, V'_2, V'_3, are both three dimensional. The sum $V'_2 \oplus V'_3$ equals $\wedge^2 V_1$. If we choose an orthonormal basis e_1, e_2, e_3, e_4 for V_1, then V'_2 is the span of the vectors

$$e_1 \wedge e_2 + e_3 \wedge e_4, \quad e_1 \wedge e_4 + e_2 \wedge e_3, \quad e_1 \wedge e_3 - e_2 \wedge e_4$$

in $\wedge^2 V_1$, while V'_3 is the span of

$$e_1 \wedge e_2 - e_3 \wedge e_4, \quad e_1 \wedge e_4 - e_2 \wedge e_3, \quad e_1 \wedge e_3 + e_2 \wedge e_4$$

in $\wedge^2 V_1$.

3.3. Reduction to representations of band one.

Proposition 3.5. *Let G be a compact Lie group whose irreducible representations can be banded. If $f \in L^2(G)$ and W is an irreducible representation of band $b > 1$, then the Fourier coefficient $F(f)(W)$ is determined from the bispectrum coefficients $a_2(f)(W_1 \otimes W_{b-1})$ and the Fourier coefficients of $F(f)(W_1)$, $F(f)(W_{b-1})$ for some W_1 of band one and some W_{b-1} of band $b-1$, provided that these coefficients are invertible.*

Proof. Since the band of W is b, there are weight vectors $\omega_1,\ldots,\omega_r$ of band one such that the highest weight vector of W is $b_1\omega_1+\cdots+b_r\omega_r$ with $b_i\in\mathbb{N}$ and $\sum_i b_i=b$. Since $b>1$, we know that one of the b_i's is positive. Take W_1 to be the irreducible representation with the highest weight ω_i and W_{b-1} to be the irreducible representation with the highest weight $b_1\omega_1+\cdots+(b_i-1)\omega_i+\cdots+b_r\omega_r$. Since weights are additive on tensor products, $b_1\omega_1+\cdots+b_r\omega_r$ is the highest weight in the tensor product $W_1\otimes W_{b-1}$. Hence, V is a summand in this tensor. Therefore, by Lemma 2.5 we conclude that $F(f)(W)$ is determined. ∎

Corollary 3.6. *With the hypotheses on G as above, if $f\in L^2(G)$ is a function which is band-limited at band $b>1$ and the Fourier coefficients of all representations of band $0\le i\le\lceil b/2\rceil$ are invertible, then all Fourier coefficients can be determined from the Fourier coefficients of band one and the bispectrum.*

Proof. Let W be an irreducible representation with the highest weight vector $\lambda=b_1\omega_1+\cdots+b_r\omega_r$, where the b_i are nonnegative integers and the ω_i have band one. We can decompose the vector $(b_1,\ldots,b_r)=(c_1,\ldots,c_r)+(d_1,\ldots,d_r)$ with b_i,c_j nonnegative integers and $\sum c_i,\sum d_i\le\lceil b/2\rceil$. If W_1 is the irreducible representation with the highest weight $c_1\omega_1+\cdots+c_r\omega_r$ and W_2 is the irreducible representation with the highest weight $d_1\omega_1+\cdots+d_r\omega_r$, then W appears as a summand in the tensor product $W_1\otimes W_2$. Thus, if $F(f)(W_1)$ and $F(f)(W_2)$ are invertible, then $F(f)(W)$ can be determined from $a_2(f)(W_1\otimes W_2)$ and $F(f)(W_1)$, $F(f)(W_2)$ regardless of whether $F(f)(W)$ is invertible. By Proposition 3.5 and induction, $F(f)(W_1)$, $F(f)(W_2)$ can be determined from the Fourier coefficients of band one. ∎

3.4. Reduction to the defining representation.

The previous propositions only required that the irreducible representations of our compact Lie group G be banded. We now state a result specific to the classical groups $\mathrm{SU}(n),\mathrm{SO}(2n+1),\mathrm{Sp}(n),\mathrm{SO}(2n)$.

Theorem 3.7. *Let G be one of the classical compact Lie groups $\mathrm{SU}(n),\mathrm{SO}(n),\mathrm{Sp}(2n)$ with defining representation V_1. If the Fourier coefficients of the irreducible representations of band one are all invertible, then the Fourier coefficient $F(f)(V_\ell)$ of any band-one representation V_ℓ is determined by $F(f)(V_1)$ and the bispectrum matrices $a_2(f)(V_1\otimes V_k)$ with V_k of band one and $k<\ell$.*

Proof. The proof is based on a case-by-case analysis, but the overall structure is the same in each case and makes use of a simple lemma.

Lemma 3.8. *Let V be a representation of a compact Lie group G. Then $\wedge^{k+1}V$ appears as a G-invariant summand in $V\otimes\wedge^k V$.*

Proof. The action of G on V defines a homomorphism $G\to U(V)$, where $U(V)$ is the group of unitary transformations of V. In particular, it suffices to prove the lemma when G is the unitary group $U(d)$, where $d=\dim V$. The statement then follows from the fact that the map $V\otimes\wedge^k V\to\wedge^{k+1}V$, defined by

$$v\otimes(v_1\wedge\cdots\wedge v_k)\mapsto v\wedge v_1\wedge\cdots\wedge v_k$$

is surjective and commutes with the respective actions of the unitary group $U(V)$ on $V\otimes\wedge^k V$ and $\wedge^{k+1}V$. ∎

3.4.1. Type A_{n-1}: the group $\mathrm{SU}(n)$. As noted above, the representation V_k with the highest weight $\omega_k = L_1 + \cdots + L_k$ is $\wedge^k V_1$, where V_1 is the defining representation.

By Lemma 2.5 and induction, it suffices to show that V_{k+1} is a summand in the tensor product $V_1 \otimes V_k$ which follows from Lemma 3.8.

3.4.2. Type B_n: the group $\mathrm{SO}(2n+1)$. Here we have a fundamental system of weights $\omega_1, \dots, \omega_{n-1}, \omega'_n$, and the corresponding irreducible representations are the exterior product $\wedge^k V_1$ for $1 \le k \le n$. Once again, by Lemma 2.5 we just need to show that V_{k+1} is a summand in $V_1 \otimes V_k$ which follows from Lemma 3.8.

3.4.3. Type C_n: the group $\mathrm{Sp}(2n)$. Unlike the case of $\mathrm{SU}(n)$ and $\mathrm{SO}(2n+1)$, the irreducibles associated to the fundamental weights are not exterior powers of the defining representation V_1. However, [16, Theorem 17.5] states that if $k > 1$, then V_k is the kernel of the contraction map $\wedge^k V_1 \to \wedge^{k-2} V_1$. Hence, $\wedge^k V_1 = V_k \oplus V_{k-2} \oplus \cdots \oplus V_0$ if k is even and $\wedge^k V_1 = V_k \oplus V_{k-2} \oplus \cdots \oplus V_1$ if k is odd. Since the Fourier coefficient of the trivial representation $V_0 = \wedge^0 V_1$ is known from the bispectrum by Proposition 2.2, we are able to inductively determine the Fourier coefficient $F(f)(V_k)$ from the bispectrum and knowledge of $F(f)(V_1)$ as follows: Assume by induction that we have determined the Fourier coefficients $F(f)(V_\ell)$ for $\ell \le k$. Since $\wedge^k(V_1) = \oplus_\ell V_{k-2\ell}$, we know the Fourier $F(f)(\wedge^k V_1)$ by induction. Since $\wedge^{k+1} V_1$ appears as a summand in $V_1 \otimes \wedge^k V_1$ and V_{k+1} is a summand in $\wedge^{k+1} V$, we see that V_{k+1} is a summand in $V_1 \otimes \wedge^k V$. Since the Fourier coefficient $F(f)(\wedge^k V_1)$ is known by induction, it follows from Lemma 2.5 that $F(f)(V_{k+1})$ is determined by $F(f)(V_1)$ and the bispectrum coefficient $a_2(f)(V_1 \otimes \wedge^k V_1)$.

3.4.4. Type D_n: the group $\mathrm{SO}(2n)$. In this case, we have $n+1$ weights of band one $\omega_1, \dots, \omega_{n-2}, \omega'_{n-1}, \omega'_n, \omega'_{n+1}$ and associated representations $V_1, \dots, V_{n+1}$. As noted above, $V_k = \wedge^k V_1$ for $1 \le k \le n-1$. Hence, the same argument used in the case of $\mathrm{SO}(2n+1)$ implies that the bispectrum and $F(f)(V_1)$ determine $F(f)(V_k)$ if $k \le n-1$. However, we also know that V_n and V_{n+1} are summands in $\wedge^n V_1$ so we can determine them from $F(f)(V_{n-1}), F(f)(V_1)$ and the bispectrum coefficient $F(f)(V_1 \otimes V_{n-1})$. ∎

4. Sharp results for $\mathrm{SO}(2n+1), \mathrm{SU}(n)$.

For the groups $G = \mathrm{SU}(n)$ and $G = \mathrm{SO}(2n+1)$, we prove that the G-orbit of a generic band- limited function in $L^2(G)$ is determined by its bispectrum.

Theorem 4.1.

(i) *If $f \in L^2(\mathrm{SU}(n))$ is band-limited with band $b \ge 1$ and all Fourier coefficients of irreducible representations whose bands are at most $\lceil b/2 \rceil$ are invertible, then the $\mathrm{SU}(n)$ orbit of f is determined by its bispectrum.*

(ii) *If $f \in L^2(\mathrm{SO}(2n+1))$ is real valued and band-limited with band $b \ge 1$ and all Fourier coefficients of irreducible representations whose band is at most $\lceil b/2 \rceil$ are invertible, then the $\mathrm{SO}(2n+1)$ orbit of f is determined by its bispectrum.*

Proof. By Theorem 3.7, we know that Fourier coefficients of all irreducibles are determined by the Fourier coefficient $F(f)(V)$ of the defining representation. Moreover, by Propositions 2.1 and 2.2, we also know $F(f)(V)F(f)(V)^*$ so we know $F(f)(V)$ up to translation by an element of $U(V)$ if f is complex valued and $O(V)$ if f is real valued.

Suppose that $f' \in L^2(\mathrm{SU}(n))$ has the same bispectrum as f. Then we know that $F(f')(V) = uF(f)(V)$ for some $u \in U(V) = U(n)$. Our goal is to show that $u \in \mathrm{SU}(n)$. Any element of $U(n)$ can be factored as $u = (\operatorname{diag} e^{i\theta})r$, where $r \in \mathrm{SU}(n)$. Replace f with the function whose Fourier coefficient of V is $rF(V)$ and has the same bispectrum. (Such a function exists because the bispectrum is invariant under the action of $\mathrm{SU}(n)$ on $L^2(\mathrm{SU}(n))$.) By doing so, we may reduce to the case that $F(f')(V) = e^{i\theta}F(f)(V)$ and has the same bispectrum. Our goal is to show that $\operatorname{diag} e^{i\theta} \in \mathrm{SU}(n)$ or, equivalently, that $e^{i\theta}$ is an nth root of unity.

Since the bispectra of f and f' are equal, we see that

$$\begin{aligned} a_2(f)(V \otimes V) &= [F(f)(V) \otimes F(f)(V)]F(f)(V \otimes V)^* \\ &= [F(f')(V) \otimes F(f')(V)]F(f')(V \otimes V)^* \\ &= e^{2i\theta}[F(f)(V) \otimes F(f)(V)]F(f')(V \otimes V)^*, \end{aligned}$$

where the last equality follows from the fact that $\operatorname{diag} e^{i\theta} \otimes \operatorname{diag} e^{i\theta}$ is $e^{2i\theta}$ times the identity operator on $V \otimes V$.

It follows that for any irreducible W appearing in $V \otimes V$, we have that $F(f')(W) = e^{2i\theta}F(f)(W)$. In particular if $V_2 = \wedge^2 V$, then $F(f')(V_2) = e^{2i\theta}F(f)(V_2)$. Continuing this way, we see that for the fundamental representations $V = V_1, \ldots, V_{n-1}$, $F(f')(V_k) = e^{ik\theta}F(f)(V_k)$. On the other hand, we know that the bispectrum uniquely determines the Fourier coefficient of the trivial representation V_0 so we must have that $F(f')(V_0) = F(f)(V_0)$. However, V_0 appears as a summand in $V \otimes V_{n-1}$ so by our previous argument we see that $F(f')(V_0) = e^{in\theta}F(f)(V_0)$. Therefore, $e^{in\theta} = 1$ as desired.

The proof for $\mathrm{SO}(2n+1)$ is similar to the proof for $\mathrm{SU}(n)$ but requires a slightly more complicated representation-theoretic argument. If $f \in L^2(\mathrm{SO}(2n+1))$ is real valued and f' is another real-valued function with the same bispectrum, then we know that $F(f')(V) = oF(f)(V)$, where $o \in O(2n+1)$. Now any element in $O(2n+1)$ can be written as $\pm r$, where $r \in \mathrm{SO}(2n+1)$. We will prove the result by showing that if $o \in O(2n+1) \setminus \mathrm{SO}(2n+1)$, we obtain a contradiction. Assuming that $o \notin \mathrm{SO}(2n+1)$, we can reduce to the case that $F(f')(V) = -F(f)(V)$ and f', f have the same bispectrum. The tensor product $V \otimes V$ contains the fundamental representation $V_2 = \wedge^2 V$ as a summand so we see that $F(f')(V_2) = (-1)^2 F(f)(V)$. Continuing this way, we see that $F(f')(V_k) = (-1)^k F(f)(V)$ for $1 \le k \le n$. Since $V_n = \wedge^n V$, we know by Lemma 3.8 that $V \otimes V_n$ contains a copy of $\wedge^{n+1} V$. Since $\dim V = 2n+1$, the exterior products $\wedge^n V$ and $\wedge^{n+1} V$ are dual representations. However, we also know that as $\mathrm{SO}(2n+1)$ representations, $\wedge^k V$ is self-dual for $k \le n$. Hence, $V \otimes V_n$ contains a copy of V_n. This implies that $F(f')(V_n) = -F(f')(V_n)$, which is a contradiction. ■

5. Examples and applications.

5.1. Counterexamples. We give two examples, one for $S^1 = \mathrm{SO}(2)$ and one for $\mathrm{SU}(2)$, that illustrate the necessity of the hypothesis in Theorem 4.1 that the Fourier coefficients of band at most $\lceil \frac{b}{2} \rceil$ be invertible. The reason we restrict ourselves to these groups is that they are both rank one, which makes the calculations more tractable.

5.1.1. S^1 counterexample. If $k \in \mathbb{Z}$ is any integer, denote by V_k the one-dimensional representation of S^1 where $e^{\iota\theta}$ acts on V_k by scalar multiplication by $e^{\iota k\theta}$. With this notation, for any $\ell > 0$ there are two one-dimensional representations of S^1 of band ℓ, namely V_ℓ and $V_{-\ell}$.

Consider the band-limited representation $W_3 = V_0 \oplus V_1 \oplus V_2 \oplus V_3$. Since every irreducible representation of S^1 is one dimensional, the Fourier coefficients are scalars, so a Fourier coefficient is invertible if and only if it is nonzero. If $f \in W_3 \subset L^2(S^1)$ is a function, then the Fourier coefficient of V_ℓ is the scalar a_ℓ in the Fourier expansion $f = \sum_{\ell=0}^3 a_\ell e^{i\ell\theta}$. As noted in Example 2.4, if the Fourier coefficient of a_2 is zero, then we cannot recover the Fourier coefficient a_3 from the bispectrum.

5.1.2. SU(2) counterexample. In this example, we identify the defining representation V_1 of SU(2) with the two-dimensional vector space of binary linear forms. The single irreducible representation V_ℓ of band ℓ is $\mathrm{Sym}^\ell V_1$ and can be identified with the $(\ell+1)$-dimensional vector space of homogeneous binary forms of degree ℓ.

Consider the 3-band-limited representation of SU(2), $W_3 = V_0 \oplus V_1 \oplus V_2 \oplus V_3$. Unlike the case for S^1, the dimension of V_ℓ depends on ℓ, as it has dimension $\ell + 1$. As a result, the Fourier coefficient of V_ℓ is not a scalar but an $(\ell+1)\times(\ell+1)$ matrix. Let $f \in W_3 \subset L^2(\mathrm{SU}(2))$ be the function whose Fourier coefficients are $F(f)(V_0) = 1, F(f)(V_1) = \mathrm{Id}_2, F(f)(V_2) = 0$, and $F(f)(V_3) = \mathrm{Id}_4$ where Id_k indicates the $k \times k$ identity matrix. Using formula (2.5) for the inverse Fourier transform, we can explicitly compute f as the function

$$A \mapsto 1 + 2\mathrm{Tr} A^{-1} + 4\mathrm{Tr}\,\mathrm{sym}^3 A^{-1}.$$

If we write $A = \left(\begin{smallmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{smallmatrix}\right)$ with $|\alpha|^2 + |\beta|^2 = 1$, then we have the explicit formula

$$A \mapsto 1 + 2(\alpha + \overline{\alpha}) + 4(\alpha + \overline{\alpha})(\alpha^2 + \overline{\alpha}^2 - 2|\beta|^2).$$

Since f has only three nonzero Fourier coefficients $F(f)(V_0), F(f)(V_1), F(f)(V_3)$, the bispectrum has at most nine nonzero Fourier coefficients $a_2(f)(V_i \otimes V_j)$ for $i, j \in \{0, 1, 3\}$. The bispectrum is also symmetric, i.e., $a_2(f)(V_i \otimes V_j) = a_2(f)(V_j \otimes V_i)$, so we need only compute the six Fourier coefficients $a_2(f)(V_i \otimes V_j)$ with $i \leq j$.

Because we have chosen the nonzero Fourier coefficients of f to be the identity matrices, the three Fourier coefficients of $a_2(f)(V_0 \otimes V_j)$ are readily calculated using formula (2.9) and are

$$\begin{aligned} a_2(f)(V_0 \otimes V_0) &= 1, \\ a_2(f)(V_0 \otimes V_1) &= \mathrm{Id}_2\,\mathrm{Id}_2^* = \mathrm{Id}_2, \\ a_2(f)(V_0 \otimes V_3) &= \mathrm{Id}_4\,\mathrm{Id}_4^* = \mathrm{Id}_4. \end{aligned}$$

We also claim that $a_2(V_1 \otimes V_3)$ is the 8×8 zero matrix. The reason is that the tensor product $V_1 \otimes V_3$ decomposes as $V_4 \oplus V_2$ and the Fourier coefficients $F(f)(V_4)$ and $F(f)(V_2)$ are zero. Thus, $F(f)(V_2 \otimes V_3) = 0$. Hence,

$$a_2(V_1 \otimes V_3) = [F(f)(V_1) \otimes F(f)(V_3)][F(f)(V_1 \otimes V_3)] = 0.$$

We now compute the Fourier coefficients $a_2(f)(V_1 \otimes V_1)$ and $a_2(f)(V_1 \otimes V_3)$.

The representation $V_1 \otimes V_1$ is the vector space of forms $q(x_0, x_1, y_0, y_1)$ which are homogeneous of degree one in (x_0, x_1) and (y_0, y_1), respectively. This representation is isomorphic to the sum of the two irreducibles $V_2 \oplus V_0$. The summand V_0 the one-dimensional subspace generated by the SU(2)-invariant form $x_0y_1 + x_1y_0$. Since the Fourier coefficient $F(f)(V_2) = 0$, the Fourier coefficient $F(f)(V_1 \otimes V_1)$ is rank-one projection P_1, which projects $V_1 \otimes V_1$ to the one-dimensional subspace spanned by the binomial $x_0y_1 + x_1y_0$. Note that $P_1 = P_1^*$ because the form $x_0y_1 + x_1y_0$ is symmetric in the x and y variables. Applying formula (2.9), we see that

$$\begin{aligned} a_2(f)(V_1 \otimes V_1) &= [F(f)(V_1) \otimes F(f)(V_1)][F(f)(V_1 \otimes V_1)]^* \\ &= [\mathrm{Id}_2 \otimes \mathrm{Id}_2]P_1^* \\ &= P_1. \end{aligned}$$

The remaining Fourier coefficient is

$$a_3(f)(V_3 \otimes V_3) = [\mathrm{Id}_4 \otimes \mathrm{Id}_4][F(f)(V_3 \otimes V_3)]^*.$$

The representation $V_3 \otimes V_3$ is isomorphic to the sum $V_6 \oplus V_4 \oplus V_2 \oplus V_0$. The only nonzero Fourier coefficient in this sum is that of the trivial representation V_0. Viewing $V_3 \otimes V_3$ as the vector space of forms $s(x_0, x_1, y_0, y_1)$ which are homogeneous of degree three in (x_0, x_1) and (y_0, y_1), respectively, the invariant subspace V_0 is spanned by the form $(x_0y_1 - x_1y_0)^3$, and the Fourier coefficient $F(f)(v_2)(V_3 \otimes V_3)$ is the rank-one projection P_3 on to this subspace. Because the form $(x_0y_1 - x_1y_0)^3$ is skew-symmetric in the x and y variables, $P_3^* = -P_3$. Thus, by formula (2.9) we see that $a_2(f)(V_3 \otimes V_3) = P_3^* = -P_3$.

It is easy to construct functions f' with the same bispectrum as f which are not in the same SU(2) orbit. The simplest example is the functions whose Fourier coefficients are $F(f')(V_0) = 1, F(f')(V_1) = \mathrm{Id}_2, F(f')(V_2) = 0, F(f')(V_3) = -\mathrm{Id}_3$ corresponding to the function on SU(2) defined by the formula

$$A \mapsto 1 + 2(\alpha + \overline{\alpha}) - 4(\alpha + \overline{\alpha})(\alpha^2 + \overline{\alpha}^2 - 2|\beta|^2).$$

More generally, if U is any 4×4 unitary matrix acting on V_3 such that $U \otimes U \circ P_3 = P_3$, where P_3 is the projection onto the subspace spanned by $(x_0y_1 - x_1y_0)^3$, then the function f' with generalized Fourier coefficients $F(f')(V_0) = 1, F(f')(V_1) = \mathrm{Id}_2, F(f')(V_2) = 0, F(f')(V_3) = U$ will have the same bispectrum as f.

5.2. Algorithmic aspects. Although our result is theoretical, the proof of Theorem 3.7 gives a potential algorithm for determining the Fourier coefficients of all irreducible representations of a band-limited function from the Fourier coefficient of the defining representation and the bispectrum. Moreover, if all nonzero generalized Fourier coefficients of a band-limited function are invertible, then the potential algorithm needs only a relatively small part of the bispectrum to compute the unknown function from the matrix Fourier coefficient of the defining representation.

Precisely, if $f \in L^2(G)$ is band-limited with band b and $W_1, \ldots, W_t$ are the irreducible representations of band one, then Proposition 3.5 implies that we only need as input the values (which are matrices) of the bispectrum at $\{W_i \otimes V\}$ where V runs through all irreducible representations of band strictly less than b. By contrast, if f is b band-limited, then the full bispectrum is determined by its values at $W \otimes V$, where W, V run over all irreducible representations of band at most b. As in the proof of Theorem 3.7, we proceed by determining the Fourier coefficients of band ℓ from the Fourier coefficients of band $\ell-1$ by performing at most $B_{\ell-1}$ matrix inversions and multiplications, where $B_{\ell-1}$ is the number of irreducible representations of band $\ell-1$. (Note that this strategy would also require knowing the decomposition of the tensor products $W_i \otimes V$ into irreducible representations.) An interesting question for further work is to investigate the robustness and stability of this approach from an algorithmic perspective.

For example, if $G = \mathrm{SU}(3)$, the number of irreducible representations of band ℓ is $\ell+1$, so the bispectrum of a b band-limited function depends on its values at $\binom{b+1}{2}^2$ pairs of irreducible representations. However, in order to determine the Fourier coefficients from the Fourier coefficient of the defining representation we need only consider $2\binom{b+1}{2}$ values of the bispectrum.

5.3. Results for the group $\mathrm{SO}(3)$. For the classical Lie groups, the number and dimensions of the irreducible representations of a given band grows exponentially in the rank of the group. However, for a group of rank one such as $\mathrm{SU}(2)$ or $\mathrm{SO}(3)$ the computations may be feasible. For $\mathrm{SO}(3)$, there is a single irreducible representation of band ℓ, the representation V_ℓ of dimension $2\ell+1$, which has a basis of spherical harmonic polynomials of $Y_{\ell,m}$ for $m = -\ell, \dots, \ell$. In this case, the coefficient of $V_1 \otimes V_{b-1}$ in the bispectrum is a $(6b-3)\times(6b-3)$ matrix. In particular, this shows that we can determine the Fourier coefficients of a b band-limited function from the Fourier coefficient $F(f)(V_1)$ and a polynomial in b number of matrix multiplications and inversions. This suggests that for a group of rank one like $\mathrm{SO}(3)$ bispectrum, inversion of a band-limited function can be done in polynomial time in the band.

5.3.1. Comparison with the work of Liu and Moitra [23]. A related result, with precise error bounds, was proved by Liu and Moitra [23] for the MRA problem of $\mathrm{SO}(3)$ acting on band-limited functions on S^2. Note that the space of b band-limited functions on S^2 is isomorphic to the sum of the representations $V_0 \oplus V_1 \otimes \cdots \oplus V_b$ where V_ℓ is the $2\ell+1$-dimensional irreducible representation of $\mathrm{SO}(3)$. This is in the contrast to the case for functions on $\mathrm{SO}(3)$ where the summand V_ℓ appears with multiplicity equal to its dimension $2\ell+1$. In particular, their algorithm determines $1+3+\cdots+(2b+1) = (b+1)^2$ unknown coefficients $f_{\ell m}$ coming from the expansion of a band-limited function in spherical harmonics as

$$\sum_{\ell \le b} \sum_{m=-\ell}^{\ell} f_{\ell m} Y_{\ell m}(\theta,\phi).$$

By comparison, our goal is to determine a collection of matrices (the matrix Fourier coefficients). The main result of [23] is a robust quasi-polynomial time algorithm which uses the degree-three invariants together with knowledge of all coefficients $f_{\ell m}$ with $\ell \le C$ to determine the remaining coefficients by frequency marching. (Here C is a fixed constant independent of the band limit.) It should be noted that it is an open theoretical problem as to whether all unknown coefficients $f_{\ell m}$ can be determined solely from the degree-three invariants [2, section 4.5].

5.4. Unprojected cryo-EM. Let $L^2(\mathbb{R}^3)$ be Hilbert space of complex-valued L^2 functions on $\mathbb{R}^3$. The action of $\mathrm{SO}(3)$ on $\mathbb{R}^3$ induces a corresponding action on $L^2(\mathbb{R}^3)$, which we view as an infinite-dimensional representation of $\mathrm{SO}(3)$. In cryo-EM, we are interested in the action of SO(3) on the subspace of $L^2(\mathbb{R}^3)$ corresponding to the Fourier transforms of real-valued functions on $\mathbb{R}^3$, representing the Coulomb potential of an unknown molecular structure.

Using spherical coordinates (ρ, θ, ϕ), we consider a finite-dimensional approximation of $L^2(\mathbb{R}^3)$ by discretizing $f(\rho, \theta, \phi)$ with R samples $r_1, \ldots, r_R$, of the radial coordinates and band limiting the corresponding spherical functions $f(r_i, \theta, \phi)$. This is a standard assumption in the cryo-EM literature; see, for example, [4]. Mathematically, this means that we approximate the infinite-dimensional representation $L^2(\mathbb{R}^3)$ with the finite-dimensional representation $V = (\oplus_{\ell=0}^L V_\ell)^R$, where L is the band limit, and V_ℓ is the $(2\ell+1)$-dimensional irreducible representation of SO(3), corresponding to harmonic polynomials of frequency ℓ. An orthonormal basis for V_ℓ is the set of spherical harmonic polynomials $\{Y_\ell^m(\theta, \phi)\}_{m=-\ell}^{\ell}$. We use the notation $Y_\ell^m[r]$ to consider the corresponding spherical harmonic as a basis vector for functions on the rth spherical shell. The dimension of this representation is $R(L^2 + 2L + 1)$.

Viewing an element of V as a radially discretized function on $\mathbb{R}^3$, we can view $f \in V$ as an R-tuple

$$f = (f[1], \ldots, f[R]),$$

where $f[r] \in L^2(S^2)$ is an L-band-limited function. Each $f[r]$ can be expanded in terms of the basis functions $Y_\ell^m(\theta, \varphi)$ as follows:

$$f[r] = \sum_{\ell=0}^{L} \sum_{m=-\ell}^{\ell} A_\ell^m[r] Y_\ell^m. \tag{5.1}$$

Therefore, the problem of determining a structure reduces to determining the unknown coefficients $A_\ell^m[r]$ in (5.1).

Note that when f is the Fourier transform of a real-valued function, the coefficients $A_\ell^m[r]$ are real for even ℓ and purely imaginary for odd ℓ [11].

For the case of SO(3), we can combine our results and obtain the following corollary.

Corollary 5.1. *If $L \geq 3$ and any $R \geq L+2$, the generic orbit in the* SO(3) *representation $V = (\oplus_{\ell=0}^L V_\ell)^R$ can be recovered from the third moment.*

Proof. By Proposition 2.3, it suffices to prove the corollary when $R = L+1$. Consider the SO(3)-module

$$W = V_0 \oplus V_1^3 \oplus \cdots \oplus V_{\lceil L/2 \rceil}^{2\lceil L/2 \rceil + 1} \oplus V_{\lceil L/2 \rceil + 1}^{L+2} \oplus \cdots \oplus V_L^{L+2}.$$

Since $L + 2 \geq \lceil L/2 \rceil + 1$, we can once more invoke Proposition 2.3 and prove the result for the representation W. We view W as an SO(3)-submodule of the vector space of L-band-limited functions in $L^2(\mathrm{SO}(3))$ since the latter representation is isomorphic to $\oplus_{\ell=0}^L V_\ell^{2L+1}$. The generic element of W viewed as a submodule of $\oplus_{\ell=0}^L V_\ell^{2\ell+1}$ has invertible Fourier coefficients up to band $\lceil L/2 \rceil$. Therefore, by Corollary 3.6, if $f \in W$, then the Fourier coefficients $F(f)(V_\ell)$ are determined by the bispectrum and the single Fourier coefficient $F(f)(V_1)$ of band one. By Proposition 2.2, the third moment determines the second moment, and by Proposition 2.1, the second moment determines $A_1(f)A_1(f)^T$, where $A_1(f)$ is the full-rank real 3×3 matrix $(-iA_1^m[r])_{-1 \leq m \leq 1, 1 \leq r \leq 3}$. (Note that the coefficients $A_1^m[r]$ are purely imaginary so we multiply by $-i$ to obtain a real-valued matrix.) In particular, the matrix $A_1(f)$ (which we can identify with the Fourier coefficient in a suitable basis) is determined up to multiplication by an element $O(3)$. By Theorem 4.1, $A_1(f)$ is determined up to rotation by an element of SO(3). Hence, the orbit of the generic vector $f \in W$ is determined from its third moment. ■

Remark 5.2. An analogous result holds for the groups $\mathrm{SO}(2n+1)$ and $\mathrm{SU}(n)$. However, because there are many representations of a given band and their dimensions vary, it cannot be stated as precisely as the corresponding statement for SO(3). The general statement is the following: Let R be at least $\max \dim V$, where V runs over all irreducible representations of band $\lceil b/2 \rceil$, and let $W = \oplus_{\{V | \mathrm{band} V \leq b\}} V^R$. Then the generic $\mathrm{SO}(2n+1)$ (resp., $\mathrm{SU}(n)$) orbit in W can be recovered from the third moment.

5.4.1. Further directions.

In [2], it is conjectured that for any L the third moment separates generic orbits, provided that $R \geq 3$. This conjecture was verified for $1 \leq L \leq 15$ using techniques from computational commutative algebra, and a computational algebra algorithm was presented for recovering the orbit using frequency marching. Note that Corollary 5.1 is weaker than the conjectured bounds of [2], in that we require the multiplicities of the irreducible representations to grow with the band. An interesting direction for further work is to refine the methods used here to determine whether the third moment carries enough information to separate orbits when the irreducible representations have constant multiplicity which is independent of the band limit.

There is an expectation in the cryo-EM community that the generic orbit can be recovered from the projected third moment. In [2, section 4.5], the authors have computationally verified that the projected third moment recovers generic orbits up to a finite list (list recovery). An important problem is to mathematically prove that the projected third moment separates generic orbits in the spherical shells model. We view Corollary 5.1 as a first step in this direction, particularly since we can recover generic orbits from a very small portion of the information carried by the bispectrum/third moment.

Another interesting avenue of investigation is the case of finite groups. It is known [2] that the third moment separates generic orbits in any representation containing the regular representation. However, there are essentially no known nontrivial examples of smaller representations of finite groups where the third moment separates generic orbits.

Appendix A. Representation theory.

A.1. Terminology on representations.

Let G be a group. A representation of G is a homomorphism, $G \xrightarrow{\pi} \mathrm{GL}(V)$, where V is a vector space over a field and $\mathrm{GL}(V)$ is the group of invertible linear transformations $V \to V$. Given a representation of a group G, we can define an action of G on V by $g \cdot v = \pi(g)v$. Since $\pi(g)$ is a linear transformation, the action of G is necessarily linear, meaning that, for any vectors v_1, v_2 and scalars $\lambda, \mu \in \mathbb{C}$, $g \cdot (\lambda v_1 + \mu v_2) = \lambda(g \cdot v_1) + \mu(g \cdot v_2)$. Conversely, given a linear action of G on a vector space V, we obtain a homomorphism $G \to \mathrm{GL}(V)$, $g \mapsto T_g$, where $T_g \colon V \to V$ is the linear transformation $T_g(v) = (g \cdot v)$. Thus, giving a representation of G is equivalent to giving a linear action of G on a vector space V. Given this equivalence, we will follow standard terminology and refer to a vector space V with a linear action of G as a *representation of* G.

A representation V of G is *finite dimensional* if $\dim V < \infty$. In this case, a choice of basis for V identifies $\mathrm{GL}(V) = \mathrm{GL}(N)$, where $N = \dim V$. If V is a complex vector space with Hermitian inner product $\langle\cdot,\cdot\rangle$ on V, we say that a representation is *unitary* if for any two vectors $v_1, v_2 \in V$ $\langle g\cdot v_1, g\cdot v_2\rangle = \langle v_1, v_2\rangle$. Likewise, if V is a real vector space with inner product $\langle\cdot,\cdot\rangle$, then we say that the representation is orthogonal if the action of G preserves the inner product. If we choose an orthonormal basis for V, then the representation of G is unitary (resp., orthogonal) if and only if the image of G under the homomorphism $G \to \mathrm{GL}(N)$ lies in the subgroup $U(N)$ (resp., $O(N)$) of unitary (resp., orthogonal) matrices.

A representation V of a group G is *irreducible* if V contains no nonzero proper G-invariant subspaces.

A.2. Representations of compact groups. Any compact group G has a G-invariant measure called a Haar measure. The Haar measure dg is typically normalized so that $\int_G dg = 1$. If V is a finite-dimensional representation of a compact group and $(\cdot,\cdot)$ is any Hermitian inner product, then the inner product $\langle\cdot,\cdot\rangle$ defined by the formula $\langle v_1, v_2\rangle = \int_G (g\cdot v_1, g\cdot v_2)\, dg$ is G-invariant. As a consequence, we obtain the following fact.

Proposition A.1. *Every finite-dimensional representation of a compact group is unitary.*

Using the invariant inner product, we can then obtain the following decomposition theorem for finite-dimensional representations of a compact group.

Proposition A.2. *Any finite-dimensional representation of a compact group decomposes into a direct sum of irreducible representations.*

If V is a representation, then $V^G = \{v \in V | g\cdot v = v\}$ is a subspace which is called the subspace of invariants.

A.3. Schur's lemma. A key property of irreducible unitary representations is Schur's lemma. Recall that a linear transformation Φ is G-invariant if $g\cdot \Phi v = \Phi g\cdot v$.

Lemma A.3. *Let $\Phi\colon V_1 \to V_2$ be a G-invariant linear transformation of finite-dimensional irreducible representations of a group G (not necessarily compact). Then Φ is either zero or an isomorphism. Moreover, if V is a finite-dimensional irreducible unitary representation of a group G, then any G-invariant linear transformation $\phi\colon V \to V$ is multiplication by a scalar.*

A.4. Dual, Hom, and tensor products of representations. If V_1 and V_2 are representations of a group G, then the vector space $\mathrm{Hom}(V_1, V_2)$ of linear transformations $V_1 \to V_2$ has a natural linear action of G given by the formula $(g\cdot A)(v_1) = g\cdot A(g^{-1}v_1)$. In particular, if V is a representation of G, then $V^* = \mathrm{Hom}(V, \mathbb{C})$ has a natural action of G given by the formula $(g\cdot f)(v) = f(g^{-1}v)$.

A choice of inner product on V determines an identification of vector spaces $V = V^*$, given by the formula $v \mapsto \langle\cdot, v\rangle$. If V is a unitary representation of G, then with the identification of $V = V^*$ the dual action of G on V is given by the formula $g \cdot_* v = \overline{g}\cdot v$. Likewise, if V_1 and V_2 are two representations, then we can define an action of G on $V_1 \otimes V_2$ by the formula $g\cdot(v_1\otimes v_2) = (g\cdot v_1)\otimes(g\cdot v_2)$.

Given two representations spaces V_1, V_2, there is an isomorphism of representations $V_1 \otimes V_2^* \to \mathrm{Hom}(V_2, V_1)$ given by the formula $v_1 \otimes f_2 \mapsto \phi$, where the linear transform $\phi\colon V_2 \to V_1$ is defined by the formula $\phi(v_2) = f_2(v_2)v_1$. In particular, we can identify $V\otimes V^*$ with $\mathrm{Hom}(V, V)$.

Appendix B. Compact Lie groups. A *compact Lie group* is a compact differentiable manifold which is also a group and with the property that the multiplication and inverse maps are differentiable. A compact Lie group is a *torus* if it is isomorphic to $(S^1)^n$ for some n. A fundamental result in the theory of Lie groups is that every maximal torus in a compact Lie group has the same dimension. The *rank* of a compact Lie group is the dimension of any maximal torus. For example, the rank of $\mathrm{SU}(n)$ is $n-1$ since the set of determinant one-diagonal matrices with nonzero entries of the form $e^{\iota\theta} \in S^1$ is a maximal torus.

The *Lie algebra* of a Lie group G is the tangent space to the Lie algebra at the identity element. A connected compact Lie group is *simple* if has no nontrivial connected normal subgroups. If G is a simple Lie group, then its Lie algebra $\mathfrak{g}$ is a simple Lie algebra, meaning that it has no nontrivial proper ideals. Given a simple Lie algebra $\mathfrak{g}$, there is a unique simply connected simple compact Lie group G whose Lie algebra is $\mathfrak{g}$.

In this paper, we are concerned with representations of the following simple groups called the *classical Lie groups:*

1. The group $\mathrm{SU}(n)$ of determinant-one $n \times n$ unitary matrices. $\mathrm{SU}(n)$ has rank $n-1$ and is simply connected.
2. The special orthogonal group $\mathrm{SO}(n)$ is the group of determinant-one real $n \times n$ matrices A that satisfy the condition $AA^t = \mathrm{Id}_n$. This group has rank $\lfloor n/2 \rfloor$ and is simple if $n \geq 3$. The group $\mathrm{SO}(2)$ is the circle group and is therefore abelian so it is not simple. The group $\mathrm{SO}(n)$ is not simply connected. The simply connected group with the same Lie algebra is the *spin group* $\mathrm{Spin}(n)$.
3. The symplectic group $\mathrm{Sp}(2n)$ is the group of $2n \times 2n$ unitary matrices A which satisfy the condition $JA = \overline{A}J$, where J is the block diagonal matrix $\left(\begin{smallmatrix} 0 & -I \\ I & 0 \end{smallmatrix}\right)$. The symplectic group is simply connected and has rank n.

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