THE SAMPLE COMPLEXITY OF SPARSE MULTI-REFERENCE ALIGNMENT AND SINGLE-PARTICLE CRYO-ELECTRON MICROSCOPY

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Abstract. Multi-reference alignment (MRA) is the problem of recovering a signal from its multiple noisy copies, each acted upon by a random group element. MRA is mainly motivated by single-particle cryo-electron microscopy (cryo-EM) that has recently joined X-ray crystallography as one of the two leading technologies to reconstruct biological molecular structures. Previous papers have shown that in the high noise regime, the sample complexity of MRA and cryo-EM is $n = \omega(\sigma^2d)$, where $n$ is the number of observations, $\sigma^2$ is the variance of the noise, and $d$ is the lowest-order moment of the observations that uniquely determines the signal. In particular, it was shown that in many cases, $d = 3$ for generic signals, and thus the sample complexity is $n = \omega(\sigma^6)$.

In this paper, we analyze the second moment of the MRA and cryo-EM models. First, we show that in both models the second moment determines the signal up to a set of unitary matrices, whose dimension is governed by the decomposition of the space of signals into irreducible representations of the group. Second, we derive sparsity conditions under which a signal can be recovered from the second moment, implying sample complexity of $n = \omega(\sigma^4)$. Notably, we show that the sample complexity of cryo-EM is $n = \omega(\sigma^4)$ if at most one third of the coefficients representing the molecular structure are non-zero; this bound is near-optimal. The analysis is based on tools from representation theory and algebraic geometry. We also derive bounds on recovering a sparse signal from its power spectrum, which is the main computational problem of X-ray crystallography.

1. Introduction. This paper studies the multi-reference alignment (MRA) model of estimating a signal from its multiple noisy copies, each acted upon by a random group element. Let $G$ be a compact group acting on an $N$-dimensional vector space $V$ that can be identified with $\mathbb{R}^N$. Each MRA observation $y$ is drawn from

$$y = g \cdot f + \varepsilon,$$

where $g \in G$, $\varepsilon \sim \mathcal{N}(0, \sigma^2I)$ is a Gaussian noise vector independent of $g$, $\cdot$ denotes the group action, and $f \in V$. We assume that the distribution over $G$ is uniform (Haar). The goal is to estimate the signal $f \in V$ from $n$ realizations

$$y_i = g_i \cdot f + \varepsilon_i \quad i = 1, \ldots, n.$$

Evidently, given a set of observations $y_1, \ldots, y_n$ and with no prior knowledge on $f$, it is impossible to distinguish between $f$ and $\tilde{g} \cdot f$ for any $\tilde{g} \in G$. Thus, we can only hope to recover the orbit of $f \in V$ under $G$.

A wide range of MRA models have been studied in recent years. The simplest and most studied model is when a signal in $V = \mathbb{R}^N$ is estimated from its multiple circularly shifted, noisy copies, namely $G = \mathbb{Z}_N$ [8, 17, 2, 10, 72]. Figure 1 illustrates observations drawn from this model. Additional MRA models include the dihedral group acting on $\mathbb{R}^N$ [20], the group of two-dimensional rotations $\text{SO}(2)$ acting on band-limited images [9, 65, 53], the group of three-dimensional rotations $\text{SO}(3)$ acting on band-limited signals on the sphere [7, 64], as well as additional setups [73, 51, 21]. The results of this paper hold for any MRA model when a compact group $G$ is acting on a finite-dimensional space $V$; specific examples are provided in Section 2.4.

The MRA model is mainly motivated by single-particle cryo-electron microscopy (cryo-EM)—an increasingly popular technology that has joined X-ray crystallography as one of the two leading technologies to reconstruct molecular structures [45, 70]. Under some simplified assumptions, the cryo-EM generative model reads

$$y = T(g \cdot f) + \varepsilon, \quad g \in G,$$
Fig. 1: An example of the one-dimensional MRA setup, where a signal in $\mathbb{R}^N$ is acted upon by random elements of the group of circular shifts $\mathbb{Z}_N$. The left column shows three shifted copies of the signal, corresponding to noiseless measurements (i.e., $\sigma = 0$). In this case, all three observations are admissible solutions as the signal can be estimated only up to a group action. The middle and right columns present the same observations, with low noise level of $\sigma = 0.2$ and high noise level of $\sigma = 1.2$. This paper focuses on the extremely high noise level $\sigma \to \infty$ when the signal is swamped by noise. Figure credit: [13].

where $G$ is the group of three-dimensional rotations $\text{SO}(3)$, and $T$ is a tomographic projection acting by

$$
Tf(x_1, x_2) = \int_{\mathbb{R}} f(x_1, x_2, x_3)dx_3.
$$

The celebrated Fourier Slice Theorem states that the 2-D Fourier transform of a tomographic projection is equal to a 2-D slice of the volume’s 3-D Fourier transform [68]. This motivates analyzing the cryo-EM model in Fourier space, which is indeed the common practice. Notably, the noise level in cryo-EM images is very high; Figure 2 shows several experimental cryo-EM images. We refer the reader to recent surveys on the mathematical and algorithmic aspects of cryo-EM [84, 13, 87].

While the random linear action of 3-D rotation followed by a tomographic projection does not constitute a group action, we will show that the results of this paper apply to the cryo-EM model as well. The emerging molecular reconstruction technology of X-ray free-electron lasers (XFEL) also obeys the model (1.3) with one important distinction: the phases in Fourier space are unavailable [89, 66].

MRA analysis in the high and low noise regimes. In the low noise regime, when the signal dominates the noise, the group elements $g_1, \ldots, g_n \in G$ can be usually estimated accurately from the observations, see for example [83, 27, 32, 76, 63]. If we denote the estimated group elements by $\hat{g}_1, \ldots, \hat{g}_n \in G$, then an estimator $\hat{f}$ can be constructed by applying the inverse group elements and averaging:

$$
\hat{f} = \frac{1}{n} \sum_{i=1}^{n} \hat{g}_i^{-1} y_i.
$$
In cryo-EM, while the statistical model is more involved (1.3), the group elements can be estimated as well based on the common-lines geometrical property [86, 81], and thus recovering the molecular structure reduces to a linear inverse problem for which many effective techniques exist [68].

Motivated by cryo-EM, this work focuses on the high noise regime, when the signal is swamped by noise, and thus the group elements cannot be accurately estimated [16, 4, 75]. Consequently, one needs to develop methods to estimate the
signal $f$ directly, without estimating the group elements as an intermediate step. In particular, two main estimation methods dominate the MRA literature. The first is based on optimizing the marginalized likelihood function, using methods such as expectation-maximization [17, 65, 22, 20, 53, 59, 24]. While these techniques are highly successful, and are the state-of-the-art methods in cryo-EM [82, 78, 74], their properties are currently not well-understood [44, 57, 29, 43]. The second approach is based on the method of moments—a classical parameter estimation technique, tracing back to the seminal paper of Pearson [71]. In the method of moments, the idea is to find a signal which is consistent with the empirical moments (which are estimates of the population moments). The method of moments was applied to a wide range of MRA models [17, 7, 72, 2, 31, 28, 65, 73, 5, 51, 64, 22, 20, 24, 46, 1], as well as to construct ab initio models in cryo-EM [25, 26, 62, 79, 16, 60, 52] and XFEL [77, 34]. In this work, we focus on the method of moments due to its appealing statistical properties that are introduced next.

**Sample complexity.** In the high noise regime $\sigma \to \infty$, when the dimension of the signal is finite, it was shown that a necessary condition for recovery is $n = \omega(\sigma^{2d})$ (namely, $n/\sigma^{2d} \to \infty$ as $n, \sigma \to \infty$), where $d$ is the lowest-order moment that determines the orbit of the signal uniquely\(^1\) [10, 3, 72]. Therefore, determining the sample complexity in the high noise regime reduces to analyzing moment equations. In [7, 38], it was shown that in many cases, if the distribution of the group elements is uniform (as we assume in this paper), $d = 3$ suffices to determine almost all signals, implying sample complexity of $n = \omega(\sigma^3)$; this is also true for cryo-EM. Moreover, in some cases, an efficient algorithm to recover the signal at the optimal estimation rate was devised. For example, if $V \in \mathbb{R}^N$ and $G = \mathbb{Z}_N$, a generic signal can be recovered efficiently from the third moment, called the bispectrum, using a variety of efficient algorithms [17, 72]; see also [64].

We mention that when the distribution of the group elements is non-uniform, the MRA problem is usually easier, and signal recovery may be possible from the second moment [2, 20, 79]. In fact, uniform distribution can be thought of as the worst-case scenario of the MRA model (1.1) since, no matter what the original distribution over the group elements is, one can force a uniform distribution by generating a new set of observations:

\[(1.5)\quad z_i = \tilde{g}_i \cdot y_i = (\tilde{g}_i \cdot f) \cdot \tilde{g}_i \cdot \epsilon_i,\]

where $\tilde{g}_i$ is drawn from a uniform distribution (and thus the distribution of $\tilde{g}g$ is also uniform). This is not necessarily true for the cryo-EM model.

**Main contributions: Signal recovery from the second moment.** This work studies signal recovery from the second moment of the MRA observations:

\[(1.6)\quad \mathbb{E}yy^* = \int_G (g \cdot f)(g \cdot f)^* dg + \sigma^2 I.\]

Since we assume to know $\sigma^2$, we henceforth omit the effect of the noise. If we view $g \cdot f$ as a column vector, then $(g \cdot f)(g \cdot f)^*$ is a rank-one matrix, and thus the second moment is an integral over rank-one Hermitian matrices. Recall that the second moment can be estimated from samples

\[(1.7)\quad \mathbb{E}yy^* \approx \frac{1}{n} \sum_{i=1}^{n} y_i y_i^*.\]

\(^1\)This is not necessarily true when the dimension of the signal grows with the noise level and the number of observations [75, 36].
When \( n = \omega(\sigma^4) \), \( \frac{1}{n} \sum_{i=1}^{n} y_i y_i^* \) almost surely convergences to \( \mathbb{E} y y^* \). In this paper, we identify a class of signals that are determined uniquely by \( \mathbb{E} y y^* \). This in turn implies that the sample complexity of the problem, for this class of signals, is \( n = \omega(\sigma^4) \) and not \( n = \omega(\sigma^6) \) as for generic signals [7, 17, 72].

The first contribution of this paper, introduced in Section 2, is a precise characterization of the set of signals having the same second moment. Through the lens of representation theory, we show in Theorem 2.3 that the second moment determines the signal up to a set of unitary matrices, whose dimension is governed by the decomposition of the space of signals into irreducible representations of the group. While the unitary matrix ambiguities have been identified before in some special cases [56, 25], we show that the same pattern of ambiguities governs all MRA models. Section 2.4 provides specific examples.

To resolve these ambiguities, we suggest assuming the signal is sparse under some basis. This is a common assumption in many problems in signal processing and machine learning, such as regression [90, 47], compressed sensing [35, 30, 41], and various image processing applications [40]. Note that the representations of compact groups that we consider are typically spaces of \( L^2 \) functions on a domain such as \( \mathbb{R}^3 \). As such, they do not come equipped with a canonical basis, so the assumption we make is that our signal is sparse with respect to a generic basis. The notion of generic basis comes from algebraic geometry and makes use of the fact that the set of all possible bases of a vector space is an algebraic variety. When we say that a result holds for a generic basis, it means that there is a Zariski open set of bases for which the statement of the result holds. In particular, it holds for almost all bases. For more detail, see Section 3.1.

Our second contribution, presented in Section 3 and summarized in Theorem 3.1, describes the sparsity level under which the orbit of a generic sparse signal can be recovered from the second moment. That is, the sparsity level that allows resolving the unknown unitary matrices. This implies that merely \( n = \omega(\sigma^4) \) observations are required for accurate signal recovery. The sparsity level is bounded by a factor that depends on the dimensions of the irreducible representations and their multiplicities. The proof of Theorem 3.1 relies on tools from algebraic geometry and representation theory. Specific results are provided in Section 3.3.

Implications to cryo-EM. In Section 4, we show that the second moment of the cryo-EM model (1.3) is the same as of the MRA model (1.1), when \( G \) is the group of three-dimensional rotations \( \text{SO}(3) \) and \( V \) is the space of band-limited functions on the ball. Namely, the tomographic projection operator (1.4) does not change the second moment of the observations. We introduce this model in detail in Section 4 and particularize the main result of this paper to cryo-EM in Theorem 4.3. We now state this result informally.

**Theorem 1.1 (Informal theorem for cryo-EM).** In the cryo-EM model (1.3) (described in detail in Section 4.1), a generic \( K \)-sparse function \( f \in \mathbb{V} \) is uniquely determined by the second moment for \( K \lesssim N/3 \), where \( N = \dim \mathbb{V} \).

Theorem 1.1 implies that sparse structures can be recovered, in the high noise regime, with only \( n = \omega(\sigma^4) \) observations, improving upon \( n = \omega(\sigma^6) \) for generic structures [7]. Figure 3 shows the distribution of wavelet coefficients (a standard choice of basis in many signal processing applications [67]) of a few molecular structures. Evidently, less than 1/3 of the coefficients capture almost all the energy of the volumes, suggesting that the bound of Theorem 1.1 is reasonable for typical molecular structures.
A recent paper [23] showed that a structure composed of ideal point masses (possibly convolved with a kernel with a non-vanishing Fourier transform) can be recovered from the second moment. However, the technique of [23] is tailored for this specific model. The same paper also suggests to recover a 3-D structure from the second moment based on a sparse expansion in a wavelet basis. Our result implies that for a given wavelet basis then with probability one the generic signal whose expansion is sufficiently sparse with respect to that basis can be recovered from its second moment. Moreover, for a given basis, there is, in principle, a computational technique to test whether Theorem 1.1 holds for that basis. See Remarks 3.2 and 3.3 for more detail.

Fig. 3: The sorted wavelet coefficients of cryo-EM structures whose experimental images are presented in Figure 2. The structures were downloaded from the Electron Microscopy Data Bank (EMDB) https://www.ebi.ac.uk/emdb. The structures were expanded using Haar wavelets, where the number of coefficients is approximately the same as the number of voxels. Besides EMD-8012, all the volumes energy (i.e., the squared norm of the coefficients) is captured by less that one third of the coefficients, which is the bound of Theorem 1.1. For EMD-8012, the same fraction of wavelet coefficients captures more than 91% of its energy.
Crystallographic phase retrieval. The second moment of the MRA model, where random elements of the group of circular shifts $\mathbb{Z}_N$ act on real signals in $\mathbb{R}^N$, is equivalent to the squared absolute values of the Fourier transform of the signal, known as the power spectrum. Recovering a signal from its power spectrum is called the phase retrieval problem and it has numerous applications in signal processing; see recent surveys and references therein [80, 14, 49, 19].

Crystals are often modeled as functions on a finite abelian group (typically $\mathbb{Z}_N$), which corresponds to the regular representation of the group. For this representation there is a natural notion of sparsity which corresponds to requiring that the function is non-zero only on a small subset of elements of the group. Real valued functions on $\mathbb{Z}_N$ are identified with $\mathbb{R}^N$ and this notion of sparsity corresponds to sparsity in the standard basis of $\mathbb{R}^N$. Recovering a sparse signal from the power spectrum is the main computational challenge in X-ray crystallography: a leading method for elucidating the atomic structure of molecules. This is by far the most important phase retrieval application. We discuss this problem in detail in Section 5 and explain how the techniques of this paper can be used to prove that a $K$-sparse signal $f \in \mathbb{R}^N$, under a generic basis, can be recovered from its power spectrum provided that $K \leq N/2$.

Organization of the paper. The rest of the paper is organized as follows. Section 2 formulates the second moment of the MRA model (1.1) and shows that it determines the signal up to a set of unitary matrices. The section also provides several examples. Section 3 derives a bound on the sparsity level that allows for unique recovery from the second moment (Theorem 3.1) in terms of the dimension and multiplicity of the irreducible representations, and provides examples. Section 4 focuses on cryo-EM: the main motivation of this paper. We formulate the cryo-EM model in detail, derive explicitly the ambiguities of the second moment, and deduce sparsity conditions allowing unique recovery (Theorem 4.3). Section 5 discusses the crystallographic phase retrieval problem. Section 6 concludes this work, and delineates future research directions. The supplementary material provides necessary background in representation theory.

2. The second moment and symmetries. This section lays out the mathematical background for the second moments of the MRA model (1.1) for a compact group $G$ acting on an $N$-dimensional real or complex vector space $V$. Following standard terminology, we refer to a vector space $V$ equipped with an action of a group $G$ as a representation of $G$. Our goal is to use classical methods from the representation theory of compact groups to understand the information obtained from the second moment. In the supplementary material, we provide a necessary background in representation theory.

Any representation of a compact group is unitary. This means that elements of $G$ act on $V$ as unitary transformations. In particular, the action preserves a Hermitian inner product. By Weyl’s unitarian trick, this inner product can be obtained by averaging any chosen inner product on $V$ over the group. If $V$ is a real vector space, then the action of $G$ is orthogonal, meaning that elements of $G$ act by orthogonal transformations.

Let $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$ be the field. Assuming that the distribution on the group $G$ is uniform (Haar), then a choice of basis for an $N$-dimensional representation $V = \mathbb{K}^N$ expresses the second moment as a function $\mathbb{K}^N \rightarrow \mathbb{K}^{N^2}$ given by the formula

\begin{equation}
\label{eq:second_moment}
f \mapsto \int_G (g \cdot f)(g \cdot f)^* dg,
\end{equation}
where $\mathbb{K}^{N^2} = \text{Hom}(V, V)$ is the vector space of linear transformations $V \to V$. The vector $f$ is viewed as column vector so $(g \cdot f)(g \cdot f)^*$ is an $N \times N$, rank-one Hermitian matrix.

The second moment can also be defined without the use of coordinates, using tensor notation, as a map $V \to V \otimes V^*$,

\begin{equation}
(2.2) \quad f \mapsto \int_G (g \cdot f) \otimes (g \cdot f^*) dg.
\end{equation}

We will use both (2.1) and (2.2) interchangeably. The reason that these formulations are equivalent is that there is isomorphism of representations $V \otimes V^* \to \text{Hom}(V, V)$ as discussed in the supplementary material. If we choose an orthonormal basis for $V$, then the tensor $f_1 \otimes f_2^*$ corresponds to the matrix $f_1 f_2^*$.

Ultimately, we will view elements of $V$ as functions $D \to \mathbb{C}$, where $D$ is some domain on which $G$ acts. For example, in cryo-EM $G = \text{SO}(3)$, and $V$ is the subspace of $L^2(\mathbb{C}^3)$ consisting of the Fourier transforms of real-valued functions in $L^2(\mathbb{R}^3)$; this problem is discussed in detail in Section 4. The second moment of a function $f : D \to \mathbb{C}$ can be viewed as the function $m_f^2 : D \times D \to \mathbb{C}$, where

\begin{equation}
(2.3) \quad m_f^2(x_1, x_2) = \int_G (g \cdot f(x_1))(g \cdot f(x_2)) \, dg,
\end{equation}

where $g \cdot f : D \to \mathbb{C}$ is defined by $g f(x) = f(g^{-1} x)$.

### 2.1. The second moment of an irreducible representation of $G$

Recall that a representation is irreducible if it has no non-zero proper $G$-invariant subspaces. Examples of reducible and irreducible representations are given in the supplementary material. If the representation $V$ is irreducible, then the following proposition shows that the second moment gives very little information about a vector $f \in V$.

**Proposition 2.1.** Let $V$ be an $N$-dimensional irreducible unitary representation of a compact group $G$ and identify $V$ with $\mathbb{C}^N$ via a choice of orthonormal basis $f_1, \ldots, f_N$ of $V$. Then, as a map $\mathbb{C}^N \to \mathbb{C}^{N^2}$, the second moment is given by the formula

\begin{equation}
(2.4) \quad f \mapsto \frac{|f|^2}{N} I_N,
\end{equation}

where $I_N$ is the $N \times N$ identity matrix. In tensor notation, the second moment is the map $V \mapsto V \otimes V^*$ given by

\begin{equation}
(2.5) \quad f \mapsto \frac{|f|^2}{N} \sum_{i=1}^N f_i \otimes f_i.
\end{equation}

**Proof.** If we identify the Hermitian matrix $m_f^2 = \int_G (g \cdot f)(g \cdot f)^* \, dg$ as giving a linear transformation $V \to V$, then the second moment defines a map $V \to \text{Hom}(V, V)$, where $\text{Hom}(V, V)$ is the group of linear transformations $V \to V$. Since the second moment is by definition invariant under the action of $G$ on $V$ (i.e., $f$ and $g \cdot f$ both yield the matrix $m_f^2$), the matrix $m_f^2$ defines a $G$-invariant linear transformation on $V$. However since $V$ is irreducible, by Schur’s Lemma, any $G$-invariant linear transformation $V \to V$ is a scalar multiple of the identity. Since $G$ acts by unitary transformations, $\text{trace}((g \cdot f)(g \cdot f)^*) = \text{trace}(ff^*) = |f|^2$ for any $g \in G$. Thus,

$$
\text{trace} m_f^2 = \int_G \text{trace}((g \cdot f)(g \cdot f)^*) \, dg = |f|^2.
$$
The formula (2.5) is equivalent to the first formula because under the identification of \(V \otimes V^*\) with Hom\((V, V) = K^{N^2}\), the tensor \(\sum_{i=1}^{N} f_i \otimes f_i\) corresponds to the identity matrix.

2.2. The second moment for multiple copies of an irreducible representation. The following discussion is motivated by the situation in cryo-EM, where we view \(\mathbb{R}^3\) as a collection of spherical shells. In other words, we model \(SO(3)\) acting on \(L^2(\mathbb{R}^3)\) by taking a number of copies of \(L^2(S^2)\). This is a standard model in cryo-EM, and is introduced in detail in Section 4.

Consider the case where the representation \(V\) decomposes as the direct sum of \(R\) copies of a single irreducible representation \(V_0\). In other words, there is a \(G\)-invariant isomorphism \(V \simeq V_0^{\oplus R}\). This means that any vector \(f \in V\) can be decomposed uniquely as \(f = f[1] + \ldots + f[R]\), with \(f[r]\) in the \(r\)-th copy of \(V_0\). The summands are invariant under the action of \(G\) so \((g \cdot f)[r] = g \cdot f[r]\).

Since \(V\) decomposes as the sum \(V_0^{\oplus R}\), the tensor product \(V \otimes V^*\) decomposes as the sum of tensor products \(\oplus_{i,j=1}^{R} V_0[i] \otimes V_0^*[j]\), where \(V_0[r]\) indicates the \(r\)-th copy of \(V_0\) in the decomposition of \(V\). In particular, using tensor notation for the second moment, we can decompose

\[
(2.6) \quad m_f^2 = \int_G (g \cdot f) \otimes (g \cdot f^*) dg = \sum_{i,j=1}^{R} m_f^2[i, j],
\]

where

\[
(2.7) \quad m_f^2[i, j] = \int_G (g \cdot f[i]) \otimes (g \cdot f[j]^*) dg \in V_0[i] \otimes V_0^*[j],
\]

is the component in the \((i, j)\)-th summand of the tensor product \(V \otimes V^*\). Each of the summands in (2.7) defines a \(G\)-invariant linear transformation \(V_0[i] \rightarrow V_0[j]\).

Let \(N_0 = \dim V_0\). For suitable orthonormal bases \(f_1[i], \ldots, f_{N_0[i]}[i]\) and \(f_1[j], \ldots, f_{N_0[j]}[j]\) of \(V_0[i]\) and \(V_0[j]\), respectively, Schur’s Lemma implies that

\[
m_f^2[i, j] = \int_G (g \cdot f[i]) \otimes (g \cdot f[j]^*) \, dg = \frac{1}{N} \left( \sum_{k=1}^{N_0} f_k[i] \otimes f_k[j]^* \right).
\]

To put this more directly, if we view an element of \(V = V_0^{\oplus R}\) as an \(R\)-tuple \(f[1], \ldots, f[R]\) of elements of \(V_0\), then the second moment determines all pairwise inner products \(\langle f[i], f[j]\rangle\). Equivalently, if we consider the vectors \(f[1], \ldots, f[R]\) as the column vectors of an \(N_0 \times R\) matrix \(A\), then the second moment determines the \(R \times R\) Hermitian matrix \(A^*A\).

Therefore, the vectors \(f[1], \ldots, f[R] \in V_0\) are determined from their pairwise inner products up to the action of the unitary group \(U(N_0)\), parameterizing the isometries of \(V_0\). If, as will be the case for cryo-EM, we know that each \(f[r]\) lies in a conjugation invariant subspace of \(V\) (for example, it is the Fourier transform of a real vector), then we can determine each \(f[r]\) up to the action of a subgroup of \(U(N_0)\), isomorphic to the real orthogonal group \(O(N_0)\).

2.3. The second moment of a general finite dimensional representation and its group of ambiguities. A general finite dimensional representation of a compact group can be decomposed as

\[
(2.8) \quad V = \bigoplus_{\ell=1}^{L} V_{\ell}^{\oplus R_{\ell}},
\]
with the $V_\ell$ are distinct (non-isomorphic) irreducible representations of $G$ of dimension $N_{\ell}$. An element of $f \in V$ has a unique $G$-invariant decomposition as a sum

\[(2.9)\]

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

where $f_{\ell}[i]$ is in the $i$-th copy of the irreducible representation $V_\ell$. In this case, the second moment decomposes as a sum of tensors $\int_{G} (g \cdot f_\ell[i]) \otimes (g \cdot f_m[j]) dg$. Each of these tensors determines a $G$-invariant map $V_\ell[i] \rightarrow V_m[j]$. Since $V_\ell[i]$ and $V_m[j]$ are non-isomorphic irreducible representations, Schur’s Lemma implies that there are no non-zero $G$-invariant linear transformations $V_\ell[i] \rightarrow V_m[j]$ for $\ell \neq m$. In other words, we have a generalized orthogonality relation that the tensors $\int_{G} (g \cdot f_\ell[i]) \otimes (g \cdot f_m[j]) dg$ are zero if $\ell \neq m$ for all $i, j$.

Hence, the second moment decomposes as a sum

\[(2.10)\]

\[m^2_f = \sum_{\ell=1}^{L} \sum_{i,j=1}^{R_{\ell}} \frac{\langle f_{\ell}[i], f_{\ell}[j] \rangle}{N_{\ell}} \left( \sum_{k=1}^{N_{\ell}} f_{k,\ell}[i] \otimes f_{k,\ell}[j] \right),\]

where the vectors $f_{1,\ell}[i], \ldots, f_{N_{\ell},\ell}[i]$ form an orthonormal basis for the $i$-th copy of the $\ell$-th irreducible representation $V_\ell$.

Remark 2.2. The second moment is a map $V \rightarrow \text{Hom}_G(V, V)$. As noted by a referee, $\text{Hom}_G(V, V)$ is the endomorphism ring of the $G$-module $V$. A result from classical representation theory, which follows from Schur’s Lemma, states that this ring decomposes into a sum of matrix algebras $\oplus_{\ell=1}^{L} \text{Mat}(R_\ell)$ and our description of the second moment can also be derived using this decomposition.

2.3.1. Functional representation of the second moment. If, as will be the case for our model of cryo-EM, we view the elements of $V$ as functions $f: D \rightarrow \mathbb{C}$, then we can reformulate (2.10) as follows. Suppose that $f_1, \ldots, f_{N_\ell}[i]$ are functions $D \rightarrow \mathbb{C}$ which form an orthonormal basis for the $i$-th copy of the $\ell$-th irreducible representation $V_\ell$. If we expand $f_\ell[i] = \sum_{m=1}^{N_\ell} A^m_{\ell}[i] f_{m,\ell}[i]$, then the second moment realized as a function $D \times D \rightarrow \mathbb{C}$ is expanded as

\[(2.11)\]

\[m^2_f(x_1, x_2) = \sum_{\ell=1}^{L} \sum_{i, j=1}^{R_{\ell}} \left( \sum_{m=1}^{N_{\ell}} A^m_{\ell}[i] A^m_{\ell}[j] \right) \left( \sum_{k=1}^{N_{\ell}} f_{k,\ell}[i](x_1) f_{k,\ell}[j](x_2) \right),\]

where $x_1, x_2$ are, respectively, the variables on the first and second copies of $D$ respectively.

2.3.2. The group of ambiguities. The main result of this section is a characterization of the group of ambiguities of the second moment. Later on, we provide a few explicit examples.

Suppose that $V$ decomposes as a sum of irreducible representations $V = \bigoplus_{\ell=1}^{L} V_{\ell}^R$, where $\dim V_\ell = N_\ell$, and let $H = \prod_{\ell=1}^{L} U(N_\ell)$. The group $H$ acts on $V$ as follows. If $f \in V$ is represented by an $L$-tuple of $(A_1, \ldots, A_L)$ with $A_\ell$ an $N_\ell \times R_\ell$ matrix and $h = (U_1, \ldots, U_L)$ with $U_\ell \in U(N_\ell)$, then $h \cdot f = (U_1 A_1, \ldots, U_L A_L)$.

Theorem 2.3. With the notation as above, a vector $f \in V$ is determined from the second moment up to the action of the ambiguity group $H = \prod_{\ell=1}^{L} U(N_\ell)$. That is, $m^2_f = m^2_{f'}$ if and only if $f = h \cdot f'$ for some $h \in H$.}

10
The vector space $C$ shows an example of two different images with the same power spectrum. The ambiguity group is of dimension $N = \sum_{\ell=1}^L N_\ell - 1/2$. If the ambiguity group is isomorphic to the real orthogonal groups, as in cryo-EM, then the ambiguity group is of dimension $N_H = \sum_{\ell=1}^L N_\ell (N_\ell - 1)/2$.

Remark 2.5. Note that the total dimension of the ambiguity group of the second moment does not depend on the multiplicities $R_\ell$. In particular, the ratio of the dimensions is

$$\frac{N_H}{N} = \frac{\sum_{\ell=1}^L N_\ell^2}{2 \sum_{\ell=1}^L R_\ell N_\ell}.$$ 

This implies that as the number of multiplicities increases, the proportional amount of information about the signal contained in the second moment increases as well.

2.4. Examples.

2.4.1. The power spectrum. Consider the group $G = \mathbb{Z}_N$ acting on $\mathbb{K}^N$ by cyclic shifts, where $\mathbb{K} = \mathbb{R}$ or $\mathbb{K} = \mathbb{C}$. In the Fourier domain, the cyclic group $G = \mathbb{Z}_N$ acts by multiplication by roots of unity. In particular, we identify $\mathbb{Z}_N = \mu_N$, where $\mu_N$ is the $N$-th roots of unity. If $\omega \in \mu_N$, then

$$\omega \cdot (f[0], \ldots, f[N-1]) = (\omega f[0], \omega f[1], \ldots, \omega^{N-1} f[N-1]).$$

The vector space $\mathbb{C}^N$ with this action of $\mu_N$ decomposes as a sum of one-dimensional irreducible representations (namely, $N_\ell = R_\ell = 1$ for all $k$ so that $N = L$) $\mathbb{V}_0 \oplus \cdots \oplus \mathbb{V}_{N-1}$, where $\omega \in \mu_N$ acts on $\mathbb{V}_i$ by $\omega \cdot f[i] = \omega^i f[i]$. The second moment of a vector $f \in \mathbb{C}^N$ in the Fourier domain is the power spectrum $(f[0]^2, \ldots, f[N-1]^2)$. This determines the vector up to the action of the group $(\mathbb{S}^1)^N$ since $U(1) = \mathbb{S}^1$. Figure 4 shows an example of two different images with the same power spectrum.

Recall that the image of $\mathbb{R}^N$ under the discrete Fourier transform is the real subspace of $\mathbb{C}^N$ given by the condition $f[N-i] = \overline{f[i]}$. Thus, if $f$ is the Fourier transform of a real vector, the ambiguity group must preserves the condition that $f[N-i] = \overline{f[i]}$ and is therefore the subgroup of

$$\{ (\lambda_0, \ldots, \lambda_{N-1} | \lambda_{N-n} = \lambda_n^{-1}) \} \subset (\mathbb{S}^1)^N.$$

Recovering a signal from its power spectrum is called the phase retrieval problem [80, 14, 49, 19]; see Section 5 for further discussion.

2.4.2. Dihedral MRA. Consider the action of the dihedral group $G = D_{2N}$ acting $\mathbb{K}^N$, where the rotation $r \in D_{2N}$ acts by cyclic shift and the reflection $s \in D_{2N}$ acts by $(s \cdot f)[i] = f[N-i]$. In the Fourier domain, $(s \cdot f)[i] = f[N-i]$ and
Fig. 4: The left panel shows an image of Albert Einstein. To generate the image of the right panel, we combined the absolute values of the Fourier transform of Einstein’s image with random phases and computed the inverse Fourier transform. This example underscores that two images with the same power spectrum may be very different. More generally, two signals which are equal up to a set of unitary matrices (e.g., have the same second moment) may differ significantly.

\[(r \cdot f)[i] = \omega^i f[i] \text{ as in (2.12). In [20], it was shown that the orbit of a generic signal is determined uniquely from the second moment if the group elements are drawn from a non-uniform distribution over the dihedral group. Here, we consider a uniform (Haar) distribution of the group elements.}

The vector space \( \mathbb{C}^N \) with this action of \( D_{2N} \) decomposes into a sum of one and two-dimensional irreducible representations, depending on the parity of \( N \) (with multiplicity \( R_\ell = 1 \)). If \( N \) is even, then

\[ \mathbb{C}^N = V_0 \oplus V_1 \oplus \ldots \oplus V_{N/2 - 1} \oplus V_{N/2}, \]

where \( V_0 \) is the one dimensional subspace spanned by the vector \( e_0 = (1, 0, \ldots, 0) \), \( V_{N/2} \) is spanned by the vector \( e_{N/2} \) (\( N_0 = N_{N/2} = 1 \)), and for \( 1 \leq \ell \leq N/2 - 1 \), \( V_\ell \) is the subspace spanned by \( \{e_\ell, e_{N-\ell}\} \) (\( N_\ell = 2 \)). Similarly, if \( N \) is odd, then

\[ \mathbb{C}^N = V_0 \oplus V_1 \oplus \ldots \oplus V_{(N-1)/2}, \]

where again \( V_0 \) is spanned by \( e_0 \) and for \( \ell \geq 1 \) \( V_\ell \), is spanned by \( \{e_\ell, e_{N-\ell}\} \).

Therefore, the second moment of a vector \( f \) in the Fourier domain determines the \( N/2 + 1 \) real numbers

\[ (|f[0]|^2, |f[1]|^2 + |f[N - 1]|^2, \ldots, |f[N/2 - 1]|^2 + |f[N/2 + 1]|^2, |f[N/2]|^2) \]

if \( N \) is even, and the \( (N + 1)/2 \) real numbers

\[ (|f[0]|^2, |f[1]|^2 + |f[N - 1]|^2, \ldots, |f[(N - 1)/2]|^2 + |f[(N + 1)/2]|^2) \]

if \( N \) is odd. When \( \mathbb{K} = \mathbb{C} \), this is less information than the power spectrum. When \( N \) is even, the ambiguity group is \( S^1 \times U(2)^{N/2} \times S^1 \) and when \( N \) is odd the ambiguity group is \( S^1 \times U(2)^{(N-1)/2} \). However, if \( \mathbb{K} = \mathbb{R} \) then the second moment gives the
power spectrum because if \( f \) is the Fourier transform of a real vector then we have \( |f[i]| = |f[N-i]| \). In this case, the ambiguity group is \( \pm 1 \times O(2)^{N/2} \times \pm 1 \) if \( N \) is even and if \( N \) is odd then it is \( \pm 1 \times O(2)^{(N-1)/2} \). These groups are isomorphic to the subgroups of \((S^1)^N\) considered in (2.13).

2.4.3. MRA with rotated images. In this model the Fourier transform of an image is represented as a radially discretized band limited function on \( \mathbb{C}^2 \). That is, our function \( f \) is expressed as \( f = (f[1], \ldots, f[R]) \), where

\[
(2.14) \quad f[r](\theta) = \sum_{k=-L'}^{L'} a_{k,r}e^{i\theta k}, \quad \theta \in [0,2\pi),
\]

for some bandlimit \( L' = (L-1)/2 \) and \( R \) radial samples. The action of a rotation \( S^1 \) on the image is given by

\[
e^{i\alpha} \cdot f[r](\theta) = \sum_{k=-L'}^{L'} a_{k,r}e^{i(\theta-\alpha)k} = \sum_{k=-L'}^{L'} a_{k,r}e^{-i\alpha k}e^{i\theta k}.
\]

With this action, the parameter space of two-dimensional images is the \( S^1 \)-representation \( V = V_{-L'} \oplus \ldots \oplus V_{L'}^R \), where \( V_k \) is the one-dimensional representation of \( S^1 \), where \( e^{i\alpha} \in S^1 \) acts with weight \(-k\). Namely, \( N_k = 1, R_k = R \) for all \( k \) so that \( N = LR \).

The \((r_1, r_2)\) component of the second moment equals

\[
(2.15) \quad m_2^2[r_1, r_2](\theta_1, \theta_2) = \int_\alpha e^{-i\alpha f[r_1](\theta_1)}e^{-i\alpha f[r_2](\theta_2)}d\alpha \\
= \sum_{k=-L'}^{L'} \sum_{k_1=-L'}^{L'} a_{k_1,r_1} \overline{a_{k_1,r_2}} e^{-i(\theta_1-\theta_2)k_1} \\
= \sum_{k=-L'}^{L'} \sum_{k_2=-L}^{L} a_{k,r_1} \overline{a_{k,r_2}} e^{i\theta_2} e^{-i\theta_1} e^{-i\alpha k_2} \\
= m_2^2[r_1, r_2](\Delta \theta),
\]

where \( \Delta \theta := \theta_1 - \theta_2 \). Following our previous discussion, a function \( f \in V \) is determined by a \( L \)-tuple of \( 1 \times R \) matrices \((A_{-L'}, \ldots, A_{L'})\), where \( A_k = (a_{k,1}, \ldots, a_{k,R})^T \). The second moment computes the \( L \)-tuple of rank-one \( R \times R \) matrices \((A_{-L'}^*, A_{-L'}, \ldots, A_{L'}^*, A_{L'})\). Since each irreducible summand in the representation \( V \) has dimension one (namely, \( N_k = 1 \) for all \( k \)), the ambiguity group of the second moment for the rotated images problem is \((S^1)^L\). If we assume that the function \( f \) is the Fourier transform of a real valued function, then \( a_{k,r} = \overline{a_{-k,r}} \) and the ambiguity group is \( O(2)^L \times \pm 1 \).

2.4.4. Two-dimensional tomography from unknown random projections.

The problem of recovering a two-dimensional image from its tomographic projections is a classical problem in computerized tomography (CT) imaging [68]. However, in some cases, the viewing angles are unknown and may be considered random. Due to the Fourier Slice Theorem, this is equivalent to randomly rotating the image, and then acquiring a single one-dimensional line of its Fourier transform. While generally
an image cannot be recovered from such random projections (in contrast to the three-dimensional counterpart (1.3), where recovery is theoretically possible based on the common-lines property [86, 81]), it was shown that unique recovery, up to rotation, requires rather mild conditions [12]. Different algorithms were later developed, see for example [33, 88, 95].

In this model, we compute the second moment of the Fourier transform of the image after tomographic projection to a line. In other words, we compute the integral

\[
\int_{S^1} T e^{i\alpha} \cdot f[r_1](\theta_1) T e^{i\alpha} \cdot f[r_2](\theta_2) d\alpha,
\]

where \( T \) is the tomographic projection to the line \( \theta = 0 \) (the two-dimensional counterpart of (1.4)). Because we are computing the second moment after tomographic projection, we cannot directly determine the ambiguity group from Theorem 2.3. In this case, the tomographic projection causes us to lose information and we obtain a function only of \( r_1, r_2 \) (compare with (2.15))

\[
m_f^2[r_1, r_2] = \sum_{k=-L'}^{L'} a_{k, r_1} \overline{a_{k, r_2}},
\]

where \( L' = (L - 1)/2 \). If we view the \( L \)-tuple of \( 1 \times R \) matrices \( (A_{-L'}, \ldots, A_{L'}) \) as a single \( L \times R \)-matrix \( A \), then the projected second moment determines the Hermitian matrix \( A^* A \). Equivalently, an element of \( V \) is determined by \( R \) vectors in \( \mathbb{C}^L \) and the projected second moment determines all pairwise inner products of these vectors. In this case, the loss of information caused by the tomographic projection means that the ambiguity group is the bigger group \( U(L) \) (or \( O(L) \) if the image is the Fourier transform of a real-valued function) compared to \( (S^1)^L \) in the unprojected case (respectively, \( O(2)^{L'} \times \pm 1 \)).

Remark 2.6. Note that when \( G = \text{SO}(3) \), the second moment is unchanged by the tomographic projection from \( \mathbb{R}^3 \to \mathbb{R}^2 \). See Lemma 4.1.

3. Retrieving the unitary matrix ambiguities for sparse signals. In the previous section, we have shown that it is generally impossible to recover a vector \( f \) in a representation \( V \) of a compact group \( G \) from its second moment due to the large group of ambiguities. To resolve these ambiguities and recover the signal in either the MRA (1.1) or cryo-EM (1.3) models, we need a prior on the sought signal. In this work, we assume that the signal is sparse in some basis. This assumption has been studied and harnessed in the MRA [24, 46] and cryo-EM literature [23, 91, 54, 58, 42, 94]. In this section, we derive bounds on the sparsity level that allows retrieving the missing unitary matrices, as a function of the dimensions and multiplicities of the irreducible representations. We also provide a couple of examples, and leave more detailed discussions on cryo-EM and phase retrieval to, respectively, Section 4 and Section 5.

3.1. Sparsity conditions. Let \( V \) be an \( N \)-dimensional vector space. The notion of sparsity depends on the choice of an orthonormal basis \( V = \{ f_1, \ldots, f_N \} \). A vector \( f \in V \) is \( K \)-sparse with respect to this ordered basis if \( f \) is a linear combination of at most \( K \) elements of this basis. The set of \( K \)-sparse vectors with respect to an ordered basis \( V \) is the union of \( \binom{N}{K} \) linear subspaces \( L_S(V) \), where \( L_S(V) \) is the subspace spanned by the vectors \( \{ f_i \}_{i \in S} \) and \( S \) is a \( K \)-element subset of \( [1, N] \).
Let
\[ V = \oplus_{\ell=1}^L V_\ell^{R_\ell}, \]
be a representation of a compact group \( G \), where \( \dim V_\ell = N_\ell \). Let \( H = \prod_{\ell=1}^L U(N_\ell) \) be the ambiguity group of the second moment (see Theorem 2.3).

The main result of this section is the following.

**Theorem 3.1.** Let \( V \) be a representation as in (3.1), let \( N = \sum_{\ell=1}^L N_\ell R_\ell \) be its total dimension and let \( M = \sum_{\ell=1}^L \min(N_\ell R_\ell, N_\ell^2) \). Then, for a generic choice of orthonormal basis \( \mathcal{V} \), a generic \( K \)-sparse vector \( f \in V \) with \( K \leq N - M \) is uniquely determined by its second moment, up to a global phase.

We note that, as in Remark 2.5, the larger the number of irreducible representation copies is, the easier the problem is. In particular, note that if \( R_\ell \gg N_\ell \) for all \( \ell \), the sparsity bound read \( K \leq \sum_{\ell=1}^L R_\ell N_\ell = N \). That is, the sparsity level is proportional to the dimension of the representation. In Theorem 4.3 we provide an explicit example for the cryo-EM case.

**Remark 3.2.** The set of ordered orthonormal bases of an \( N \)-dimensional vector space \( V \) can be identified with the real algebraic group \( O(N) \) if \( V \) is real, and \( U(N) \) if \( N \) is complex. When we say that our result holds for a **generic basis** we mean that there is a real Zariski open subset of \( O(N) \) (resp. \( U(N) \)) parametrizing bases for which the conclusion of Theorem 3.1 holds. Since the complement of a Zariski open set has Lebesgue measure zero, this means that given an orthonormal basis which the conclusion of Theorem 3.1 holds. Since the complement of a Zariski open set has Lebesgue measure zero, this means that given an orthonormal basis \( \mathcal{V} \) for \( V \), then with probability one Theorem 3.1 holds for that basis.

**Remark 3.3.** Given a basis \( \mathcal{V} = \{f_1, \ldots, f_N\} \) for \( V \), we can express \( f \in V \) as \( \sum_{n=1}^N x_i f_i \) and the second moment is a collection of homogeneous quadratic functions in \( x_1, \ldots, x_N \), which we denote by \( m_f^2(x_1, \ldots, x_N) \). The following computational test is a simple generalization of the test used in [18, Sections 4.3.3, 4.3.4] that can be used to decide whether \( \mathcal{V} \) satisfies the theorem with a sparsity level of \( K \):

If \( S \subset [1, N] \) is a subset of size \( K \), let
\[ I_S = \{(x_1, \ldots, x_N), (y_1, \ldots, y_N) \mid m_f^2(x_1, \ldots, x_N) = m_f^2(y_1, \ldots, y_N)\} \subset \mathbb{L}_S(\mathcal{V}) \times \mathbb{L}_S(\mathcal{V}), \]
where \( \mathbb{L}_S(\mathcal{V}) \) is the subspace spanned by \( \{f_i\}_{i \in S} \). Likewise, if \( S, S' \) are two distinct \( K \)-element subsets of \([1, N]\), let
\[ I_{S,S'} = \{(x_1, \ldots, x_N), (y_1, \ldots, y_N) \mid m_f^2(x_1, \ldots, x_N) = m_f^2(y_1, \ldots, y_N)\} \subset \mathbb{L}_S(\mathcal{V}) \times \mathbb{L}_{S'}(\mathcal{V}). \]

The conclusion of Theorem 3.1 holds if \( I_S \) has dimension exactly \( K \) and degree one, and \( \dim I_{S,S'} < K \). For small values of \( N \), these conditions can be checked using a computer algebra system, but not in polynomial time [18, Appendix D].

**Remark 3.4 (Frames).** Recall that a collection \( \mathcal{F} \) of vectors in a finite-dimensional vector space \( V \) is a **frame** if the vectors span \( V \). The methods used to prove Theorem 3.1 can also be used to prove a corresponding result where orthonormal bases are replaced by arbitrary frames. The only difference between working with frames instead of bases is that definition of a vector being sparse with respect to an ordered frame is more subtle. The reason is that for a generic frame \( \mathcal{F} \), any \( N \)-element subset consists of linearly independent vectors, so any \( f \in V \) which has zero frame coefficients with respect to \( N \) elements in \( \mathcal{F} \) must necessarily be zero. In particular, if we work with frames, then the condition that a vector is \( K \)-sparse should be replaced by
the condition that at least \( N - K \) of the frame coefficients are zero. Otherwise, the statements and proofs remain the same.

3.1.1. Strategy and remarks on the proof. The proof of Theorem 3.1 involves a number of steps. Suppose that \( V \) is a generic orthonormal basis and consider the set of vectors which are \( K \)-sparse with respect to \( V \). The set of such vectors form the union of \( \binom{N}{K} \) \( K \)-dimensional linear subspaces of \( V \). The strategy of the proof is to show that with bounds on \( K \) given in the Theorem 3.1, the following is true: if \( f \) is a generic \( K \)-sparse vector with respect to the orthonormal basis \( V \), the only vectors in the \( H \)-orbit of \( f \) which are also \( K \)-sparse are of the form \( e^{i\alpha}f \).

Although the \( H \)-orbit of \( f \) is a real algebraic subvariety of \( V \) containing \( \{e^{i\alpha}f\} \), we know of no general algebraic geometry result which can be used to analyze when a generic linear subspace of \( V \) will intersect the orbit \( HF \) exactly in \( \{e^{i\alpha}f\} \). To prove our result, we will actually prove something stronger. Rather than consider the \( H \)-orbit of a vector \( f \), we will consider the linear span of its orbit and prove that the only \( K \)-sparse vectors in the linear span of the orbit of \( f \) are scalar multiples of \( f \). The advantage of working with the linear span is that we can use techniques from linear algebra to understand when a linear subspace (the linear span of our orbit) intersects the \( \binom{N}{K} \) \( K \)-dimensional linear subspaces consisting of vectors which are \( K \)-sparse with respect to the given orthonormal basis \( V \).

The price we pay for working with the linear span of an orbit instead of directly working with the orbit is that if the \( H \)-orbit of \( f \) has real dimension \( M \), then its linear span is a complex linear subspace of complex dimension \( M \) or equivalently real dimension \( 2M \) (see Proposition 3.5). As a result, the sparseness bound we obtain may not be optimal. However, when \( \dim H << \dim V \), as is the case in cryo-EM, this gap is not significant.

Finally, we remark that for the general MRA problem with group \( G \) (1.1), we can at best recover the \( G \)-orbit of a vector \( f \) from its moments. However, by imposing the prior condition that the vector is sparse with respect to a given basis we have the possibility of recovering a vector up to a global phase. The reason is that for a general orthonormal basis \( V \) of \( V \), the sparse vectors are not invariant under the action of \( G \).

3.2. Proof of Theorem 3.1. Let \( H \) be a group acting on a vector space \( V \) and \( f \in V \) any vector. We denote by \( \mathbb{L}_f \) the linear span of the \( H \)-orbit \( Hf \). By definition \( \mathbb{L}_f = \{ \sum \alpha_i (h_i \cdot f) | h_i \in H \} \) and it is the smallest linear subspace containing the orbit \( Hf \).

Let \( V = \bigoplus_{\ell=1}^{L} V^{R_{\ell}}_\ell \) be a unitary representation of a compact group \( G \) and let \( H = \prod_{\ell=1}^{L} U(N_{\ell}) \). Given a vector \( f \in V \), we can write \( f = \sum_{\ell=1}^{L} \sum_{r=1}^{R_{\ell}} f_{\ell}[r] \), where \( f_{\ell}[r] \) is in the \( r \)-th copy of the irreducible representation \( V_{\ell} \). As above, we can view our vector \( f \) as an \( L \)-tuple \( (A_1, \ldots, A_L) \) of \( N_{\ell} \times R_{\ell} \) matrices with \( A_{\ell} = (f_{\ell}[1]^T, \ldots, f_{\ell}[R_{\ell}]^T) \).

Viewing \( V^{R_{\ell}}_\ell \) as the vector space of \( N_{\ell} \times R_{\ell} \) matrices, the linear span \( \mathbb{L}_f \) of the orbit \( Hf \) is the product of the \( \ell \) linear spans of the \( U(N_{\ell}) \) orbits of the matrices \( A_{\ell} \), where elements of \( U(N_{\ell}) \) acts on \( A_{\ell} \) by left multiplication.

Proposition 3.5. Let \( V = \bigoplus_{\ell=1}^{L} V^{R_{\ell}}_\ell \) be a unitary representation of a compact group \( G \) and let \( H = \prod_{\ell=1}^{L} U(N_{\ell}) \). If \( f \in V \) is represented by an \( L \)-tuple \( (A_1, \ldots, A_L) \) of \( N_{\ell} \times R_{\ell} \) matrices, then

\[
\dim_{\mathbb{C}} \mathbb{L}_f = \sum_{\ell=1}^{L} \text{rank}(A_{\ell}) N_{\ell},
\]
where $\dim_{\mathbb{C}}$ denotes the dimension of $L_f$ as a complex vector space. In particular,

$$\dim_{\mathbb{C}} L_f \leq \sum_{\ell=1}^{L} M_{\ell},$$

where $M_{\ell} = \min(N_{r\ell}, N_{r\ell}^2)$.

Proof. Since the linear span of the $H$-orbit of $f = (A_1, \ldots, A_L)$ is the product of the linear spans of the $U(N_{\ell})$-orbits of the matrices $A_{\ell}$, it suffices to prove that the linear span of the $U(N_{\ell})$-orbit of the matrix $A_{\ell}$ in $V_{\ell}^{R_{\ell}}$ has dimension $(\text{rank } A_{\ell}) N_{\ell}$.

Let $r_{\ell} = \text{rank } A_{\ell}$ and to simplify notation assume that the first $r_{\ell}$ columns $f_{\ell}[1]^T, \ldots, f_{\ell}[r_{\ell}]^T$ of $A_{\ell}$ are linearly independent. Since $\text{rank } A_{\ell} = r_{\ell}$, for $r > r_{\ell}$ there are unique scalars $b_{r,r}, \ldots, b_{r_{\ell},r}$ such that $f_{\ell}[r] = \sum_{i=r_{\ell}+1}^{r} b_{i,r} f_{\ell}[i]$.

Let $L_{A_{\ell}}$ be the $r_{\ell} N_{\ell}$-dimensional linear subspace of $V_{\ell}^{R_{\ell}}$ consisting of $N_{\ell} \times R_{\ell}$ matrices $B$ such that for $r > r_{\ell}$, $B_r = \sum_{i=1}^{r_{\ell}} b_{i,r} B_i$, where $B_i$ denotes the $i$-th column of the matrix $B$. Since $U(N_{\ell})$ acts linearly, the linear relations on the columns of $A_{\ell}$ are preserved by the action of $U(N_{\ell})$, so the linear span of $U(N_{\ell}) A_{\ell}$ lies in the subspace $L_{A_{\ell}}$. Conversely, we note that the linear span of $U(N_{\ell}) A_{\ell}$ contains the open set $L_{A_{\ell}}^o$ of $L_{A_{\ell}}$, parameterizing matrices whose first $r_{\ell}$ columns are linearly independent. The reason this holds is because any invertible $N_{\ell} \times N_{\ell}$ matrix is a linear combination of unitary matrices and any element of $L_{A_{\ell}}^o$ can be obtained by applying some invertible matrix to $A_{\ell}$. 

Remark 3.6. Note that the real dimension of the $U(N_{\ell})$-orbit of the matrix $A_{\ell}$ considered in the proof of Proposition 3.5 has real dimension $r_{\ell} N_{\ell}$. It follows that for any vector $f \in V$, $\dim_{\mathbb{R}} L_f = \dim_{\mathbb{R}} H f$. In particular, the real dimension of $L_f$ is twice the real dimension of the orbit $H f$.

To prove the theorem, we need to show that the set $\mathcal{U}$ of orthonormal bases $\mathcal{V}$, such that for every subset $S \subset [1, N]$ with $|S| = K$ and with $K \leq M = \sum_{\ell=1}^{L} \min(N_{r\ell}, N_{r\ell}^2)$ the following statement hold.

1. For generic $f \in L_{S}(\mathcal{V})$, $L_f \cap L_{S}(\mathcal{V})$ is the line spanned by $f$.

2. For generic $f \in L_{S}(\mathcal{V})$, if $|S'| = K$ and $S' \neq S$ then $L_f \cap L_{S}(\mathcal{V}) = \{0\}$.

For a fixed subset $S$ with $|S| = K$, let $\mathcal{U}_{S}$ be the set of orthonormal bases such that (1) and (2) hold for $S$. Then, $\mathcal{U} = \cap S \mathcal{U}_{S}$. Since the intersection of a finite number of Zariski open sets is Zariski open, it suffices to prove that each $\mathcal{U}_{S}$ contains a Zariski open set. Moreover, the proof is identical up to indexing for each subset $S$ so we will assume, for simplicity of notation, that $S = \{1, \ldots, K\}$.

Given a vector $f \in V$, let $\mathcal{B}_{f}$ be the set of orthonormal bases such that $f \in L_{\{1, \ldots, K\}}$. Note that $\mathcal{B}_{f}$ is a Zariski closed subset of $O(N)$ (resp. $U(N)$) defined by the equation $f_1 \wedge \ldots \wedge f_K \wedge f = 0$, where $f_1, \ldots, f_K$ are the first $K$ vectors of an ordered basis.

Proposition 3.7. Let $f \in V$ be any non-zero vector and let $L_f$ be the linear span of its orbit under $H$. Let $M = \sum_{\ell=1}^{L} \min(N_{r\ell}, N_{r\ell}^2)$. Then, if $K \leq N - M$, for the generic orthonormal basis $\mathcal{V} \in \mathcal{B}_{f}$:

1. $L_f$ intersects $L_{\{1, \ldots, K\}}(\mathcal{V})$ in the line spanned by $f$;

2. $L_f \cap L_{S}(\mathcal{V}) = \{0\}$ if $S \neq \{1, \ldots, K\}$.

The set of orthonormal bases $\mathcal{V} \in \mathcal{B}_{f}$ for which conditions (1) and (2) of Proposition 3.7 are not satisfied is defined by polynomial equations. This means that the set of bases satisfying (1) and (2) is Zariski open, and to prove Proposition 3.7 we just
need to show that this set is non-empty; i.e., we just need to show that there exists a
basis \( V \in \mathcal{B}_f \) which satisfies conditions (1) and (2). To do this we need to introduce
some notation and prove a lemma.

Fix an orthonormal basis \( e_1, \ldots, e_N \) of a Hermitian vector space \( V \) of dimension
\( N \). For \( S \subset [1, N] \) with \( |S| = K \), let \( L_S = \text{span}\{e_i\}_{i \in S} \) and \( L_S^c \) be the open subset
of \( L_S \) of vectors whose expansion with respect to the basis \( \{e_i\}_{i \in S} \) have all non-zero
coordinates. In other words, \( L_S^c = L_S \setminus ( \bigcup_{S' \neq S} L_{S'} ) \).

For a given vector \( w \in V \), let \( \text{Gr}_w(M, V) \) be the subvariety of the Grassmannian
of \( M \)-dimensional linear subspaces of \( V \) that contain \( w \).

**Lemma 3.8.** If \( K \leq N - M \), then for any vector \( w \in \mathbb{L}_{\{1, \ldots, K\}} \) the generic \( M \)
dimensional linear subspace \( L \in \text{Gr}_w(M, V) \) satisfies the following conditions:
1. \( L \cap \mathbb{L}_{\{1, \ldots, K\}} \) is the line spanned by \( w \);
2. \( L \cap \mathbb{L}_S = \{0\} \) for \( S \neq \{1, \ldots, K\} \) and \( |S| = K \).

**Proof of Lemma 3.8.** The subset of \( \text{Gr}_w(M, V) \) parameterizing linear subspaces
intersecting \( \mathbb{L}_{\{1, \ldots, K\}} \) in dimension greater than one is locally defined by a polynomial
equation and therefore a proper algebraic subset. Likewise, for any \( S \neq \{1, \ldots, K\} \)
the subset of \( \text{Gr}_w(M, V) \) parameterizing linear subspace \( L \) such that \( L \cap \mathbb{L}_S = \{0\} \) is
also defined by a polynomial equation, and thus is again a proper algebraic subset.
In particular, the set of \( L \in \text{Gr}_w(M, V) \) which do not satisfy conditions (1) and
(2) lie in a proper algebraic subset of \( \text{Gr}_w(M, V) \). Therefore, the generic subspace
\( \mathbb{L} \in \text{Gr}_w(M, V) \) satisfies conditions (1) and (2).

**Proof of Proposition 3.7.** Choose a fixed orthonormal basis \( \{e_1, \ldots, e_N\} \) and let
\( (L, w) \) be an \( M \)-dimensional linear subspace and vector satisfying the conclusions (1)
and (2) of Lemma 3.8. If we choose \( w \) so that \( |w| = |f| \), then we can find a rotation
g \in U(N) such that \( g \cdot (L, w) = (L_f, f) \). The orthonormal basis \( \{v_i = g \cdot e_i\}_{i=1, \ldots, N} \)
satisfies conditions (1) and (2) of the proposition.

**Proposition 3.9.** Let \( V \) be an ordered orthonormal basis for \( V \) and assume that
there is a non-zero vector \( f_0 \in \mathbb{L}_{\{1, \ldots, K\}}(\mathbb{V}) \) such that \( \dim \mathbb{L}_{f_0} \cap \mathbb{L}_{\{1, \ldots, K\}}(\mathbb{V}) = 1 \) and
\( \mathbb{L}_{f_0} \cap \mathbb{L}_{S}(\mathbb{V}) = \{0\} \) for \( S \neq \{1, \ldots, K\} \). Then, for a generic \( f \in \mathbb{L}_{\{1, \ldots, K\}}(\mathbb{V}) \) the
same property holds.

**Proof.** Given an orthonormal basis \( \mathcal{V} \), the set \( D \) of \( f \in \mathbb{L}_{\{1, \ldots, K\}}(\mathbb{V}) \) which satisfy
the condition that \( \dim \mathbb{L}_f \cap \mathbb{L}_{\{1, \ldots, K\}}(\mathbb{V}) > 1 \) or \( \dim \mathbb{L}_f \cap \mathbb{L}_{S}(\mathbb{V}) > 0 \) for \( S \neq \{1, \ldots, K\} \)
is defined by polynomial equations. By hypothesis, we know that \( D \neq \mathbb{L}_{\{1, \ldots, K\}} \) since
\( f_0 \notin D \) so its complement is necessarily Zariski dense.

At this point we have proved the following. For a fixed vector non-zero \( f_0 \in V \),
there is a Zariski open set \( \mathcal{U}_{f_0} \subset \mathcal{B}_{f_0} \) such that for every \( \mathcal{V} \in \mathcal{U}_{f_0} \) the generic vector
\( f \in \mathbb{L}_{\{1, \ldots, K\}} \) satisfies conditions (1) and (2) of Proposition 3.7. To complete the
proof, we observe that the set of all bases is \( \bigcup_{f_0 \in \mathcal{P}(\mathcal{V})} \mathcal{B}_{f_0} \) and our desired set of bases
is \( \bigcup_{f_0 \in \mathcal{P}(\mathcal{V})} \mathcal{U}_{f_0} \), where \( \mathcal{P}(\mathcal{V}) \) is the projective space of lines in \( V \). This set is open in
\( O(N) \) (resp. \( U(N) \)) because it is the complement of the projection to the first of the
Zariski closed set \( Z = \{(\mathcal{V}, f) | \mathcal{V} \in \mathcal{B}_f \setminus \mathcal{U}_f \} \subset O(N) \times \mathcal{P}(\mathcal{V}) \) (resp. \( U(N) \times \mathcal{P}(\mathcal{V}) \))
and this projection is proper (meaning it takes Zariski closed sets to Zariski closed
sets) because the projective space \( \mathcal{P}(\mathcal{V}) \) is a proper variety.

### 3.3. Examples

3.3.1. **MRA with rotated images model.** Using Theorem 3.1 we can obtain
sparsity bounds for recovering a generic image from its second moment as in Section
2.4.3. Recall that in this model the Fourier transform of an image is represented as a radially discretized band-limited function on \( \mathbb{C}^2 \), and the function \( f \) is determined by an \( L \)-tuple \((A_{-L}, \ldots, A_L)\) vectors in \( \mathbb{C}^R \), where \( L' = (L-1)/2 \) is the bandlimit and \( R \) is the number of radial samples. The ambiguity group is \( H = \left(S^1 \right)^{2L+1} \). In the notation of Theorem 3.1, we have \( M_\ell = 1 \) for \( \ell = -L', \ldots, L' \). In particular, for any vector \( f \in V \), \( \dim f \leq L \). Hence, by Theorem 3.1 we can conclude that if \( K \leq \dim V - L \), then for a generic orthonormal basis, a generic \( K \)-sparse vector can be recovered from its second moment. Since \( \dim V = RL \), if the number of radial samples \( R \geq 2 \), then the sparsity level required for signal recovery is \( K \leq \frac{R-1}{R}N \), namely, linear in \( \dim V \). If only one radial sample is taken \( (R = 1) \), then this problem reduces to the MRA model on the circle, which is equivalent to the Fourier phase retrieval problem [14].

3.3.2. Sparsity bounds for two-dimensional tomography from unknown random projections. Following the model of Section 2.4.4, the unknown image \( f \) is viewed as a \( L \times R \) matrix \( A \) and the projected second moment determines the matrix \( A^*A \). Thus, the ambiguity group is \( U(L) \) (complex images) or \( O(L) \) (real images). The orbit of a generic signal \( f \) has dimension \( M \), where \( M = \min(\dim V, L^2) \). Since \( \dim V = LR \), we have \( M = \min(RL, L^2) \). In order to be able to recover sparse signals, we need to take \( R > L \); i.e., the number of radial samples must exceed the number of frequencies. Specifically, Theorem 3.1 implies that for a generic ordered orthonormal basis \( V \) we can recover \( K \)-sparse signals where \( K = \frac{(R-L)}{p}N \), with \( p > 1 \), then a generic \( K \)-sparse signal is uniquely determined by its second moment if \( K \leq \frac{p-1}{p}N \), where \( N = \dim V \).

4. Application to cryo-EM. This section is devoted to the application of the results of Section 2 and Section 3 to single-particle cryo-EM: the main motivation of this work.

Recent technological breakthroughs in cryo-EM have sparked a revolution in structure biology—the field that studies the structure and dynamics of biological molecules—by recovering an abundance of new molecular structures at near-atomic resolution. In particular, cryo-EM allows recovering molecules that were notoriously difficult to crystallize (e.g., different types of membrane proteins), the sample preparation procedure is significantly simpler (compared to alternative technologies) and preserves the molecules in a near-physiological state, and it allows reconstructing multiple functional states.

In this section, we describe the mathematical model of cryo-EM in detail, formulate the ambiguities of recovering the three-dimensional structure from the second moment, and then derive the sparsity level that allows resolving these ambiguities based on Theorem 3.1.

4.1. Mathematical model. Let \( L^2(\mathbb{R}^3) \) be Hilbert space of complex valued \( L^2 \) functions on \( \mathbb{R}^3 \). The action of \( SO(3) \) on \( \mathbb{R}^3 \) induces a corresponding action on \( L^2(\mathbb{R}^3) \), which we view as an infinite-dimensional representation of \( SO(3) \). 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 \((r, \theta, \phi)\) we consider a finite dimensional approximation of \( L^2(\mathbb{R}^3) \) by discretizing \( f(r, \theta, \phi) \) with \( R \) samples \( r_1, \ldots, r_R \), of the radial coordinates and bandlimiting the corresponding spherical functions \( f(r_i, \theta, \phi) \). This is
a standard assumption in the cryo-EM literature, see for example [9]. 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 bandlimit, and \( V_\ell \) is the \((2\ell + 1)\)-dimensional irreducible representation of \( SO(3) \), corresponding to harmonic polynomials of frequency \( \ell \). An orthonormal basis for \( V_\ell \) 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 \( r \)-th 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 \( L \)-bandlimited function. Each \( f[r] \) can be expanded in terms of the basis functions \( Y_\ell^m(\theta, \varphi) \) as follows

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

Therefore, the problem of determining a structure reduces to determining the unknown coefficients \( A_\ell^m[r] \) in (4.1).

Note that when \( f \) is the Fourier transform of a real valued function, the coefficients \( A_\ell^m[r] \) are real for even \( \ell \) and purely imaginary for odd \( \ell \) [25].

### 4.2. The second moment of the cryo-EM model.

In this section, we first formulate the second moment of the MRA model (1.1) for \( G = SO(3) \) and functions of the form (4.1). Then, we show that this is equivalent to the second moment of the cryo-EM model (Lemma 4.1) and derive the ambiguity group of this model (Corollary 4.2).

Consider the MRA model with \( G = SO(3) \) and functions of the form (4.1). Using the expansion from the previous section and the functional representation of the second moment (2.11), we can write

\[
 m^2_f = \sum_{r_1, r_2=1}^R \sum_{\ell=0}^L \left( \sum_{m=-\ell}^{\ell} A_\ell^m[r_1] \overline{A_\ell^m[r_2]} \right) \sum_{m'=-\ell}^{\ell} \overline{Y_\ell^{m'}[r_1]} Y_\ell^{m'}[r_2],
\]

where the notation \( Y_\ell^{m'}[r] \) denotes the corresponding spherical harmonic in the \( r \)-th copy of \( V_\ell \subset L^2(S^2) \). To simplify notation, set

\[
 B_\ell[r_1, r_2] = \sum_{m=-\ell}^{\ell} A_\ell^m[r_1] \overline{A_\ell^m[r_2]}.
\]

This can be viewed as an inner product of the coefficient vector \( (A_\ell^m[r_1], \ldots, A_\ell^m[r_1]) \) from the \( r_1 \)-shell and the coefficient vector \( (A_\ell^{-m}[r_2], \ldots, A_\ell^{-m}[r_2]) \) from the \( r_2 \) shell. Let \( A_\ell \in \mathbb{C}^{(2\ell+1) \times R} \) and \( B_\ell \in \mathbb{C}^{R \times R} \) be matrices consisting of the coefficients

\[
 A_\ell = (A_\ell^m[r_i])_{m=-\ell, \ldots, \ell, i=1, \ldots, R},
\]

and

\[
 B_\ell = (B_\ell[r_i, r_j])_{i, j=1, \ldots, R}.
\]
Then, the second moment determines the matrices
\[(4.4) \quad B_\ell = A_\ell^T A_\ell, \quad \ell = 0, \ldots, L.\]
Remarkably, unlike the tomographic projection $\mathbb{R}^2 \to \mathbb{R}^1$, the tomographic projection operator (1.4) does not affect the second moment for $SO(3)$. Therefore, in the context of the second moment, we can treat cryo-EM as a special case of the MRA model (1.1), where $G$ is the group of three-dimensional rotations $SO(3)$ and $V$ is a discretization of $L^2(\mathbb{R}^3)$ as in (4.1). This fact has been recognized (implicitly) already by Zvi Kam [56]. For completeness, we prove the following lemma.

**Lemma 4.1.** Assume a function of the form (4.1). Then, the second moment of the cryo-EM model (1.3) is the same as the second moment of the MRA model (1.1) with $G = SO(3)$. Namely, the tomographic projection operator in (1.3) does not affect the second moment.

**Proof.** Consider the projected second moment of a function $f \in V$ for fixed $(r_1, r_2)$:
\[(4.5) \quad \int_{SO(3)} T(g \cdot f[r_1](\theta_1, \phi_2))T(g \cdot f[r_2](\theta_2, \phi_2)) \, dg = (T \times T) \int_{SO(3)} (g \cdot f[r_1](\theta_1, \phi_1)(g \cdot f[r_2])(\theta_2, \phi_2)) \, dg = (T \times T)(m^2 r_1, r_2)(\theta_1, \phi_1, \theta_2, \phi_2)) = \sum_{\ell=0}^L B_\ell[r_1, r_2] \sum_{m=-\ell}^\ell Y_\ell^m(\pi/2, \varphi_1)Y_\ell^m(\pi/2, \varphi_2).\]
Here, $T \times T$ is the product of tomographic projections so $(T \times T)f(\theta_1, \phi_1, \theta_2, \phi_2) = f(\pi/2, \phi_1, \pi/2, \phi_2)$. Note that the first equality holds because the linear operator $T$ commutes with integration over the group $SO(3)$. Let $P_\ell$ be the Legendre polynomial of degree $\ell$. Since, up to constants [6, Section 2.2],
\[(4.6) \quad \sum_{m=-\ell}^\ell Y_\ell^m(\pi/2, \varphi_1)Y_\ell^m(\pi/2, \varphi_2) = P_\ell(\cos(\varphi_1 - \varphi_2)),\]
we have
\[(4.7) \quad \int_G T(g \cdot f[r_1])T(g \cdot f[r_2]) \, dg = \sum_{\ell=0}^L B_\ell[r_1, r_2] P_\ell(\cos(\varphi_1 - \varphi_2)).\]
Since the Legendre polynomials are orthonormal functions of $\varphi = \varphi_1 - \varphi_2$, we can determine the coefficients $B_\ell[r_1, r_2]$ from (4.7). Thus we can conclude that no information is lost from the taking the projected second moment. \[\square\]

**Corollary 4.2.** Assume a function of the form
\[f[r] = \sum_{\ell=0}^L \sum_{m=-\ell}^\ell A_\ell^m[r] Y_\ell^m.\]
Then, the second moment of the cryo-EM model (1.3) is given by (4.4). Therefore, the second moment determines the coefficient matrices $A_\ell$, $\ell = 0, \ldots, L$ up to the action of the ambiguity group $\prod_{\ell=0}^L U(2\ell + 1)$. Moreover, if we consider functions $f[r]$ which are the Fourier transforms of real-valued functions on $\mathbb{R}^3$ (which is the scenario in cryo-EM), then the coefficients $A_\ell^m[r]$ are real for even $\ell$ and purely imaginary for odd $\ell$ [25], and the ambiguity group is $\prod_{\ell=0}^L O(2\ell + 1)$. 

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4.3. Recovery of sparse structures from the second moment. Based on Theorem 3.1, we now prove that in cryo-EM a $K$-sparse signal can be recovered from the second moment when $K \lesssim N/3$.

**Theorem 4.3.** Assume a function of the form (4.1), where the number of shells satisfies $R \geq 2L + 1$. Let $V = \oplus_{\ell=0}^{L} V^{R}_{\ell}$ and let $N = \dim V$. Then, if

$$\frac{K}{N} \leq \frac{2/3L^{3} + L^{2} + L/3}{2L^{3} + 5L^{2} + 4L + 1} \approx \frac{1}{3},$$

then for a generic choice of orthonormal basis, a generic $K$-sparse function $f \in V$ is uniquely determined by its second moment, up to a global phase.

**Proof.** The dimension of the representation $V$ is $N = R(L + 1)^{2}$. Thus, if $R \geq 2L + 1$, then $N = \dim V \geq 2L^{3} + 5L^{2} + 4L + 1$. On the other hand, since $R \geq \dim \mathbb{V}_{\ell}$ for all $\ell$, we know by Proposition 3.5 that for $f \in V$ the linear span $\mathbb{L}_{f}$ of the orbit of $f$ under the ambiguity group $\oplus_{\ell=0}^{L} O(2\ell + 1)$ has dimension at most

$$\sum_{\ell=0}^{L}(2\ell + 1)^{2} = 4/3L^{3} + 4L^{2} + 11L/3 + 1.$$

Therefore, by Theorem 3.1, if $K \leq 2/3L^{3} + L^{2} + L/3$ then for a generic choice of orthonormal basis, a generic $K$-sparse vector $f \in V$ is uniquely determined by its second moment.

**Corollary 4.4.** Under the conditions of Theorem 4.3, a three-dimensional structure of the form (4.1) can be recovered from $n$ realization from the cryo-EM model when $n = \omega(\sigma^{4})$.

**Remark 4.5 (Near-optimality).** While the sparsity level of Theorem 4.3 is not necessarily optimal, it is optimal up to a constant. Thus, we say that our sparsity bound is near-optimal.

**Remark 4.6.** A recent paper [23] showed that a three-dimensional structure composed of a finite number of ideal point masses (or its convolution with a fixed kernel with a non-vanishing Fourier transform) can be recovered from the second moment. Theorem 4.3 is far more general as it includes sparse structures under almost any basis. Yet, [23] also suggests an algorithm which harnesses sparsity in the wavelet domain, for which our result does not necessarily hold (since Theorem 4.3 holds for generic bases and we cannot verify that any particular basis satisfies the generic condition).

**Remark 4.7 (Spherical-Bessel expansion).** Our analysis assumes a model of multiple shells as in (4.1). However, a similar analysis can be carried out to related models, such as spherical-Bessel expansion, where the coefficients $A_{\ell}^{m}[r]$ are expanded by

$$A_{\ell}^{m}[r] = \sum_{s=1}^{S_{\ell}} \tilde{A}_{\ell}^{m}[s] j_{\ell,s}[r],$$

where the $j_{\ell,s}[r]$ are the normalized spherical Bessel functions. The “bandlimit” $S_{\ell}$ is determined by a sampling criterion, akin to Nyquist sampling criterion [26]. This expansion has been useful in various cryo-EM tasks, see for example [62, 16, 24]. Our analysis can be applied to molecular structures represented using the spherical-Bessel expansion, where the only difference is the way we count the dimension of the representation.
5. Crystallographic phase retrieval. The crystallographic phase retrieval problem is the problem of recovering a signal in $\mathbb{R}^N$ or $\mathbb{C}^N$ from its power spectrum. As seen from Section 2.4.1, this is equivalent to recovering a signal from its second moment for the action of either the cyclic group $\mathbb{Z}_N$ or the dihedral group. However, because each irreducible representation appears exactly once, Theorem 3.1 provides an uninformative bound of $K \leq 0$.

In [18], the authors conjectured that when $\mathbb{R}^N$ is given by the standard basis, a generic $K$-sparse vector in $\mathbb{R}^N$ can be recovered, up to unavoidable ambiguities, from its power spectrum if $K \leq N/2$ if the support is not an arithmetic progression. This conjecture was proved for a few specific cases but a complete proof of this conjecture is beyond current techniques. In [46], it was shown that for large enough $N$, $K$-sparse, symmetric signals are determined uniquely from their power spectrum for $K = O(N/\log^5 N)$.

On the other hand, for generic bases, the following provable optimal bound for phase retrieval was recently obtained [39] using the techniques of this paper. Unlike the conjectures of [18], this result makes no assumption on the support of the signal with respect to the given basis.

**Theorem 5.1.** [39, Theorem 1.1] Let $V$ be a generic basis for $\mathbb{R}^N$. Then, if $K \leq N/2$, a generic $K$-sparse vector can be recovered from its power spectrum, up to a global phase.

6. Discussion and future work. In this paper, we have derived general sparsity conditions under which the sample complexity of the MRA model (1.1) is only $n = \omega(\sigma^4)$ rather than $n = \omega(\sigma^6)$ in the general case. We have further applied the result to cryo-EM, showing that if a molecular structure can be represented with $\sim N/3$ coefficients in a generic basis, then the sample complexity is quadratic in the variance of the noise. Next, we delineate a few possible extensions of these results.

*Linear transformations which are not compact groups.* Our MRA model (1.1) assumes a compact group. However, in some important situations, the group is non-compact, for instance, the group of rigid motions $\text{SE}(d)$ [21]. One challenge of working with non-compact groups is that their representations do not necessarily decompose into a sum of irreducibles which makes the representation-theoretic analysis of the second moment more difficult. The problem is even more challenging when considering a combination of a group action with a general linear operator; this is for example the situation when considering sub-pixel measurements [22].

*Sample complexity for specific bases.* Our main theoretical result, Theorem 3.1, holds for almost all bases but it is very difficult to say if they hold for a specific basis, such as wavelets, since the algebraic conditions on the bases are implicit. An important future work is to derive conditions for recovery from the second moment for specific bases, and ideally for all bases. (In [24], recovery from the second moment of structures composed of ideal point masses was proven.)

*Unified theoretical framework with phase retrieval.* In Section 5, Theorem 5.1, we discussed sparsity conditions for recovering a signal from its power spectrum, which is the second moment of the simplest MRA model, where a signal in $\mathbb{R}^N$ is acted upon by $\mathbb{Z}_N$. This problem is called the phase retrieval problem. We wish to consolidate the proof techniques of Theorem 3.1 and those used to prove Theorem 5.1 in one general theoretical framework, which should yield optimal dimension bounds for recovering a signal from its second moment.
Multi-target detection. The multi-target detection model was devised to design a new computational paradigm for recovering small molecular structure using cryo-EM [15]. Without delving into the technical details, the second moment of this model is provided by the diagonals of the matrices $B_\ell$, $\ell = 0, \ldots, L$, that describe the second moment of the cryo-EM model (4.4) [16]. Deriving the conditions for signal recovery from these diagonals will have important implications to the sample complexity of the multi-target detection model and to understanding the fundamental limitations of the cryo-EM technology.

Alternative priors. This work shows that the sample complexity of MRA and cryo-EM can be significantly improved if the signal can be sparsely represented. An interesting future research thread is studying alternative priors that can improve the sample complexity, such as statistical priors, data-driven priors (e.g., based on AlphaFold [55]), semi-algebraic priors [37], or priors based on the statistical properties of proteins [92, 85].

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Appendix A. Representation theory.

A.1. Terminology on representations. Let $G$ be a group. A (complex) representation of $G$ is a homomorphism, $G \rightarrow \text{GL}(V)$, where $V$ is a complex vector space and $\text{GL}(V)$ is the group of invertible linear transformations $V \rightarrow V$. 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 $\lambda, \mu \in \mathbb{C}$, $\lambda v_1 + \mu v_2 = \lambda (g \cdot v_1) + \mu (g \cdot v_2)$. Conversely, given a linear action of $G$ on a vector space $V$, we obtain a homomorphism $G \rightarrow \text{GL}(V)$, $g \rightarrow T_g$, where $T_g : V \rightarrow V$ 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 $\text{GL}(V) = \text{GL}(N)$, where $N = \dim V$. Given a Hermitian inner product $\langle \cdot, \cdot \rangle$ on $V$, we say that a representation is unitary if for any two vectors $v_1, v_2 \in V$, $\langle v_1, v_2 \rangle = (g \cdot v_1, g \cdot v_2)$. If we choose an orthonormal basis for $V$, then the representation of $G$ is unitary if and only if the image of $G$ under the homomorphism $G \rightarrow \text{GL}(N)$ lies in the subgroup $U(N)$ of unitary matrices.

A representation $V$ of a group $G$ is irreducible if $V$ contains no non-zero 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 $\langle \cdot, \cdot \rangle$ 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 compact group.

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

**Example A.3.** Most representations that naturally occur in imaging and signal processing are not irreducible. For example, consider the action of the cyclic group \( \mathbb{Z}_N \) on \( \mathbb{C}^N \) by cyclic shifts; i.e., if \( T \) is the generator of \( \mathbb{Z}_N \), then \( T \cdot (x_0, \ldots, x_{N-1}) = (x_1, x_2, \ldots, x_{N-1}, x_0) \). To see that this representation is reducible, let \( e_0, \ldots, e_{N-1} \) be the standard basis and take \( \omega = e^{2\pi i/N} \). With this notation, if \( 0 \leq n \leq N - 1 \), the one-dimensional subspace \( V_n \) spanned by the vector \( f_n = e_0 + \omega^n e_1 + \omega^{2n} e_2 + \cdots + \omega^{(n-1)n} e_{N-1} \) is invariant under \( T \) because \( T \cdot f_n = \omega^n f_n \). The vectors \( f_0, \ldots, f_{N-1} \) are the Fourier basis for \( \mathbb{C}^N \) and \( \mathbb{C}^N \) decomposes as the sum of one-dimensional representations \( V_0 \oplus \cdots \oplus V_{N-1} \). In general, if \( G \) is an abelian compact group then any complex representation of \( G \) will decompose into a sum of one-dimensional representations.

For non-abelian groups, or even real representations of abelian groups, this need not be the case. If we consider the action of \( \mathbb{Z}_N \) on \( \mathbb{R}^N \) by cyclic shifts, then \( \mathbb{R}^N \) decomposes into a sum of one and two-dimensional irreducible representations. For example if \( N = 4 \), then \( \mathbb{R}^4 \) decomposes as the sum \( V_0 \oplus V_1 \oplus V_2 \), where \( V_0 = \text{span}(e_0 + e_1 + e_2 + e_3) \), \( V_1 = \text{span}(e_0 - e_2, e_1 - e_3) \) and \( V_2 = \text{span}(e_0 - e_1 + e_2 - e_3) \).

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 \( \Phi \) is \( G \)-invariant if \( g \cdot \Phi v = \Phi g \cdot v \).

**Lemma A.4.** Let \( \Phi : V_1 \to V_2 \) be a \( G \)-invariant linear transformation of finite dimensional irreducible representations of a group \( G \) (not necessarily compact). Then, \( \Phi \) 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 \( \phi : V \to V \) 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 \( \text{Hom}(V_1, V_2) \) 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 \( V^* = \text{Hom}(V, \mathbb{C}) \) 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 \( g \cdot v = g^{-1} v \). Likewise, if \( V_1 \) and \( V_2 \) are 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 \( V_1, V_2 \) there is an isomorphism of representations \( V_1 \otimes V_2^* \to \text{Hom}(V_2, V_1) \) given by the formula \( v_1 \otimes f_2 \mapsto \phi \), where the linear transform \( \phi : V_2 \to V_1 \) is defined by the formula \( \phi(v_2) = f_2(v_2) v_1 \). In particular, we can identify \( V \otimes V^* \) with \( \text{Hom}(V, V) \).

**Appendix B. Grassmannians.** The set \( \text{Gr}(M, V) \) of \( M \)-dimensional linear subspaces of an \( N \)-dimensional vector space \( V \) has the natural structure as a projective manifold, called the Grassmannian of \( M \) planes in \( V \). The Grassmannian \( \text{Gr}(M, V) \) has dimension \( M(N - M) \) and there are a number of ways to see the manifold structure and compute the dimension.
Given an ordered basis \( v_1, \ldots, v_M \) for an \( M \)-dimensional linear subspace \( \Lambda \), we can associate a full rank \( M \times N \) matrix \( A_{\Lambda} = [v_1 \ldots v_M] \). Conversely, given a full rank \( M \times N \) matrix \( A \), the columns of \( A \) determine an ordered basis for an \( M \)-dimensional linear subspace of \( V \). Two matrices \( A, A' \) correspond to the same linear subspace if an only there is an invertible \( M \times M \) matrix \( P \) such that \( A = PA' \). Hence, the Grassmannian can be identified as the quotient \( F(M, N)/\text{GL}(M) \), where \( F(M, N) \) is the set of full rank \( M \times N \) matrices. Since \( F(M, N) \) has dimension \( MN \) and \( \text{GL}(M) \) has dimension \( M^2 \), the quotient has dimension \( MN - M^2 = (N - M)M \).

To see that \( \text{Gr}(M, V) \) is a projective variety, we note that if \( v_1, \ldots, v_M \) and \( v'_1, \ldots, v'_M \) are two bases for an \( M \)-dimensional linear subspace \( \Lambda \) then, \( v_1 \wedge \ldots \wedge v_M = \lambda(v'_1 \wedge \ldots \wedge v'_M) \) for some scalar \( \lambda \). Here \( \wedge \) denotes the exterior product. Thus there is a well-defined map \( \text{Gr}(M, V) \rightarrow \mathbb{P}(\Lambda^M V) \) which sends the point representing the linear subspace \( \Lambda \) to the exterior product \( v_1 \wedge \ldots \wedge v_M \) where \( v_1, \ldots, v_M \) is any basis for \( \Lambda \). Moreover, this map is an embedding because \( v_1 \wedge \ldots \wedge v_M = \lambda(v'_1 \wedge \ldots \wedge v'_M) \) for some scalar \( \lambda \) if and only if \( v_1, \ldots, v_M \) and \( v'_1, \ldots, v'_M \) span the same \( M \)-dimensional linear subspace. This is embedding is called the Plücker embedding.

For more on Grassmannians, see [48, Chapter 1, Section 5] or [50, Lecture 6].

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