

# Isometric Embeddings of Quotients of the Rotation Group Modulo Finite Symmetries

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## Abstract

The analysis of manifold valued data using embedding based methods is linked to the problem of finding suitable embeddings. In this paper we are interested in embeddings of quotient manifolds  $SO(3)/\mathcal{S}$  of the rotation group modulo finite symmetry groups. Data on such quotient manifolds naturally occur in crystallography, material science and biochemistry. We provide a generic framework for the construction of such embeddings which generalizes the embeddings constructed in [1]. The central advantage of our larger class of embeddings is that it comprises isometric embeddings for all crystallographic symmetry groups.

*Keywords:* Euclidean Embedding, Isometric Embedding, Rotation Group

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## 1. Introduction

In the analysis of manifold valued data there are two different approaches - intrinsic and extrinsic. Intrinsic methods solely rely on intrinsic properties of the manifold, e.g. the Riemannian curvature tensor, the exponential map or the Levi-Cevita connection. Those methods often work locally like moving least squares [2], multiscale methods [3] or subdivision schemes [4]. Other intrinsic approaches make use of function systems that are adapted to the geometry of the manifold, e.g. diffusion maps [5] or the eigenfunctions of the manifold Laplacian [6, 7, 8, 9, 10].

On the other hand, extrinsic methods rely on an embedding of the manifold into some higher dimensional vector space [1, 11, 12]. The advantage of embedding based methods is that they often are straight forward generalizations of the corresponding linear methods. The central challenges for applying an embedding based method to a specific manifold  $\mathcal{M}$  are

1. Find a suitable embedding  $\mathcal{E}: \mathcal{M} \rightarrow \mathbb{R}^d$  of the manifold  $\mathcal{M}$  that approximately preserves distances and has moderate dimension.
2. Find an efficient algorithm for the projection  $P_{\mathcal{M}}: U \rightarrow \mathcal{M}$  from some neighborhood  $U \supset \mathcal{E}(\mathcal{M})$  back to the manifold.

In our paper we are concerned with the specific case when the manifold  $\mathcal{M}$  is the quotient  $SO(3)/\mathcal{S} = \{[\mathbf{R}]_{\mathcal{S}}: \mathbf{R} \in SO(3)\}$  of the rotational group  $SO(3)$  with respect to some finite symmetry group  $\mathcal{S} \subset SO(3)$ . Data that

represents rotations modulo symmetries are of central importance in various scientific areas. For instance, they are used to describe the alignment of crystals in crystallography, material science and geology [13, 14, 15], the alignment of molecules and proteins in biochemistry [16] or movements in robotics [17] and motion tracking [18].

Since, locally, the quotient manifolds  $SO(3)/\mathcal{S}$  are isometric to the rotation group  $SO(3)$  itself all intrinsic methods for the rotation group can be easily adapted to work on the quotients as well. Unfortunately, this is not true for embedding based methods, e.g. for the interpolation methods described in [19]. Explicit embeddings for the quotient manifolds  $SO(3)/\mathcal{S}$  have been investigated first by R. Arnold, P. Jupp and H. Schaeben in [1]. Our paper aims to extend their results by developing a general framework for the construction of embeddings of the quotient manifolds  $SO(3)/\mathcal{S}$  that include the embeddings described in [1]. Our embeddings pose several nice properties, e.g. they are all  $SO(3)$  homomorphisms, their image is contained in a sphere and the pushforward of the Haar measure on  $SO(3)$  has zero mean in  $\mathbb{R}^d$ . Furthermore, we find within our framework isometric embeddings of  $SO(3)/\mathcal{S}$  for all crystallographically relevant symmetry groups  $\mathcal{S}$  and provide an efficient numerical method for the projection  $P_{\mathcal{M}}$ .

Our paper is organized as follows. In Section 2.1 we introduce the generic embeddings and prove in the Theorem 2.3 that they are  $SO(3)$  homomorphisms that map the quotient manifold into a subsphere of an Euclidean vector space. Furthermore, we provide in Table 1 the parameters such that our embeddings coincide with the embeddings found in [1]. In Section 2.2 we further investigate the submanifold and show in Theorem 2.9 that our embedding can be generalized such that the pushforward of the Haar measure on  $SO(3)$  has zero mean in the embedding. Eventually, we propose in Section 2.3 an iterative algorithm for the numerical computation of the projection  $P_{\mathcal{M}}$  of an arbitrary point in some neighborhood of the manifold back to the manifold. To this end, we derive in Theorem 2.11 the gradient of the distance functional.

In Section 3 we are interested in the discrepancy between the geodesic distance on the quotient manifold and the Euclidean distance in the embedding. A smooth embedding into  $\mathbb{R}^d$ , such that the pull back of the Euclidean metric tensor coincides with the metric tensor of the manifold, is called isometric. According to the Nash embedding Theorem there exists for every  $m$ -dimensional Riemannian manifold an isometric embedding into  $\mathbb{R}^{m(3m+1)/2}$ . As all our quotient manifolds are three dimensional the result guaranties the existence of an isometric embedding into the space  $\mathbb{R}^{30}$ . It turns out that our generic embeddings are sufficiently general to comprise isometric embeddings for the quotient manifolds  $SO(3)/\mathcal{S}$  modulo all crystallographic symmetry groups  $\mathcal{S}$ . This result is proven separately for the different types of symmetry groups in Theorems 3.6, 3.7, 3.8, 3.9, 3.10. The corresponding parameters as well as the dimension of the linear space are summarized in Table 2. The dimensions of the isometric embeddings vary from 8 to 32 depending on the symmetry group.

In the last Section 3.2 we investigate the global relationship between the geodesic distance on  $SO(3)/\mathcal{S}$  and the Euclidean distance in the embedding.

According to [20] it is possible to construct for each smooth and compact manifold  $\mathcal{M}$  an embedding  $\mathcal{E}: \mathcal{M} \rightarrow \mathbb{R}^d$  such that the geodesic distance on the manifold and the Euclidean distance in the embedding differ only by a given  $\varepsilon > 0$ , i.e.,

$$(1 - \varepsilon)d_{\mathcal{M}}(m_1, m_2) \leq d(\mathcal{E}(m_1), \mathcal{E}(m_2)) \leq (1 + \varepsilon)d_{\mathcal{M}}(m_1, m_2). \quad (1)$$

However, the dimension  $d$  of the vector space required for such an embedding is much too large for numerical applications. In Table 3 we provide similar bounds as in equation (1) for the isometric embeddings defined in this paper. It turns out that locally isometric embeddings do not necessarily lead to globally optimal bounds. Parameters for our embeddings optimized with respect to global preservation of distances are provided in Table 4.

## 2. Embeddings of the Rotation Group

### 2.1. General Framework

The group of rotations  $SO(3)$  interpreted as a matrix group has a canonical embedding  $\mathcal{E}: SO(3) \rightarrow \mathbb{R}^9$  given by

$$\mathcal{E}(\mathbf{R}) = (\mathbf{R}\mathbf{e}_1, \mathbf{R}\mathbf{e}_2, \mathbf{R}\mathbf{e}_3) \quad (2)$$

where  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$  is the standard basis in  $\mathbb{R}^3$ . Replacing the basis vectors  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$  by any other list of vectors  $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n$  will always result in an embedding as long as at least two of the vectors are linearly independent. Unfortunately, this approach is not applicable to quotients  $SO(3)/\mathcal{S}$  since this requires that  $\mathcal{E}(\mathbf{R}\mathbf{S}) = \mathcal{E}(\mathbf{R})$  for all symmetry operations  $\mathbf{S} \in \mathcal{S}$ . For that reason, we generalize the embedding (2) to tensor products of vectors  $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_n$ . In the next definition we will make use of the following notation. Let  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$  be a multiindex. Then  $\mathbb{R}^{3^\alpha}$  is defined as the linear space

$$\mathbb{R}^{3^\alpha} = \times_{i=1}^n (\otimes^{\alpha_i} \mathbb{R}^3) \cong \mathbb{R}^{(\sum_{i=1}^n 3^{\alpha_i})}.$$

**Definition 2.1.** Let  $n \in \mathbb{N}$ ,  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}^n$  a multiindex and  $\mathbf{u} = (\mathbf{u}_1, \dots, \mathbf{u}_n) \in \mathbb{R}^{3n}$  be a list of  $n$  directions  $\mathbf{u}_j \in \mathbb{R}^3$ . Then we define the mapping  $\mathcal{E}_{\mathbf{u}}^{\boldsymbol{\alpha}}: SO(3) \rightarrow \mathbb{R}^{3^\alpha}$  as

$$\mathcal{E}_{\mathbf{u}}^{\boldsymbol{\alpha}}(\mathbf{R}) = (\otimes^{\alpha_1} \mathbf{R}\mathbf{u}_1, \dots, \otimes^{\alpha_n} \mathbf{R}\mathbf{u}_n).$$

In order to define mappings that are invariant with respect to a finite subgroup  $\mathcal{S} \subset SO(3)$  we utilize the averaging idea.

**Definition 2.2.** Let  $\mathcal{S} \subset SO(3)$  be a finite subgroup and  $\mathcal{E}_{\mathbf{u}}^{\boldsymbol{\alpha}}: SO(3) \rightarrow \mathbb{R}^{3^\alpha}$  as defined in Definition 2.1. Then we denote by

$$\mathcal{E}_{\mathbf{u}, \mathcal{S}}^{\boldsymbol{\alpha}}: SO(3)/\mathcal{S} \rightarrow \mathbb{R}^{3^\alpha}, \quad \mathcal{E}_{\mathbf{u}, \mathcal{S}}^{\boldsymbol{\alpha}}([\mathbf{O}]_{\mathcal{S}}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{S} \in \mathcal{S}} \mathcal{E}_{\mathbf{u}}^{\boldsymbol{\alpha}}(\mathbf{O}\mathbf{S}), \quad [\mathbf{O}]_{\mathcal{S}} \in SO(3)/\mathcal{S}$$

its symmetrized version.

In order to examine the properties of  $\mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha$  it is useful to consider both, the quotient  $SO(3)/\mathcal{S}$  as well as the vector space  $\mathbb{R}^{3^\alpha}$  of dimension  $\sum_{i=1}^n 3^{\alpha_i}$  as  $SO(3)$  manifolds with respect to the group actions

$$\mathbf{R} \triangleright [\mathbf{O}]_{\mathcal{S}} = [\mathbf{R}\mathbf{O}]_{\mathcal{S}}, \quad \mathbf{R} \triangleright \mathbf{v} = (\otimes^\alpha \mathbf{R}) \mathbf{v},$$

where  $\mathbf{R} \in SO(3)$ ,  $[\mathbf{O}]_{\mathcal{S}} \in SO(3)/\mathcal{S}$  and  $\mathbf{v} \in \mathbb{R}^{3^\alpha}$ .

**Theorem 2.3.** *The mapping  $\mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha: SO(3)/\mathcal{S} \rightarrow \mathbb{R}^{3^\alpha}$  is an  $SO(3)$  homomorphism, i.e.,*

$$\mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha(\mathbf{R} \triangleright [\mathbf{O}]_{\mathcal{S}}) = \mathbf{R} \triangleright \mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}})$$

for all  $\mathbf{R} \in SO(3)$  and  $[\mathbf{O}]_{\mathcal{S}} \in SO(3)/\mathcal{S}$ .

*Proof.* Let  $\mathbf{R} \in SO(3)$  and  $[\mathbf{O}]_{\mathcal{S}} \in SO(3)/\mathcal{S}$ . Then straight forward computation reveals

$$\begin{aligned} \mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha(\mathbf{R} \triangleright [\mathbf{O}]_{\mathcal{S}}) &= \frac{1}{|\mathcal{S}|} \sum_{\mathbf{S} \in \mathcal{S}} \mathcal{E}_{\mathbf{u}}^\alpha(\mathbf{R}\mathbf{O}\mathbf{S}) \\ &= \frac{1}{|\mathcal{S}|} \sum_{\mathbf{S} \in \mathcal{S}} (\otimes^{\alpha_1} \mathbf{R}\mathbf{O}\mathbf{S}\mathbf{u}_1, \dots, \otimes^{\alpha_n} \mathbf{R}\mathbf{O}\mathbf{S}\mathbf{u}_n) = \mathbf{R} \triangleright \mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}}). \end{aligned}$$

□

**Corollary 2.4.** *The image  $\mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha(SO(3))$  is contained in a sphere, i.e.,*

$$\|\mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}})\| = \text{const.}$$

for all  $[\mathbf{O}]_{\mathcal{S}} \in SO(3)/\mathcal{S}$ .

*Proof.* The assertion is a direct consequence of Theorem 2.3 and the fact that the Kronecker product of orthogonal matrices is again an orthogonal matrix. □

## 2.2. Rotational Invariant Subspaces

In order to prove further properties of the embeddings  $\mathcal{E}_{\mathbf{u},\mathcal{S}}^\alpha$  we continue by investigating subspaces of  $\mathbb{R}^{3^\alpha}$  that are invariant with respect to the group action  $\triangleright$ .

**Lemma 2.5.** *Let  $\alpha = (\alpha_i)_{i=1}^n$  be a multiindex. Then the tensor  $\mathbf{M}_\alpha \in \mathbb{R}^{3^\alpha}$  defined by*

$$(\mathbf{M}_{\alpha_i})_{j_1, \dots, j_{\alpha_i}} = \text{symm}(\otimes^{\alpha_i/2} \mathbf{I}_3) = \frac{1}{\alpha_i!} \sum_{\sigma \in \Sigma_{\alpha_i}} \prod_{k=1}^{\alpha_i/2} \delta_{j_{\sigma(2k-1)}, j_{\sigma(2k)}},$$

if  $\alpha_i$  is even and  $\mathbf{M}_{\alpha_i} = \mathbf{0} \in \otimes^{\alpha_i} \mathbb{R}^3$  if  $\alpha_i$  is odd, is  $SO(3)$  invariant, i.e.,  $\mathbf{R} \triangleright \mathbf{M}_\alpha = \mathbf{M}_\alpha$ ,  $\mathbf{R} \in SO(3)$ .

*Proof.* For odd  $\alpha_i$  there is nothing to prove. For  $\mathbf{R} = (r_{ij})_{i,j=1}^3 \in SO(3)$  and even  $\alpha \in \mathbb{N}_0$  we have

$$\begin{aligned}
(\mathbf{R} \triangleright \mathbf{M}_\alpha)_{i_1, \dots, i_\alpha} &= ((\otimes^\alpha \mathbf{R}) \mathbf{M}_\alpha)_{i_1, \dots, i_\alpha} \\
&= \sum_{j_1, \dots, j_\alpha=1}^3 (\mathbf{M}_\alpha)_{j_1, \dots, j_\alpha} \cdot r_{i_1 j_1} r_{i_2 j_2} \cdots r_{i_\alpha j_\alpha} \\
&= \frac{1}{\alpha!} \sum_{j_1, \dots, j_\alpha=1}^3 \left( \left( \sum_{\sigma \in \Sigma_\alpha} \prod_{k=1}^{\frac{\alpha}{2}} \delta_{j_{\sigma(2k-1)}, j_{\sigma(2k)}} \right) r_{i_1 j_1} r_{i_2 j_2} \cdots r_{i_\alpha j_\alpha} \right) \\
&= \frac{1}{\alpha!} \sum_{j_1, \dots, j_\alpha=1}^3 \left( \sum_{\sigma \in \Sigma_\alpha} \prod_{k=1}^{\frac{\alpha}{2}} \delta_{j_{\sigma(2k-1)}, j_{\sigma(2k)}} \right) \prod_{l=1}^\alpha r_{i_l j_l} \\
&= \frac{1}{\alpha!} \sum_{\sigma \in \Sigma_\alpha} \prod_{k=1}^{\frac{\alpha}{2}} \sum_{j_1, \dots, j_\alpha=1}^3 \delta_{j_{\sigma(2k-1)}, j_{\sigma(2k)}} r_{i_{\sigma(2k-1)} j_{\sigma(2k-1)}} r_{i_{\sigma(2k)} j_{\sigma(2k)}} \\
&= \frac{1}{\alpha!} \sum_{\sigma \in \Sigma_\alpha} \prod_{k=1}^{\frac{\alpha}{2}} \sum_{j_1, \dots, j_\alpha=1}^3 r_{i_{\sigma(2k-1)} j_{\sigma(2k-1)}} r_{i_{\sigma(2k)} j_{\sigma(2k)}}.
\end{aligned}$$

All the sums and products are finite, so we can interchange them. Using the orthogonality of  $\mathbf{R}$  we obtain

$$\begin{aligned}
\sum_{j_{\sigma(2k-1)}=1}^3 \prod_{k=1}^{\frac{\alpha}{2}} r_{i_{\sigma(2k-1)} j_{\sigma(2k-1)}} r_{i_{\sigma(2k)} j_{\sigma(2k)}} &= \langle r_{i_{\sigma(2k-1)}}, r_{i_{\sigma(2k)}} \rangle \\
&= \begin{cases} 0 & \text{if } i_{\sigma(2k-1)} \neq i_{\sigma(2k)} \\ 1 & \text{if } i_{\sigma(2k-1)} = i_{\sigma(2k)} \end{cases}
\end{aligned}$$

and eventually,

$$(\mathbf{R} \triangleright \mathbf{M}_\alpha)_{i_1, \dots, i_\alpha} = \frac{1}{\alpha!} \sum_{\sigma \in \Sigma_\alpha} \prod_{k=1}^{\frac{\alpha}{2}} \delta_{i_{\sigma(2k-1)}, i_{\sigma(2k)}} = (\mathbf{M}_\alpha)_{i_1, \dots, i_\alpha}.$$

Applying this argument element-wise for all  $\alpha \in \{\alpha_i\}_{i=1}^n$ , yields the assertion.  $\square$

Since,  $\mathcal{E}_{\mathbf{u}, \mathcal{S}}^\alpha$  is an  $SO(3)$  homomorphism, any rotational invariant subspace is orthogonal to the embedding  $\mathcal{E}_{\mathbf{u}, \mathcal{S}}^\alpha(SO(3))$ . More precisely, we have the following result:

**Lemma 2.6.** *For even  $\alpha \in \mathbb{N}$  and  $\mathbf{R} \in SO(3)$  it holds*

$$\langle \mathcal{E}_{\mathbf{u}}^\alpha(\mathbf{R}), \mathbf{M}_\alpha \rangle = 1.$$

*Proof.* We can rewrite the definition of  $\mathbf{M}_\alpha$  for even  $\alpha$  to

$$\begin{aligned}\mathbf{M}_\alpha &= \frac{1}{\alpha!} \sum_{\sigma \in \Sigma_\alpha} \delta_{j_{\sigma(1)}, j_{\sigma(2)}} \cdot \delta_{j_{\sigma(3)}, j_{\sigma(4)}} \cdots \delta_{j_{\sigma(\alpha-1)}, j_{\sigma(\alpha)}} \\ &= \frac{1}{\alpha!} 2^{\frac{\alpha}{2}} \left(\frac{\alpha}{2}\right)! \underbrace{(\delta_{j_1, j_2} \cdot \delta_{j_3, j_4} \cdots \delta_{j_{\alpha-1}, j_\alpha} + \cdots)}_{(\alpha-1)(\alpha-3)\cdots 1 \text{ summands}}.\end{aligned}\quad (3)$$

The product of the  $\delta$  is only 1, if pairwise two  $j_i$  are equal. Hence, we obtain the following for the scalar product if  $\mathbf{v} = (v_1, v_2, v_3)^\top = \mathbf{R}\mathbf{u}$

$$\langle \mathcal{E}_\mathbf{u}^\alpha(\mathbf{R}), \mathbf{M}_\alpha \rangle = \langle \otimes^\alpha(\mathbf{R}\mathbf{u}), \mathbf{M}_\alpha \rangle = \sum_{\substack{i, j, k \\ 2i+2j+2k=\alpha}} a(i, j, k) v_1^{2i} v_2^{2j} v_3^{2k}$$

with coefficients  $a(i, j, k)$ . These coefficients have to be determined:

$$\begin{aligned}a(i, j, k) &= \underbrace{\frac{1}{\alpha!} 2^{\frac{\alpha}{2}} \left(\frac{\alpha}{2}\right)!}_{\text{factor in (3)}} \cdot \underbrace{\binom{\alpha}{2i} \binom{\alpha-2i}{2j} \binom{\alpha-2i-2j}{2k}}_{\text{number of entries}} \\ &\quad \cdot \underbrace{(2i-1)(2i-3)\cdots 1 \cdot (2j-1)(2j-3)\cdots 1 \cdot (2k-1)(2k-3)\cdots 1}_{\text{number of summands unequal to 0 in (3)}} \\ &= \left(\frac{\alpha}{2}\right)! \cdot \frac{2^i (2i-1)(2i-3)\cdots 1}{(2i)!} \cdot \frac{2^j (2j-1)(2j-3)\cdots 1}{(2j)!} \cdot \frac{2^k (2k-1)(2k-3)\cdots 1}{(2k)!} \\ &= \left(\frac{\alpha}{2}\right)! \cdot \frac{1}{i!j!k!} = \binom{\frac{\alpha}{2}}{i, j, k}.\end{aligned}$$

With the multinomial theorem it follows that

$$\langle \otimes^\alpha \mathbf{v}, \mathbf{M}_\alpha \rangle = (v_1^2 + v_2^2 + v_3^2)^\alpha = 1.$$

□

The previous lemma states that the embedded manifold is contained in an affine subspace of  $\mathbb{R}^{3^\alpha}$ . Next we want to shift the embedding into the corresponding linear subspace. To this end we need to compute the Frobenius norms  $\|\mathbf{M}_\alpha\|_F$  of the invariant tensors  $\mathbf{M}_\alpha$ . This requires the following two technical lemmas.

**Lemma 2.7.** *It holds for  $\alpha \in 2\mathbb{N}$*

$$(\alpha+1) \binom{\alpha}{\frac{\alpha}{2}} = \sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{2i_1}{i_1} \binom{2i_2}{i_2} \binom{2i_3}{i_3}.\quad (4)$$

*Proof.* With the general definition of the binomial coefficient  $\binom{n}{k} = \frac{n(n-1)\cdots(n-(k-1))}{k!}$  for  $k > 0$  we obtain

$$\binom{2n}{n} = (-1)^n \cdot 4^n \cdot \binom{-\frac{1}{2}}{n}.\quad (5)$$

With this equation and the Chu-Vandermonde-identity it follows that

$$\begin{aligned}
\sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{2i_1}{i_1} \binom{2i_2}{i_2} \binom{2i_3}{i_3} &= \sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} (-1)^{i_1+i_2+i_3} \cdot 4^{i_1+i_2+i_3} \binom{-\frac{1}{2}}{i_1} \binom{-\frac{1}{2}}{i_2} \binom{-\frac{1}{2}}{i_3} \\
&= (-1)^{\frac{\alpha}{2}} \cdot 4^{\frac{\alpha}{2}} \sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{-\frac{1}{2}}{i_1} \binom{-\frac{1}{2}}{i_2} \binom{-\frac{1}{2}}{i_3} \\
&= (-1)^{\frac{\alpha}{2}} \cdot 4^{\frac{\alpha}{2}} \binom{-\frac{3}{2}}{\frac{\alpha}{2}} \\
&= (-1)^{\frac{\alpha}{2}} \cdot 4^{\frac{\alpha}{2}} \left( \frac{-\frac{3}{2}(-\frac{3}{2}-1) \cdots (-\frac{3}{2}-(\frac{\alpha}{2}-1))}{(\frac{\alpha}{2})!} \right) \\
&= 4^{\frac{\alpha}{2}} \left( \frac{\frac{3}{2}(\frac{3}{2}+1) \cdots (\frac{3}{2}+(\frac{\alpha}{2}-1))}{(\frac{\alpha}{2})!} \right) \\
&= 2^{\frac{\alpha}{2}} \left( \frac{3 \cdot 5 \cdot 7 \cdots (\alpha+1)}{(\frac{\alpha}{2})!} \right) \\
&= (\alpha+1) \frac{2^{\frac{\alpha}{2}} (\frac{\alpha}{2})! \cdot 3 \cdot 5 \cdot 7 \cdots (\alpha+1)}{(\frac{\alpha}{2})!^2} \\
&= (\alpha+1) \binom{\alpha}{\frac{\alpha}{2}}.
\end{aligned}$$

□

**Lemma 2.8.** *Let  $\alpha \in 2\mathbb{N}$ . Then the Frobenius norm of the tensor  $\mathbf{M}_\alpha$  satisfies*

$$\|\mathbf{M}_\alpha\|_F^2 = \langle \mathbf{M}_\alpha, \mathbf{M}_\alpha \rangle = \alpha + 1.$$

*Proof.* Let  $\alpha \in 2\mathbb{N}$ . We use the formulation for the tensor  $\mathbf{M}_\alpha$  from equation (3). Let  $i_1, i_2, i_3 \in \{0, 1, 2, \dots, \frac{\alpha}{2}\}$  with  $i_1 + i_2 + i_3 = \frac{\alpha}{2}$  such that

$$\begin{aligned}
j_1, \dots, j_{2i_1} &= 1, \\
j_{2i_1+1}, \dots, j_{2i_1+2i_2} &= 2, \\
j_{2i_1+2i_2+1}, \dots, j_{2i_1+2i_2+2i_3} &= 3.
\end{aligned}$$

The respective entry in  $\mathbf{M}_\alpha$  is

$$\begin{aligned}
&\frac{1}{\alpha!} 2^{\frac{\alpha}{2}} \binom{\alpha}{2}! \cdot (2i_1-1)(2i_1-3) \cdots 1 \cdot (2i_2-1)(2i_2-3) \cdots 1 (2i_3-1)(2i_3-3) \cdots 1 \\
&= \frac{1}{\alpha!} \binom{\frac{\alpha}{2}}{i_1, i_2, i_3} (2i_1)! (2i_2)! (2i_3)! = \frac{(\frac{\alpha}{2})! (2i_1)! (2i_2)! (2i_3)!}{\alpha! i_1! i_2! i_3!}.
\end{aligned}$$

The values in  $\mathbf{M}_\alpha$  are equal, no matter which  $j_i$  are 1 and similarly for  $i_2$  and  $i_3$ . Hence, there are  $\binom{\alpha}{2i_1, 2i_2, 2i_3}$  such entries in  $\mathbf{M}_\alpha$ . Overall we obtain

$$\begin{aligned}
\|\mathbf{M}_\alpha\|_F^2 &= \sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{\alpha}{2i_1, 2i_2, 2i_3} \left( \frac{(\frac{\alpha}{2})! (2i_1)! (2i_2)! (2i_3)!}{r! i_1! i_2! i_3!} \right)^2 \\
&= \sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \frac{\alpha!}{(2i_1)! (2i_2)! (2i_3)!} \left( \frac{(\frac{\alpha}{2})!^2 (2i_1)!^2 (2i_2)!^2 (2i_3)!^2}{\alpha!^2 i_1!^2 i_2!^2 i_3!^2} \right) \\
&= \sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \left( \frac{(\frac{\alpha}{2})!^2 (2i_1)! (2i_2)! (2i_3)!}{\alpha! i_1!^2 i_2!^2 i_3!^2} \right) \\
&= \frac{1}{\binom{\alpha}{\frac{\alpha}{2}}} \sum_{\substack{i_1, i_2, i_3=0 \\ i_1+i_2+i_3=\frac{\alpha}{2}}}^{\frac{\alpha}{2}} \binom{2i_1}{i_1} \binom{2i_2}{i_2} \binom{2i_3}{i_3}.
\end{aligned}$$

With Lemma 2.7 follows the assertion.  $\square$

Shifting the embedding into the affine subspace found in Lemma 2.8 results in an embedding that maps the uniform distribution into a distribution with zero mean.

**Theorem 2.9.** *Let  $\mathcal{E}_{\mathbf{u}, \mathcal{S}}^\alpha: SO(3)/\mathcal{S} \rightarrow \mathbb{R}^{3^\alpha}$  be the embedding defined in Definition 2.2 and let  $\mu$  be the Haar measure on  $SO(3)/\mathcal{S}$ . Then the centered embedding*

$$\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}}) = \mathcal{E}_{\mathbf{u}, \mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}}) - \left( \frac{1}{\alpha_1 + 1} \mathbf{M}_{\alpha_1}, \dots, \frac{1}{\alpha_n + 1} \mathbf{M}_{\alpha_n} \right)$$

is an  $SO(3)$  homomorphism with

$$\|\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}})\| = \text{const}, \quad [\mathbf{O}]_{\mathcal{S}} \in SO(3)/\mathcal{S}$$

and satisfies that the push forward measure  $\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha \mu$  is centered as well, i.e., its first moment satisfies

$$\mathbb{E} \tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha \mu = 0.$$

*Proof.* The homomorphism property follows from Theorem 2.3 together with Lemma 2.5. For  $\mathbf{R} \in SO(3)$  and  $\mathbf{O} \in SO(3)/\mathcal{S}$  there holds

$$\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha(\mathbf{R} \triangleright [\mathbf{O}]_{\mathcal{S}}) = \mathcal{E}_{\mathbf{u}, \mathcal{S}}^\alpha(\mathbf{R} \triangleright [\mathbf{O}]_{\mathcal{S}}) - \mathbf{M}_\alpha = \mathbf{R} \triangleright \mathcal{E}_{\mathbf{u}, \mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}}) - \mathbf{R} \triangleright \mathbf{M}_\alpha = \mathbf{R} \triangleright \tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha([\mathbf{O}]_{\mathcal{S}}).$$

Assume  $\mathbf{R}$  to be distributed according to the Haar measure on  $SO(3)$ . Then  $\mathbf{R}\mathbf{u}$  is distributed according to the spherical Borel measure  $\sigma$  normalized to



$\sigma(\mathbb{S}^2) = 1$  for any  $\mathbf{u} \in \mathbb{S}^2$ . For the inner products with any vector  $\mathbf{v} \in \mathbb{S}^2$  we calculate

$$\begin{aligned} \langle \mathbb{E}(\otimes^\alpha \mathbf{R}\mathbf{u}), \otimes^\alpha \mathbf{v} \rangle &= \mathbb{E} \langle \otimes^\alpha \mathbf{R}\mathbf{u}, \otimes^\alpha \mathbf{v} \rangle = \mathbb{E}((\mathbf{R}\mathbf{u})^\top \mathbf{v})^\alpha \\ &= \int_{\mathbb{S}^2} (\boldsymbol{\xi}^\top \mathbf{v})^\alpha d\sigma(\boldsymbol{\xi}) = \begin{cases} \frac{1}{\alpha+1} & \text{if } \alpha \text{ odd} \\ 0 & \text{if } \alpha \text{ even} \end{cases}. \end{aligned}$$

If  $\alpha$  is odd, the assertion follows directly, because  $\mathbf{M}_\alpha = \mathbf{0}$  in this case. By Lemma 2.6 we have for even  $\alpha$

$$\begin{aligned} \langle \mathbb{E}\tilde{\mathcal{E}}_\mathbf{u}^\alpha(\mathbf{R}), \otimes^\alpha \mathbf{v} \rangle &= \langle \mathbb{E}(\otimes^\alpha(\mathbf{R}\mathbf{u}) - \frac{1}{\alpha+1}\mathbf{M}_\alpha), \otimes^\alpha \mathbf{v} \rangle = \mathbb{E} \langle \otimes^\alpha(\mathbf{R}\mathbf{u}) - \frac{1}{\alpha+1}\mathbf{M}_\alpha, \otimes^\alpha \mathbf{v} \rangle \\ &= \mathbb{E}(((\mathbf{R}\mathbf{u})^\top \mathbf{v})^\alpha) - \frac{1}{\alpha+1} = 0. \end{aligned}$$

Thanks to the rotational invariance of the tensors  $\mathbf{M}_\alpha$  the image of centered embedding is also contained in a sphere.  $\square$

In [1] the authors where especially interested in embeddings of the rotation group modulo crystallographic point groups. These consist of the cyclic groups  $C_k$ , and the dihedral groups  $D_k$  with  $k \in \{1, 2, 3, 4, 6\}$ , the tetrahedral group  $T$  and the octahedral group  $O$ . For all the corresponding quotients Table 1 lists specific choices of the parameters  $\boldsymbol{\alpha} \in \mathbb{R}^n$  and  $\mathbf{u}_1, \dots, \mathbf{u}_n \in \mathbb{R}^3$  such that the generic embeddings  $\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha$  coincide with the embeddings reported in Table 2 of [1].

$\mathcal{S}$	$\mathbf{u}$	$\boldsymbol{\alpha}$	Dimension
$C_1$	$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$	$(1, 1, 1)$	9
$C_2$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(1, 2)$	8
$C_\alpha$ ( $\alpha$ even, $\alpha \geq 4$ )	$(\mathbf{e}_1, \mathbf{e}_2)$	$(1, \alpha)$	$\frac{(\alpha+2)(\alpha+1)}{2} + 2$
$C_\alpha$ ( $\alpha$ odd, $\alpha \geq 3$ )	$(\mathbf{e}_1, \mathbf{e}_2)$	$(1, \alpha)$	$\frac{(\alpha+2)(\alpha+1)}{2} + 3$
$D_2$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(2, 2)$	10
$D_\alpha$ ( $\alpha$ even, $\alpha \geq 4$ )	$\mathbf{e}_1$	$\alpha$	$\frac{(\alpha+2)(\alpha+1)}{2} - 1$
$D_\alpha$ ( $\alpha$ odd, $\alpha \geq 3$ )	$\mathbf{e}_1$	$\alpha$	$\frac{(\alpha+2)(\alpha+1)}{2}$
$O$	$\mathbf{e}_1$	4	14
$T$	$\mathbf{e}_1$	3	10

Table 1: Choices of the vectors  $\mathbf{u}$  and the parameter  $\boldsymbol{\alpha}$  such that  $\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha$  coincides with the embeddings reported in Table 2 of [1].

It is important to note that at this point we have not yet proven that the mappings  $\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^\alpha$  are indeed embeddings, i.e., that they are injective. This will be done in the next chapter, where we shall prove that with some modifications they are even isometries.

The images of the embeddings  $\mathcal{E}_{\mathbf{u}, \mathcal{S}}^\alpha$  lie in the linear space  $\mathbb{R}^{3^\alpha}$ , but these tensors are additionally symmetric. That means, for  $\mathbf{T} = \otimes^\alpha \mathbf{v}$  we have  $\mathbf{T}_{i_1, \dots, i_\alpha} =$

$\mathbf{T}_{\sigma(i_1), \dots, \sigma(i_\alpha)}$  for any permutation  $\sigma$  of  $\{1, \dots, \alpha\}$ . In [21, 3.4] it is shown that the linear space of the symmetric  $\alpha$ -tensors  $S^\alpha(\mathbb{R}^3)$  has the dimension  $\binom{\alpha+2}{\alpha}$ . That means the images  $\mathcal{E}_{\mathbf{u}}^\alpha(SO(3))$  are contained in a subspace of  $\mathbb{R}^{3^\alpha}$  with dimension  $\sum_{i=1}^n \binom{\alpha_i+2}{\alpha_i}$ . Since the embeddings  $\tilde{\mathcal{E}}_{\mathbf{u}}^\alpha$  are centered, the images  $\tilde{\mathcal{E}}_{\mathbf{u}}^\alpha(SO(3))$  lie in a hyperplane, so we reduce the dimension of every component with even  $\alpha$  by 1. Hence, the images  $\tilde{\mathcal{E}}_{\mathbf{u}}^\alpha(SO(3))$  have dimension

$$\sum_{i=1}^n \binom{\alpha_i + 2}{\alpha_i} - \sum_{i=1}^n (\alpha_i + 1 \bmod 2).$$

### 2.3. Projection onto the Embedding

A central operation of embedding based methods is projecting a point of the vector space back onto the manifold. For our embeddings  $\mathcal{E}: SO(3)/S \rightarrow \mathbb{R}^{3^\alpha}$  this means that for an arbitrary tensor  $\mathbf{T} \in \mathbb{R}^{3^\alpha}$  we ask for the rotation  $\mathbf{R}^* \in SO(3)/S$  with minimum distance  $\|\mathcal{E}(\mathbf{R}^*) - \mathbf{T}\|$  in the embedding. This problem has a unique solution whenever  $\mathbf{T}$  is sufficiently close to the submanifold, cf. [22].

Since, by Corollary 2.4, the submanifold  $\mathcal{E}_{\mathbf{u}, S}^\alpha(SO(3)/S) \subset \mathbb{R}^{3^\alpha}$  is contained in a sphere, i.e., has constant norm, the above minimization problem is equivalent to the maximization problem

$$\mathbf{R}^* = \operatorname{argmax}_{\mathbf{R} \in SO(3)/S} J(\mathbf{R}), \quad J(\mathbf{R}) = \langle \mathcal{E}_{\mathbf{u}, S}^\alpha(\mathbf{R}), \mathbf{T} \rangle. \quad (6)$$

For the symmetry group  $C_1$ , i.e. no symmetry,  $\mathbf{u} = (\mathbf{u}_1, \dots, \mathbf{u}_n)$ ,  $\boldsymbol{\alpha} = (1, \dots, 1) \in \mathbb{R}^n$  and  $\mathbf{T} = (\mathbf{T}_1, \dots, \mathbf{T}_n) \in \mathbb{R}^{3n}$  the functional  $J: SO(3) \rightarrow \mathbb{R}$  simplifies to

$$J(\mathbf{R}) = \sum_{i=1}^n \langle \mathbf{R}\mathbf{u}_i, \mathbf{T}_i \rangle. \quad (7)$$

An explicit formula for its maximum is known as the Kabsch Algorithm [23].

**Lemma 2.10.** *Let  $\mathbf{u}_1, \dots, \mathbf{u}_n, \mathbf{v}_1, \dots, \mathbf{v}_n \in \mathbb{R}^3$  be two lists of vectors. Then the solution of the maximization problem*

$$\sum_{i=1}^n \langle \mathbf{R}\mathbf{u}_i, \mathbf{v}_i \rangle \rightarrow \max, \quad \mathbf{R} \in SO(3)$$

is given by

$$\mathbf{R} = \mathbf{V} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \det \mathbf{V}\mathbf{U}^T \end{pmatrix} \mathbf{U}^T,$$

where  $\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{H}$  is the singular value decomposition of the matrix

$$\mathbf{H} = \sum_{i=1}^n \mathbf{u}_i \otimes \mathbf{v}_i.$$

In the case of arbitrary symmetry groups and a general embedding  $\mathcal{E}_{\mathbf{u},S}^\alpha$  we are not able to give such a closed form solution. For this reason, we propose to solve the maximization problem in equation (6) numerically using a manifold gradient method [24]. The next theorem provides an explicit formula for the required gradient of  $J$ .

**Theorem 2.11.** *Let  $\mathbf{T} \in \mathbb{R}^{3^\alpha}$ ,  $\mathbf{R} \in SO(3)$ ,  $\mathbf{s}$  an arbitrary skew symmetric matrix and hence,  $\mathbf{sR} \in T_{\mathbf{R}}SO(3)$  a tangential vector at  $\mathbf{R}$ . Then the gradient of  $J$  in direction  $\mathbf{sR}$  is given by the inner product*

$$\nabla_{\mathbf{sR}}J(\mathbf{R}) = \alpha \langle \mathbf{s} \triangleright_1 (\mathbf{R} \triangleright \mathbf{E}), \mathbf{T} \rangle$$

where  $\mathbf{E} = \mathcal{E}_{\mathbf{u}}^\alpha(\mathbf{I}) \in \mathbb{R}^{3^\alpha}$  denotes the embedding of the identity matrix and  $\triangleright_1$  denotes the multiplication of the matrix  $\mathbf{s}$  with a tensor  $\mathbf{T} \in \mathbb{R}^{3^\alpha}$  with respect to the first dimension of  $\mathbf{T}$ , i.e.,

$$[\mathbf{s} \triangleright_1 \mathbf{T}]_{k_1, \dots, k_\alpha} = \sum_{\ell_1=1}^3 \mathbf{s}_{k_1 \ell_1} \mathbf{T}_{\ell_1, k_2, \dots, k_\alpha}.$$

*Proof.* First of all we note that by Theorem 2.3 the functional  $J$  can be written as

$$J(\mathbf{R}) = \langle \mathbf{R} \triangleright \mathbf{E}, \mathbf{T} \rangle, \quad \mathbf{R} \in SO(3).$$

Considering now a tangential vector  $\mathbf{sR} \in T_{\mathbf{R}}SO(3)$  the corresponding directional derivative evaluates to

$$\begin{aligned} \nabla_{\mathbf{sR}}J(\mathbf{R}) &= \lim_{h \rightarrow 0} \frac{1}{h} \left( \langle (\mathbf{R} + h\mathbf{sR}) \triangleright \mathbf{E}, \mathbf{T} \rangle - \langle \mathbf{R} \triangleright \mathbf{E}, \mathbf{T} \rangle \right) \\ &= \lim_{h \rightarrow 0} \frac{1}{h} \left\langle \left( \otimes^\alpha (\mathbf{R} + h\mathbf{sR}) - \otimes^\alpha \mathbf{R} \right) \mathbf{E}, \mathbf{T} \right\rangle. \end{aligned}$$

In the difference of the tensor products only the terms with  $h^1$  remain as all terms with higher power of  $h$  converge to zero. Since the tensor  $\mathbf{E}$  is symmetric the derivative simplifies further to

$$\nabla_{\mathbf{sR}}J(\mathbf{R}) = \sum_{i=0}^{\alpha-1} \left\langle \left( \otimes^i \mathbf{R} \otimes \mathbf{sR} \otimes^{\alpha-1-i} \mathbf{R} \right) \mathbf{E}, \mathbf{T} \right\rangle = \alpha \langle \mathbf{s} \triangleright_1 (\mathbf{R} \triangleright \mathbf{E}), \mathbf{T} \rangle.$$

□

**Remark 2.12.** *In the theorem above, we just considered the case  $\alpha \in \mathbb{R}$ , i.e.  $n = 1$ . For the case with multiple components, we have to sum over all components in the function*

$$J(\mathbf{R}) = \sum_{i=1}^n \langle \mathcal{E}_{\mathbf{u}_i}^{\alpha_i}(\mathbf{R}), \mathbf{T}_i \rangle,$$

as well as in the gradient

$$\nabla_{\mathbf{sR}}J(\mathbf{R}) = \sum_{i=1}^n \alpha_i \langle \mathbf{s} \triangleright_1 (\mathbf{R} \triangleright \mathcal{E}_{\mathbf{u}_i}^{\alpha_i}(\mathbf{I})), \mathbf{T}_i \rangle.$$

### 3. Distance Preservation

In this section we are going to investigate how well the embeddings defined in Section 2.1 preserve the geodesic distance between any two rotations. We first analyze this problem locally.

#### 3.1. Isometric Embeddings

Lets recall that a differentiable embedding  $\mathcal{E}: \mathcal{M} \rightarrow \mathbb{R}^d$  is isometric if its differential  $d\mathcal{E}: T_m\mathcal{M} \rightarrow T_{\mathcal{E}(m)}\mathcal{E}(\mathcal{M})$  at each point  $m \in \mathcal{M}$  is an isometry between vector spaces. Since in our setting in both spaces,  $SO(3)/\mathcal{S}$  and  $\mathbb{R}^{3\alpha}$ , the metric is invariant with respect to the action  $\triangleright$  of  $SO(3)$  and the embedding is an  $SO(3)$  homomorphism it suffices to prove isometry at the identity  $[\mathbf{I}]_{\mathcal{S}} \in SO(3)/\mathcal{S}$  only.

In order to identify isometric embeddings within our framework we need to generalize it slightly by multiplying the components by different weights  $\boldsymbol{\beta} = (\beta_1, \dots, \beta_n) \in \mathbb{R}^n$ , i.e., we define

$$\mathcal{E}_{\mathbf{u}}^{\boldsymbol{\beta}}(\mathbf{R}) = (\beta_1 \otimes^{\alpha_1} \mathbf{R}\mathbf{u}_1, \dots, \beta_n \otimes^{\alpha_n} \mathbf{R}\mathbf{u}_n)$$

together with its symmetrization

$$\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}: SO(3)/\mathcal{S} \rightarrow \mathbb{R}^{3\alpha}, \quad \mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}([\mathbf{O}]_{\mathcal{S}}) = \frac{1}{|\mathcal{S}|} \sum_{\mathbf{S} \in \mathcal{S}} \mathcal{E}_{\mathbf{u}}^{\boldsymbol{\beta}}(\mathbf{O}\mathbf{S}). \quad (8)$$

Choosing the weights  $\boldsymbol{\beta}$  carefully will allow us to explicitly define isometric embeddings for the quotients  $SO(3)/\mathcal{S}$  of  $SO(3)$  with respect to all crystallographic symmetry groups.

We shall analyze the derivative  $d\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}([\mathbf{I}]_{\mathcal{S}})\mathbf{s}^{(k)}$  of the embedding with respect to the canonical orthonormal basis of the tangential space  $T_{\mathbf{I}}SO(3)$  which consists of the skew symmetric matrices

$$\mathbf{s}^{(1)} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{s}^{(2)} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \mathbf{s}^{(3)} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (9)$$

**Lemma 3.1.** *The mapping  $\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}: SO(3)/\mathcal{S} \rightarrow \mathbb{R}^{3\alpha}$  as defined in (8) is isometric if and only if the vectors  $d\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}([\mathbf{I}]_{\mathcal{S}})\mathbf{s}^{(k)}$  are orthonormal in  $\mathbb{R}^{3\alpha}$ .*

*Proof.* The mapping  $d\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}([\mathbf{I}]_{\mathcal{S}})$  is linear and  $\{\mathbf{s}^{(k)}\}_{k=1}^3$  is a basis in  $T_{\mathbf{I}}SO(3)$ . Hence,  $\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}$  is isometric if and only if the vectors  $d\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}([\mathbf{I}]_{\mathcal{S}})\mathbf{s}^{(k)}$  are orthonormal in the tangent space  $T_{\mathcal{E}(\mathbf{I})}\mathbb{R}^{3\alpha}$ .  $\square$

For the differential of the mapping  $\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\boldsymbol{\beta}}$  we have the following lemma.

**Lemma 3.2.** *Let  $\alpha \in \mathbb{N}$ ,  $\mathbf{u} \in \mathbb{S}^2$  an arbitrary direction and  $\mathbf{s} \in T_{\mathbf{I}}SO(3)$  an arbitrary skew symmetric matrix. Then*

$$d\mathcal{E}_{\mathbf{u}}^{\boldsymbol{\beta}}(\mathbf{I})\mathbf{s} = \sum_{i=0}^{\alpha-1} (\otimes^i \mathbf{u}) \otimes \mathbf{s}\mathbf{u} \otimes (\otimes^{\alpha-i-1} \mathbf{u}).$$

*Proof.* Let  $\gamma(t)$  be a curve in  $SO(3)$  such that  $\dot{\gamma}(0) = \mathbf{s}$  and  $\gamma(0) = \mathbf{I}$ . The image of the map  $d\mathcal{E}_{\mathbf{u},\mathcal{S}}^{\alpha,\beta}([\mathbf{I}]_{\mathcal{S}})$  of  $\mathbf{s}$  is given by

$$d\mathcal{E}_{\mathbf{u}}^{\alpha}(\mathbf{I})\mathbf{s} = \left. \frac{d}{dt} (\otimes^{\alpha} (\gamma(t) \cdot \mathbf{u})) \right|_{t=0}.$$

With the chain-rule it follows

$$\begin{aligned} d\mathcal{E}_{\mathbf{u}}^{\alpha}(\mathbf{I})\mathbf{s} &= \sum_{i=0}^{\alpha-1} (\otimes^i (\gamma(t) \cdot \mathbf{u}) \otimes \dot{\gamma}(t)\mathbf{u} \otimes (\otimes^{\alpha-i-1} \gamma(t)\mathbf{u})) \Big|_{t=0} \\ &= \sum_{i=0}^{\alpha-1} (\otimes^i \mathbf{u}) \otimes \mathbf{s}\mathbf{u} \otimes (\otimes^{\alpha-i-1} \mathbf{u}). \end{aligned}$$

□

In the following we will find isometric embeddings for all crystallographic symmetry groups. Therefore, we will proceed as follows. First we consider the cyclic groups  $C_k$ ,  $k \in \mathbb{N}$ , followed by the dihedral groups  $D_k$ ,  $k \in \mathbb{N}$  and finally the tetraeder group  $T$  and the octaeder group  $O$ . The parameters for these isometric embeddings are summarized in Table 2. For the cyclic and the dihedral groups we assume the major rotational axis to be align in  $\mathbf{e}_1$ -direction and the two fold axis parallel to  $\mathbf{e}_2$ .

For the symmetry group  $C_1$  the isometry follows directly from Lemma 3.1. The symmetry group  $C_2$  is a special case, because in contrast to  $C_k$  for  $k > 2$  the vectors  $\mathbf{O}\mathbf{e}_2$  for  $\mathbf{O} \in C_k$  do not span the plane orthogonal to  $\mathbf{e}_1$ . For this reason we need to add an additional component in contrast to the embedding in [1].

**Theorem 3.3.** *Let  $\mathbf{u} = (e_1, e_2, e_3)$ ,  $\alpha = (1, 2, 2)$  and  $\beta = (\frac{1}{\sqrt{2}}, \frac{1}{2}, \frac{1}{2})$ . Then  $\mathcal{E}_{\mathbf{u},C_2}^{\alpha,\beta}$  is an isometric embedding.*

*Proof.* There holds

$$\begin{aligned} d\mathcal{E}_{\mathbf{u},C_2}^{\alpha,\beta}([\mathbf{I}]_{C_2})\mathbf{s}^{(1)} &= \left( \beta_1 \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \beta_2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \beta_3 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \right), \\ d\mathcal{E}_{\mathbf{u},C_2}^{\alpha,\beta}([\mathbf{I}]_{C_2})\mathbf{s}^{(2)} &= \left( \beta_1 \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \beta_2 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \beta_3 \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \right), \\ d\mathcal{E}_{\mathbf{u},C_2}^{\alpha,\beta}([\mathbf{I}]_{C_2})\mathbf{s}^{(3)} &= \left( \beta_1 \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \beta_2 \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \beta_3 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right). \end{aligned}$$

These three vectors are orthogonal. To normalize them, we have to solve

$$2\beta_2^2 + 2\beta_3^2 = \beta_1^2 + 2\beta_3^2 = \beta_1^2 + 2\beta_2^2 = 1,$$

which yields  $\beta_1 = \frac{1}{\sqrt{2}}, \beta_2 = \beta_3 = \frac{1}{2}$ . □

For the symmetry groups  $C_k$  for  $k > 2$  we first show the orthogonality of the tangent vectors  $d\mathcal{E}_{\mathbf{u}, C_k}^\alpha([I]_{C_k})$ .

**Lemma 3.4.** *Let  $k \in \mathbb{N}$  with  $k > 2$ ,  $\mathbf{u} = (\mathbf{e}_1, \mathbf{e}_2)$  and  $\alpha = (1, k)$ . Then the vectors  $d\mathcal{E}_{\mathbf{u}, C_k}^\alpha$  are orthogonal.*

*Proof.* For the rank one component  $d\mathcal{E}_{\mathbf{e}_1, C_k}^{1, \beta_1}([I]_{C_k})$  of  $d\mathcal{E}_{\mathbf{u}, C_k}^{\alpha, \beta}([I]_{C_k})$  orthogonality follows from

$$d\mathcal{E}_{\mathbf{e}_1, C_k}^{1, \beta_1}([I]_{C_k})[\mathbf{s}^{(1)} \mathbf{s}^{(2)} \mathbf{s}^{(3)}] = \beta_1 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \quad (10)$$

For the rank  $k$  component  $d\mathcal{E}_{\mathbf{e}_2, C_k}^{k, \beta_2}([I]_{C_k})$  we use the Lemma 3.2 and define for  $l = 1, 2, 3$

$$\mathbf{B}_l := d\mathcal{E}_{\mathbf{e}_2, C_k}^k([I]_{C_k})\mathbf{s}^{(l)} = \sum_{i=0}^{k-1} \frac{1}{k} \sum_{j=0}^{i-1} (\otimes^i \mathbf{v}_j) \otimes \mathbf{s}^{(l)} \mathbf{v}_j \otimes (\otimes^{k-i-1} \mathbf{v}_j), \quad (11)$$

where the vectors  $\mathbf{v}_j = (0, \cos \frac{2\pi j}{k}, \sin \frac{2\pi j}{k})^\top$  result from applying all symmetries from  $C_k$  to  $\mathbf{e}_2$ . The inner product between these rank  $k$  tensors  $\mathbf{B}_l$ ,  $l = 1, \dots, 3$  evaluates to

$$\begin{aligned} \langle \mathbf{B}_{l_1}, \mathbf{B}_{l_2} \rangle &= \frac{k(k-1)}{k^2} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^{k-2} \langle \mathbf{s}^{(l_1)} \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle \langle \mathbf{s}^{(l_2)} \mathbf{v}_{j_2}, \mathbf{v}_{j_1} \rangle \\ &\quad + \frac{k}{k^2} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^{k-1} \langle \mathbf{s}^{(l_1)} \mathbf{v}_{j_1}, \mathbf{s}^{(l_2)} \mathbf{v}_{j_2} \rangle. \end{aligned} \quad (12)$$

Using

$$\mathbf{s}^{(1)} \mathbf{v}_j = \begin{pmatrix} 0 \\ -\sin \frac{2\pi j}{k} \\ \cos \frac{2\pi j}{k} \end{pmatrix}, \quad \mathbf{s}^{(2)} \mathbf{v}_j = \begin{pmatrix} -\sin \frac{2\pi j}{k} \\ 0 \\ 0 \end{pmatrix}, \quad \mathbf{s}^{(3)} \mathbf{v}_j = \begin{pmatrix} -\cos \frac{2\pi j}{k} \\ 0 \\ 0 \end{pmatrix}$$

we observe for all  $j_1, j_2$  and  $l = 2, 3$  the orthogonality  $\langle \mathbf{s}^{(l)} \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle = 0$  and hence, the first double sum in (12) is zero whenever  $l_1 \neq l_2$ .

In the second double sum we have  $\langle \mathbf{s}^{(l_1)} \mathbf{v}_{j_1}, \mathbf{s}^{(l_2)} \mathbf{v}_{j_2} \rangle = 0$  for all  $l_1 \neq l_2$

except for the pair  $l_1, l_2 \in \{2, 3\}$ . For this specific case we calculate

$$\begin{aligned}
\langle \mathbf{B}_2, \mathbf{B}_3 \rangle &= \sum_{j_1, j_2=0}^{k-1} \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^{k-1} \left\langle \mathbf{s}^{(2)} \mathbf{v}_{j_1}, \mathbf{s}^{(3)} \mathbf{v}_{j_2} \right\rangle \\
&= \sum_{j_1, j_2=0}^{k-1} \cos^{k-1} \frac{2\pi(j_1-j_2)}{k} \sin \frac{2\pi j_1}{k} \cos \frac{2\pi j_2}{k} \\
&= \frac{1}{2} \sum_{j_1, j_2=0}^{k-1} \cos^{k-1} \frac{2\pi(j_1-j_2)}{k} \left( \sin \frac{2\pi(j_1-j_2)}{k} + \sin \frac{2\pi(j_1+j_2)}{k} \right) \\
&= \frac{1}{2} \sum_{j_1, j_2=0}^{k-1} \cos^{k-1} \frac{2\pi j_1}{k} \left( \sin \frac{2\pi j_1}{k} + \sin \frac{2\pi j_2}{k} \right) = 0.
\end{aligned}$$

□

In order to prove  $\|d\mathcal{E}_{\mathbf{u}, C_k}^{\alpha, \beta}([\mathbf{I}]_{C_k})\mathbf{s}^{(k)}\| = 1$  we continue by calculating  $\|\mathbf{B}_l\|^2 = \langle \mathbf{B}_l, \mathbf{B}_l \rangle$  for  $l = 1, 2, 3$ .

**Lemma 3.5.** *For the tensors  $\mathbf{B}_l$  defined in equation (11) we have*

$$\begin{aligned}
\|\mathbf{B}_1\|^2 &= \begin{cases} \frac{k^2}{2^{k-1}} & \text{if } k \text{ odd} \\ -\frac{k(k-1)}{2^{k-2}} \binom{k-2}{\frac{k}{2}-1} + \frac{k^2}{2^k} \left( \binom{k}{\frac{k}{2}} + 2 \right) & \text{if } k \text{ even} \end{cases}, \\
\|\mathbf{B}_2\|^2 = \|\mathbf{B}_3\|^2 &= \begin{cases} \frac{k}{2^k} & \text{if } k \text{ is odd} \\ \frac{k}{2^{k+1}} \left( 2 + \binom{k-1}{\frac{k}{2}} + \binom{k-1}{\frac{k}{2}-1} \right) & \text{if } k \text{ is even} \end{cases}.
\end{aligned}$$

*Proof.* First we need the sums of the following geometric series:

$$\begin{aligned}
\sum_{j=0}^{k-1} \cos^k \left( \frac{2\pi j}{k} \right) &= \begin{cases} \frac{k}{2^{k-1}} & \text{if } k \text{ odd} \\ \frac{1}{2^k} \left( \binom{k}{\frac{k}{2}} \cdot k + 2k \right) & \text{if } k \text{ even} \end{cases}, \\
\sum_{j=0}^{k-1} \cos^{k-2} \left( \frac{2\pi j}{k} \right) &= \begin{cases} 0 & \text{if } k \text{ odd} \\ \frac{k}{2^{k-2}} \binom{k-2}{\frac{k}{2}-1} & \text{if } k \text{ even} \end{cases}.
\end{aligned}$$

By equation (12) we obtain

$$\begin{aligned}
\|\mathbf{B}_1\|^2 &= \frac{(k-1)}{k} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^{k-2} \langle \mathbf{s}^{(1)} \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle \langle \mathbf{s}^{(1)} \mathbf{v}_{j_2}, \mathbf{v}_{j_1} \rangle \\
&\quad + \frac{1}{k} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^{k-1} \langle \mathbf{s}^{(1)} \mathbf{v}_{j_1}, \mathbf{s}^{(1)} \mathbf{v}_{j_2} \rangle \\
&= -\frac{(k-1)}{k} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \cos^{k-2} \left( \frac{2\pi(j_1 - j_2)}{k} \right) \sin^2 \left( \frac{2\pi(j_1 - j_2)}{k} \right) \\
&\quad + \frac{1}{k} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \cos^{k-1} \left( \frac{2\pi(j_1 - j_2)}{k} \right) \cos \left( \frac{2\pi(j_1 - j_2)}{k} \right) \\
&= -(k-1) \sum_{j=0}^{k-1} \cos^{k-2} \left( \frac{2\pi j}{k} \right) \sin^2 \left( \frac{2\pi j}{k} \right) + \sum_{j=0}^{k-1} \cos^k \left( \frac{2\pi j}{k} \right) \\
&= -(k-1) \sum_{j=0}^{k-1} \cos^{k-2} \left( \frac{2\pi j}{k} \right) + k \sum_{j=0}^{k-1} \cos^k \left( \frac{2\pi j}{k} \right) \\
&= \begin{cases} \frac{k^2}{2^{k-1}} & \text{if } k \text{ odd} \\ -\frac{k(k-1)}{2^{k-2}} \binom{k-2}{\frac{k}{2}-1} + \frac{k^2}{2^k} \left( \binom{k}{\frac{k}{2}} + 2 \right) & \text{if } k \text{ even} \end{cases} .
\end{aligned}$$



Next we investigate the tensor  $\mathbf{B}_3$ .

$$\begin{aligned}
\|\mathbf{B}_3\|^2 &= \frac{1}{k} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^{k-1} \langle \mathbf{s}^{(3)} \mathbf{v}_{j_1}, \mathbf{s}^{(3)} \mathbf{v}_{j_2} \rangle \\
&= \frac{1}{k} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \cos^{k-1} \left( \frac{2\pi(j_1 - j_2)}{k} \right) \cos \left( \frac{2\pi j_1}{k} \right) \cos \left( \frac{2\pi j_2}{k} \right) \\
&= \frac{1}{k} \frac{1}{2^{k+1}} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \left( e^{\frac{2\pi i(j_1 - j_2)}{k}} + e^{-\frac{2\pi i(j_1 - j_2)}{k}} \right)^{k-1} \left( e^{\frac{2\pi i j_1}{k}} + e^{-\frac{2\pi i j_1}{k}} \right) \left( e^{\frac{2\pi i j_2}{k}} + e^{-\frac{2\pi i j_2}{k}} \right) \\
&= \frac{1}{k} \frac{1}{2^{k+1}} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \left( e^{\frac{2\pi i(j_1 + j_2)}{k}} + e^{-\frac{2\pi i(j_1 + j_2)}{k}} + e^{\frac{2\pi i(j_1 - j_2)}{k}} + e^{\frac{2\pi i(j_2 - j_1)}{k}} \right) \sum_{l=0}^{k-1} \binom{k-1}{l} e^{\frac{2\pi i(j_1 - j_2)(2l+1)}{k}} \\
&= \frac{1}{k} \frac{1}{2^{k+1}} \sum_{l=0}^{k-1} \binom{k-1}{l} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \left( e^{\frac{2\pi i((j_1 - j_2)(2l+1) + j_1 + j_2)}{k}} + e^{\frac{2\pi i((j_1 - j_2)(2l+1) - j_1 - j_2)}{k}} \right. \\
&\quad \left. + e^{\frac{2\pi i(j_1 - j_2)(2l+2)}{k}} + e^{\frac{2\pi i(j_1 - j_2)(2l)}{k}} \right) \\
&= \frac{1}{k} \frac{1}{2^{k+1}} \sum_{l=0}^{k-1} \binom{k-1}{l} \sum_{j_1=0}^{k-1} \sum_{j_2=0}^{k-1} \left( e^{\frac{2\pi i(j_1(2l+2) - 2lj_2)}{k}} + e^{\frac{2\pi i(2lj_1 - j_2(2l+2))}{k}} \right. \\
&\quad \left. + e^{\frac{2\pi i(j_1 - j_2)(2l+2)}{k}} + e^{\frac{2\pi i(j_1 - j_2)(2l)}{k}} \right) \\
&= \frac{k}{k} \frac{1}{2^{k+1}} \sum_{l=0}^{k-1} \binom{k-1}{l} \sum_{j=0}^{k-1} e^{\frac{2\pi i j(2l+2)}{k}} + e^{\frac{2\pi i j(2l)}{k}} \\
&= \begin{cases} \frac{k}{2^k} & \text{if } k \text{ is odd} \\ \frac{k}{2^{k+1}} \left( 2 + \binom{k-1}{\frac{k}{2}} + \binom{k-1}{\frac{k}{2}-1} \right) & \text{if } k \text{ is even} \end{cases} .
\end{aligned}$$

For the norm  $\|\mathbf{B}_2\|^2$  we only have to change some signs in the previous calculation and receive in the end  $\|\mathbf{B}_2\|^2 = \|\mathbf{B}_3\|^2$ .  $\square$

Summarizing these Lemmas we find weights  $\beta$  for all crystallographic symmetry groups  $\mathcal{S}$  such that the corresponding embeddings are isometries.

**Theorem 3.6.** *Let  $k \in \mathbb{N}$  with  $k > 2$ ,  $\mathbf{u} = (\mathbf{e}_1, \mathbf{e}_2)$  and  $\alpha = (1, k)$ . Then the embeddings  $\mathcal{E}_{\mathbf{u}, C_k}^{\alpha, \beta}$  with the factors*

$$\beta = \left( \sqrt{1 - \frac{\|\mathbf{B}_2\|^2}{\|\mathbf{B}_1\|^2}}, \frac{1}{\|\mathbf{B}_1\|} \right)^\top$$

with the norms from Lemma 3.5 are isometric embeddings. The concrete factors for  $k = 3, 4, 6$  are listed in table 2.

*Proof.* We use equation (10) for the rank 1 tensor. To normalize the vectors  $d\mathcal{E}_{\mathbf{u}, C_k}^{\alpha, \beta}([\mathbf{I}]_{C_k})\mathbf{s}^{(l)}$  for  $l = 1, 2, 3$  we have to solve for every  $k$  equations of the form

$$\beta_2^2 \cdot \|\mathbf{B}_1\|^2 = \beta_1^2 + \beta_2^2 \cdot \|\mathbf{B}_2\|^2 = \beta_1^2 + \beta_2^2 \cdot \|\mathbf{B}_3\|^2 = 1,$$

which always has a solution since  $\|\mathbf{B}_2\| = \|\mathbf{B}_3\|$ . We receive the positive solution by

$$\beta_1 = \sqrt{1 - \frac{\|\mathbf{B}_2\|^2}{\|\mathbf{B}_1\|^2}}, \quad \beta_2 = \frac{1}{\|\mathbf{B}_1\|}.$$

□

$\mathcal{S}$	$\mathbf{u}$	$\alpha$	$\beta$	Dimension
$C_1$	$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$	$(1, 1, 1)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$	9
$C_2$	$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$	$(1, 2, 2)$	$(\frac{1}{\sqrt{2}}, \frac{1}{2}, \frac{1}{2})$	13
$C_3$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(1, 3)$	$(\sqrt{\frac{5}{6}}, \frac{\sqrt{4}}{3})$	13
$C_4$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(1, 4)$	$(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$	17
$C_6$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(1, 6)$	$(\frac{1}{\sqrt{12}}, \frac{2\sqrt{2}}{3})$	30
$D_2$	$(\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$	$(2, 2, 2)$	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	15
$D_3$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(2, 3)$	$(\sqrt{\frac{5}{12}}, \frac{\sqrt{4}}{3})$	15
$D_4$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(2, 4)$	$(\frac{1}{2}, \frac{1}{\sqrt{2}})$	19
$D_6$	$(\mathbf{e}_1, \mathbf{e}_2)$	$(2, 6)$	$(\frac{1}{\sqrt{24}}, \frac{2\sqrt{2}}{3})$	32
$O$	$\mathbf{e}_1$	4	$\frac{3}{2\sqrt{2}}$	14
$T$	$\mathbf{e}_1$	3	$\frac{3}{2\sqrt{2}}$	10

Table 2: Choices of the vectors  $\mathbf{u}$  and the parameters  $\alpha, \beta$  such that the embeddings  $\tilde{\mathcal{E}}_{\mathbf{u}, \mathcal{S}}^{\alpha, \beta}$  are isometric.

For the symmetry groups  $D_k$  the case  $k = 2$  is a special case for the same reasons as  $C_2$ .

**Theorem 3.7.** *Let  $\mathbf{u} = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_2)$ ,  $\alpha = (2, 2, 2)$  and  $\beta = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . Then  $\mathcal{E}_{\mathbf{u}, D_2}^{\alpha, \beta}$  is an isometric embedding.*

*Proof.* The second and third component are the same like for the case  $C_2$ . Analog to this case we have to solve

$$2\beta_1^2 + 2\beta_2^2 = 2\beta_2^2 + 2\beta_3^2 = 1,$$

which yields  $\beta_1 = \beta_2 = \beta_3 = \frac{1}{2}$ . □

**Theorem 3.8.** Let  $k \in \mathbb{N}$  with  $k > 2$ ,  $\mathbf{u} = (\mathbf{e}_1, \mathbf{e}_2)$  and  $\boldsymbol{\alpha} = (2, k)$ . Then there exist factors  $\beta$ , such that  $\mathcal{E}_{\mathbf{u}, D_k}^{\boldsymbol{\alpha}, \beta}$  is an isometric embedding.

*Proof.* As in the case  $C_k$  we get the same second components  $B_1, B_2$  and  $B_3$ . Only the first component is now a  $3 \times 3$ -matrix and not just a vector. The three vectors  $d\mathcal{E}([\mathbf{I}]_{D_k})\mathbf{s}^{(l)}$  are again orthogonal. For the normalization we have to solve

$$\beta_2^2 \cdot \|B_1\|^2 = 2\beta_1^2 + \beta_2^2 \cdot \|B_2\|^2 = 2\beta_1^2 + \beta_2^2 \cdot \|B_3\|^2 = 1,$$

which yields the same solutions for  $\beta_2$  as in the case  $C_k$ , but for  $\beta_1$  we have to divide the solution from  $C_k$  by  $\sqrt{2}$ .  $\square$

For the cubic symmetry group the isometric embedding requires only a single vector. More precisely, we have the following result.

**Theorem 3.9.** Let  $\mathbf{u} = \mathbf{e}_1$ ,  $\boldsymbol{\alpha} = 4$  and  $\beta = \frac{3}{2\sqrt{2}}$ . Then  $\mathcal{E}_{\mathbf{u}, O}^{\boldsymbol{\alpha}, \beta}$  is an isometric embedding.

*Proof.* The vectors  $\mathbf{R}\mathbf{e}_1$  for  $\mathbf{R} \in O$  are in the set  $\{\pm\mathbf{e}_1, \pm\mathbf{e}_2, \pm\mathbf{e}_3\}$ . Since  $\otimes^4 \mathbf{x} = \otimes^4(-\mathbf{x})$ , we only have to consider the three vectors  $\mathbf{v}_i = \mathbf{e}_i$  for  $i = 1, 2, 3$ . With respect to the skew symmetric basis  $\mathbf{s}^{(k)}$ ,  $k = 1, 2, 3$  we obtain

$$\begin{array}{lll} \mathbf{s}^{(1)}\mathbf{v}_1 = \mathbf{0}, & \mathbf{s}^{(1)}\mathbf{v}_2 = \mathbf{e}_3, & \mathbf{s}^{(1)}\mathbf{v}_3 = -\mathbf{e}_2, \\ \mathbf{s}^{(2)}\mathbf{v}_1 = \mathbf{e}_3, & \mathbf{s}^{(2)}\mathbf{v}_2 = \mathbf{0}, & \mathbf{s}^{(2)}\mathbf{v}_3 = -\mathbf{e}_1, \\ \mathbf{s}^{(3)}\mathbf{v}_1 = \mathbf{e}_2, & \mathbf{s}^{(3)}\mathbf{v}_2 = -\mathbf{e}_1, & \mathbf{s}^{(3)}\mathbf{v}_3 = \mathbf{0}. \end{array}$$

By Lemma 3.2 the scalar products in the embedding calculate to

$$\begin{aligned} \left\langle dE_{\mathbf{u}, O}^{\boldsymbol{\alpha}, \beta} \mathbf{s}^{(l_1)}, dE_{\mathbf{u}, O}^{\boldsymbol{\alpha}, \beta} \mathbf{s}^{(l_2)} \right\rangle &= \frac{4 \cdot 3}{3^2} \sum_{j_1=1}^3 \sum_{j_2=1}^3 \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^2 \left\langle \mathbf{s}^{(l_1)} \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \right\rangle \left\langle \mathbf{s}^{(l_2)} \mathbf{v}_{j_2}, \mathbf{v}_{j_1} \right\rangle \\ &\quad + \frac{4}{3^2} \sum_{j_1=1}^3 \sum_{j_2=1}^3 \langle \mathbf{v}_{j_1}, \mathbf{v}_{j_2} \rangle^3 \left\langle \mathbf{s}^{(l_1)} \mathbf{v}_{j_1}, \mathbf{s}^{(l_2)} \mathbf{v}_{j_2} \right\rangle \\ &= \frac{4 \cdot 3}{3^2} \sum_{j=1}^3 \left\langle \mathbf{s}^{(l_1)} \mathbf{v}_j, \mathbf{v}_j \right\rangle \left\langle \mathbf{s}^{(l_2)} \mathbf{v}_j, \mathbf{v}_j \right\rangle + \frac{4}{3^2} \sum_{j=1}^3 \left\langle \mathbf{s}^{(l_1)} \mathbf{v}_j, \mathbf{s}^{(l_2)} \mathbf{v}_j \right\rangle \\ &= \frac{4}{3^2} \sum_{j=1}^3 \left\langle \mathbf{s}^{(l_1)} \mathbf{v}_j, \mathbf{s}^{(l_2)} \mathbf{v}_j \right\rangle = \frac{8}{9} \delta_{l_1, l_2}. \end{aligned}$$

Hence, the tangential vectors are orthogonal and normalized for  $\beta_1 = \frac{3}{2\sqrt{2}}$ .  $\square$

Finally, we consider tetrahedral symmetry  $T$ .

**Theorem 3.10.** Let  $\mathbf{u} = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ ,  $\boldsymbol{\alpha} = 3$  and  $\beta = \frac{3}{2\sqrt{2}}$ . Then  $\mathcal{E}_{\mathbf{u}, T}^{\boldsymbol{\alpha}, \beta}$  is an isometric embedding.

Proof. The vectors  $Ru_i$  for  $R \in \mathbb{R}^{2 \times 2}$  are

$$v_1 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A; \quad v_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A; \quad v_3 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A; \quad v_4 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A$$

and satisfy  $\langle v_i, v_j \rangle = \frac{1}{3}$  for  $i \neq j$ . By Lemma 3.2 we have

$$dE_{u,T}(I) s^{(l)} = \sum_{j=1}^4 \sum_{i=0}^2 \langle v_j, s^{(l)} v_j \rangle v_j$$

and hence, the scalar products of the basis vectors evaluate to

$$\begin{aligned} \langle dE_{u,T} s^{(l_1)}; dE_{u,T} s^{(l_2)} \rangle &= \frac{3}{4^2} \sum_{j_1=1}^4 \sum_{j_2=1}^4 \langle v_{j_1}, v_{j_2} \rangle \langle s^{(l_1)} v_{j_1}; s^{(l_2)} v_{j_2} \rangle \\ &+ \frac{3}{4^2} \sum_{j_1=1}^4 \sum_{j_2=1}^4 \langle v_{j_1}, v_{j_2} \rangle^2 \langle s^{(l_1)} v_{j_1}; s^{(l_2)} v_{j_2} \rangle \end{aligned}$$

Using the symmetry of vectors  $v_j$  and  $s^{(l)} v_j$

$$\begin{aligned} s^{(1)} v_1 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} A; & s^{(1)} v_2 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} A; & s^{(1)} v_3 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} A; & s^{(1)} v_4 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix} A \\ s^{(2)} v_1 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A; & s^{(2)} v_2 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A; & s^{(2)} v_3 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A; & s^{(2)} v_4 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} A \\ s^{(3)} v_1 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \end{pmatrix} A; & s^{(3)} v_2 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \end{pmatrix} A; & s^{(3)} v_3 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \end{pmatrix} A; & s^{(3)} v_4 &= \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \end{pmatrix} A \end{aligned}$$

it is sufficient to consider the scalar products for  $l_1 = 1; l_2 = 2$  and  $l_1 = l_2 = 1$ :

$$\begin{aligned} \langle dE_{u,T} s^{(1)}; dE_{u,T} s^{(2)} \rangle &= \frac{3}{8} \sum_{\substack{j_1, j_2=1 \\ j_1 \neq j_2}}^4 \langle v_{j_1}, v_{j_2} \rangle \langle s^{(1)} v_{j_1}; s^{(2)} v_{j_2} \rangle = 0; \\ \langle dE_{u,T} s^{(1)}; dE_{u,T} s^{(1)} \rangle &= \frac{3}{8} \sum_{\substack{j_1, j_2=1 \\ j_1 \neq j_2}}^4 \langle v_{j_1}, v_{j_2} \rangle \langle s^{(1)} v_{j_1}; s^{(1)} v_{j_2} \rangle \\ &+ \frac{3}{8} \sum_{j_1=1}^4 \frac{2}{6} + \frac{3}{4^2} \sum_{\substack{j_1, j_2=1 \\ j_1 \neq j_2}}^4 \frac{1}{9} \langle s^{(1)} v_{j_1}; s^{(1)} v_{j_2} \rangle \\ &= \frac{3}{8} \frac{1}{3} \frac{64}{18} + \frac{3}{8} \frac{4}{6} \frac{2}{6} + \frac{3}{4^2} \frac{1}{9} \frac{16}{6} = \frac{8}{9}. \end{aligned}$$

Hence, with  $\alpha = \frac{3}{2\sqrt{2}}$  the proposed embedding is isometric.  $\square$

### 3.2. Global Inequalities

Although the embeddings found in the previous section are isometric they obviously do not preserve the metric globally. In this section we are interested in inequalities of the form

$$c_{\min} d([\mathbf{O}_1]_S, [\mathbf{O}_2]_S) \leq d(\mathcal{E}_S([\mathbf{O}_1]_S), \mathcal{E}_S([\mathbf{O}_2]_S)) \leq c_{\max} d([\mathbf{O}_1]_S, [\mathbf{O}_2]_S) \quad (13)$$

that relate the Euclidean distance in  $\mathbb{R}^{3^\alpha}$  and the geodesic distance

$$d([\mathbf{O}_1]_S, [\mathbf{O}_2]_S) = \min_{\mathbf{R} \in S} d(\mathbf{O}_1 \mathbf{R}, \mathbf{O}_2), \quad d(\mathbf{O}_1, \mathbf{O}_2) = \arccos \left( \frac{1}{2} \left( -1 + \text{tr}(\mathbf{O}_1^\top \mathbf{O}_2) \right) \right)$$

on the manifold  $SO(3)/S$ .

The situation is most easiest for  $S = C_1$ , i.e., we just look at  $SO(3)$ . In this case the Euclidean distance in the embedding is directly related to the geodesic distance on the manifold via

$$d(\mathcal{E}_{C_1}(\mathbf{R}_1), \mathcal{E}_{C_1}(\mathbf{R}_2)) = 2 \sqrt{1 - \cos(d(\mathbf{R}_1, \mathbf{R}_2))}.$$

and we have  $c_{\min} = \frac{\sqrt{8}}{\pi}$  and  $c_{\max} = 1$ .

For higher symmetries there is no such one to one relationship. In order to illustrate the dependency between the geodesic distance on the manifold and the Euclidean distance in the embedding for higher symmetries we have visualized the regions of suitable combinations in Figure 1 and 2. While Figure 1 illustrates the embeddings from [1], Figure 2 visualizes the isometric embeddings from Table 2.

In Table 3 the upper and lower bounds  $c_{\min}$  and  $c_{\max}$  are listed for isometric embeddings from Table 2. We would like to stress that non isometric embeddings might very well lead to better global bounds. Indeed, Table 4 provides alternative coefficients for the embeddings  $\mathcal{E}_{\mathbf{u}, S}^{\alpha, \beta}$  which have better upper and lower bounds.

$S$	$c_{\min}$	$c_{\max}$	$c_{\max}/c_{\min}$
$C_2$	0.4518	1	2.2134
$C_3$	0.5827	1	1.7161
$C_4$	0.4520	1	2.2124
$C_6$	0.1864	1	5.3648
$D_2$	0.5896	1	1.6961
$D_3$	0.5807	1	1.7221
$D_4$	0.5455	1	1.8332
$D_6$	0.4433	1	2.2558
$O$	0.6041	1	1.6554
$T$	0.6085	1	1.6434

Table 3: The constants in equation (13) for all crystallographic symmetry groups  $S$

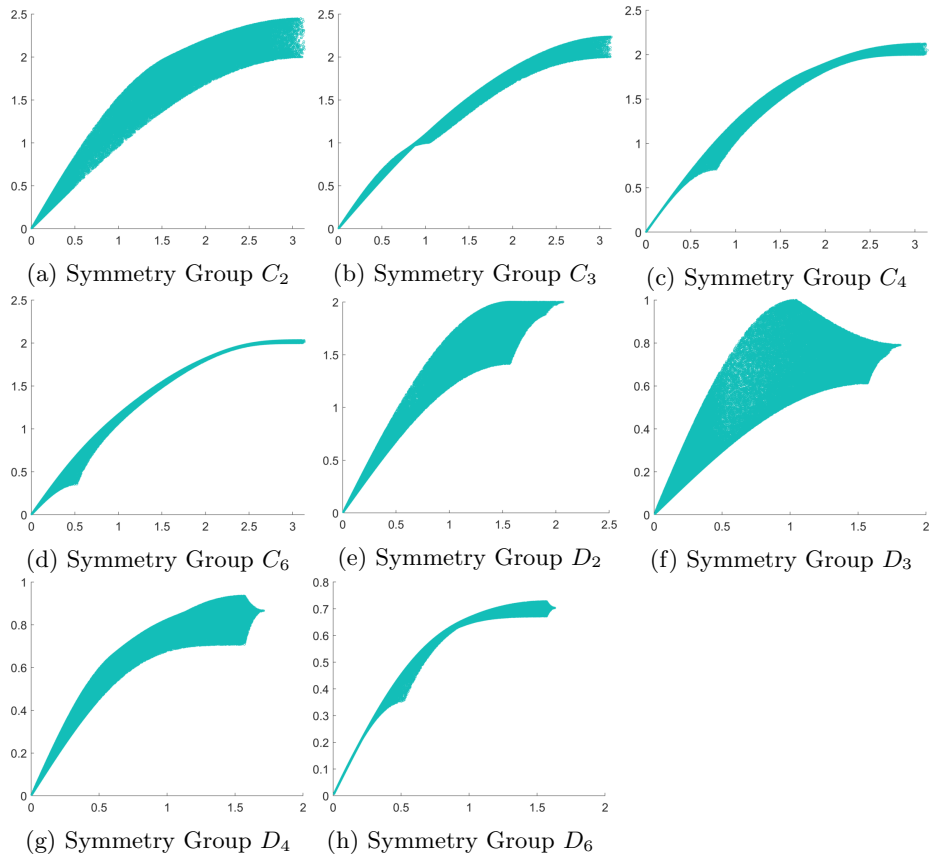


Figure 1: Relation between the geodesic distance on the manifold and the Euclidean distance in the embedding for the embeddings reported in [1].

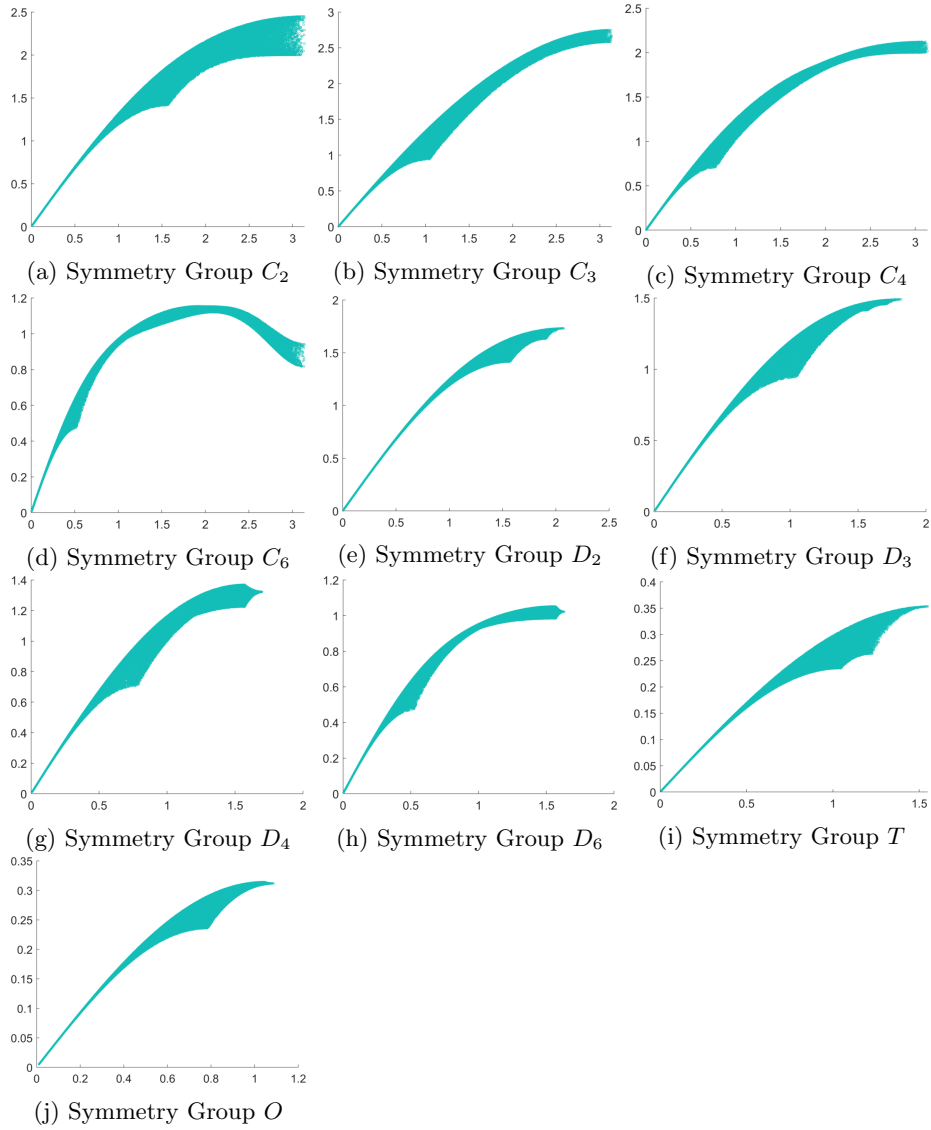


Figure 2: Relation between the geodesic distance on the manifold and the Euclidean distance in the embedding for the isometric embeddings summarized in Table 2.

$\mathcal{S}$	$\beta$	$c_{\max}/c_{\min}$
$C_2$	(1, 0.5, 0.5)	1.9217
$C_3$	(1, 0.67)	1.6813
$C_4$	(1, 0.6)	1.9107
$C_6$	(1, 0.93)	2.1488
$D_3$	(1, 1.03)	1.7192
$D_4$	(1, 1.11)	1.7968
$D_6$	(1, 1.65)	1.9540

Table 4: factors for globally almost isometric embeddings for some symmetry groups  $\mathcal{S}$

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