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Isometric and metamorphic operations on the space of local fundamental measures

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We consider symmetry operations on the four-dimensional vector space that is spanned by the local versions of the Minkowski functionals (or fundamental measures): volume, surface, integral mean curvature, and Euler characteristic, of an underlying three-dimensional geometry. A bilinear combination of the measures is used as a (pseudo) metric with $++--$ signature, represented by a 4×4 matrix with unit entries on the counter-diagonal. Six different types of linear automorphisms are shown to leave the metric invariant. Their generators form a Lie algebra that can be grouped into two mutually commuting triples with non-trivial structure constants. We supplement these six isometric operations by a further 10 transformations that have a metamorphic (altering) effect on the underlying geometry. When grouped together, four different linear combinations of the metamorphic generators form a previously obtained third-rank tensor. This is shown to describe four different types of mutually commuting 'shifting' operations in fundamental measure space. The relevance for fundamental measures density functional theory is discussed briefly.

Keywords: density functional theory; fundamental measure theory

1. Introduction

Applying classical density functional theory (DFT) requires having an approximation for the Helmholtz free energy as a functional of the one-body density distribution(s) [1,2]. For the case of additive hard sphere mixtures, Rosenfeld's fundamental measures theory (FMT) [3] is an approximate DFT that unified several earlier liquid state theories, including the Percus–Yevick integral equation theory and scaled-particle theory, and encapsulates their results in a free energy functional. Several recent reviews give a detailed account of FMT and some of its extensions and modifications [4–6]. The theory was used to address a broad variety of interesting equilibrium phenomena, ranging from freezing to the capillary behavior of liquids. When compared with computer simulation data, theoretical results for, for example, density profiles and interfacial tension were typically found to be very reliable. FMT rests on building weighted densities via convolution with the bare density profile(s). The microscopic density profile $\rho_i(\mathbf{r})$ of species i gives the mean number of particles of species i in an infinitesimal volume element at given position $\mathbf{r}$ and hence carries dimensions of $(\text{length})^{-3}$. The weighted densities in FMT are smoothed versions of these 'real' density distributions. In Kierlik and Rosinberg's (KR) version [7] of FMT [3], there are four scalar weight functions for each hard sphere species. Rosenfeld's original approach that involves additional weight functions was shown to be equivalent to the KR version [8], and was later carried much further by Tarazona [9] and Cuesta *et al.* [10]. FMT has intimate connections to methods from integral geometry [11] via the Gauss–Bonnet theorem [12].

The weight functions in FMT are quantities with dimension of negative integer powers of length, ranging from $(\text{length})^{-3}$ to $(\text{length})^{0}$. A linear combination of pairs of weight functions that are convolved with each other is used to express the Mayer bond $f_{ij}(r)$, as a function of distance r. Recall that, for hard sphere mixtures, the Mayer bond equals $f_{ij}(r) = -1$ for distances $r < R_i + R_j$, i.e. when two spheres with radii R_i and R_i overlap, and it vanishes otherwise. Here the subscripts i, j label the different species. Originally proposed for hard spheres, this framework was sufficient to derive FMTs for models such as the Asakura–Oosawa colloid–polymer mixture [13] and the Widom–Rowlinson model [14]. However, the treatment of binary non-additive hard sphere mixtures required significant modification of the mathematical structure of FMT [15]. In particular, further weight functions were introduced in order to correctly model the deviation of the hard core interaction range between species i and j from the sum of their radii, $R_i + R_j$

The fact that this deviation is non-vanishing is the defining feature of non-additive hard sphere mixtures. The additional weight (or kernel) functions possess dimensionalities up to $(\text{length})^{-6}$. They can be grouped in a double-indexed tensorial form [15] and were shown to possess a remarkable group structure [16]. In very recent work, the FMT for non-additive hard spheres was applied successfully to bulk structure [17,18] and to interfacial phenomena [18].

Several features of the mathematics that underlies the FMT weight functions have emerged [15,16]. (i) The four different position-dependent fundamental measures (in the KR formulation) can be viewed as elements of an abstract four-dimensional vector space. (ii) Based on dimensional analysis, a (pseudo) metric can be defined that can be represented by a 4×4 matrix with unit entries on the counter-diagonal. All other entries in this matrix vanish. The metric has a $++--$ signature, hence it differs both from that of Minkowski spacetime in special relativity $(+---)$ and from that of four-dimensional Euclidian space $(++++)$. (iii) Operations that are common in linear algebra, i.e. matrix multiplication and more general contraction of tensor indices, possess a meaningful interpretation (see, for example, the shifting transform described in Ref. [16]). Here, all product operations are carried out in Fourier space and hence correspond to convolutions in real space.

In the present paper we explore the mathematical structure further by focusing on symmetry operations that leave the fundamental measure metric invariant. Our motivation comes from the fact that careful analysis of the symmetries is central to exploiting the properties of any (abstract) space. Typically, this tasks requires the identification of the linear automorphisms that leave the metric invariant. Recall that an automorphism is a bijective function that maps a space onto itself (i.e. both function value and argument are elements of the same space). Much structure can be revealed by considering infinitesimal versions, or generators, of the transformations. In a *Lie algebra* the commutator of any pair of generators can be represented as a linear combination of, again, the same generators. The coefficients of the linear combinations form the structure constants of the algebra.

In Euclidian space, the symmetry operations that leave the metric invariant are orthogonal transformations, or rotations. These possess three (six) independent generators in three (four) spatial dimensions. For the case of Minkowski spacetime with three spatial and one time-like dimension, there are three spatial rotations and three Lorentz transformations, or boosts, the latter coupling time and one of the spatial dimensions. The number of degrees of freedom, and hence the dimensionality of the group of isometries, is independent of the signature of the metric. However, the algebraic structure, as expressed by commutator relations between the respective (infinitesimal) generators of the transforms, differs for both cases. For the case of spacetime, the resulting mathematical structure is the Lorentz group. (One refers to the Poincaré group when four translations in the different spacetime directions are added.) Here we present in detail a similar analysis for the space of Minkowski functionals [11]. We describe four boosts and two rotations that leave the metric invariant. These are complemented by a further 10 operations that change the metric and that we refer to as metamorphic operations. We show that the spherical shifting operation of Ref. [16] is readily generalized to four different types of shifting, and that the corresponding generators can be expressed as linear combinations of the metamorphic generators.

The paper is organized as follows. In Section 2 the theory is laid out, including the description of inner boosts and inner rotations as isometric transformations (Section 2.2), of metamorphic operations (Section 2.3), and the relationship of Jeffrey's third-rank tensor [16] to the latter (Section 2.4). Concluding remarks are given in Section 3.

2. Transforming the fundamental measures

2.1. *Metric and inner scalar product*

We consider a four-dimensional real vector space with elements $\mathsf{u}=(u_0,u_1,u_2,u_3)$, where u depends on the three-dimensional argument $\mathbf{q}$ in Fourier space. The dependence on three-dimensional position $\mathbf{r}$ is then obtained by inverse Fourier transform, $(2\pi)^{-3}\int d\mathbf{q}e^{i\mathbf{q}\cdot\mathbf{r}}\mathsf{u}$. The vector components u_ν, with index $\nu=0,1,2,3$, are dimensional objects: u_ν possesses the dimension $(\text{length})^\nu$. Hence u_3 is a measure of volume, u_2 of surface, u_1 of mean curvature, and u_0 of Gaussian curvature. We let the u_ν take on arbitrary (real) values, and hence restrict ourselves not to cases where the measures describe an underlying geometrical body. The interpretation of the u_ν in terms of geometric measures is only intended to guide the intuition, the mathematics that we present in the following is based on formal arguments.

We use the metric represented by the matrix

$$\mathsf{M}=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix}, \tag{1}$$

hence a measure of squared 'length' of a vector u is given by $\mathsf{u}^t\cdot\mathsf{M}\cdot\mathsf{u}=2(\mathsf{u}_0\mathsf{u}_3+\mathsf{u}_1\mathsf{u}_2)$, where the

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superscript t indicates matrix transposition, and the dot indicates matrix multiplication. The scalar product between two vectors u and v is $\mathsf{u}^t \cdot \mathsf{M} \cdot \mathsf{v} = \mathsf{u}_0\mathsf{v}_3 + \mathsf{u}_1\mathsf{v}_2 + \mathsf{u}_2\mathsf{v}_1 + \mathsf{u}_3\mathsf{v}_0$. Clearly, this is symmetric upon interchange of the vectors, i.e. $\mathsf{u}^t \cdot \mathsf{M} \cdot \mathsf{v} = \mathsf{v}^t \cdot \mathsf{M} \cdot \mathsf{u}$. The eigenvalues of M are -1 and 1, both being doubly degenerate; hence M possesses $(++--)$ signature. As M is not positive definite (i.e. not all of its eigenvalues are positive), it can yield negative squared distances and hence constitutes not a metric in the strict sense, but one refers to a pseudo-metric. While it is entirely possible to discriminate between covariant and contravariant vectors and correspondingly introduce lower and upper indices, which can be interchanged by application of the metric, we will not do so in the following. The present paper is primarily concerned with second-rank tensors, and we find the (index-free) matrix notation to be simpler, and will primarily rely on this in what follows.

The hard sphere weight functions of FMT can serve as an example. These are functions of the squared wave number q^2 and the radius R of the hard spheres. The Fourier space expressions of the KR version of the weight functions are $w_0 = c + (qRs/2)$, $w_1 = (qRc + s)/(2q)$, $w_2 = 4\pi Rs/q$, $w_3 = 4\pi(s - qRc)/q^3$, where $s = \sin(qR)$ and $c = \cos(qR)$. The real space expression that corresponds, via inverse Fourier transform, to w_3 is a unit step function with range R, i.e. $\Theta(R - |\mathbf{r}|)$, where $\Theta(\cdot)$ is the Heaviside (step) function. Within our framework we view the w_ν as the four components of a vector w. By straightforward explicit algebra, one can show that $\mathsf{w}^t \cdot \mathsf{M} \cdot \mathsf{w}$ yields the Fourier transform of a unit step function with range $2R$, i.e. the expression for w_3 given above, but with R replaced by $2R$. Explicitly, this is $2(w_0w_3 + w_1w_2) = 4\pi[\sin(2qR) - 2qR\cos(2qR)]/q^3$. The significance in statistical physics stems from the fact this is the Fourier transform of the negative Mayer function of the pair potential of hard spheres of radius R. For a mixture, the additional species possesses weight functions v_ν of range R', given by the above expressions for w_ν, but with R being replaced by R'. It is straightforward to verify that $\mathsf{v} \cdot \mathsf{M} \cdot \mathsf{w} = 4\pi[\sin(q(R+R')) - q(R+R') \times\cos(q(R+R'))]/q^3$, which again is the above expression for the unit step, w_3, but with R replaced by the sum of the radii, $R + R'$. These identities constitute one of the central building blocks of KR's formulation of FMT. The generalization to non-additive mixtures [15] amounts to introducing 4×4 matrices that change the range of the weight functions w_ν. This shifting operation is discussed in detail in Ref. [16]. Below in Section 2.4 we give a further three such 'internal' shifting operations. We emphasize that all transformations that are considered here are of internal nature, i.e. act on the four-dimensional space of fundamental measures, as opposed to, for example, translations and rotations of the underlying three-dimensional Euclidian space, which we do not consider here.

The central aim of this paper is to formulate linear automorphisms that leave the metric (1) invariant. We refer to such operations as isometries on the space of fundamental measures. Hence one has to identify 4×4 transformation matrices A that obey

$$\mathsf{A}^t \cdot \mathsf{M} \cdot \mathsf{A} = \mathsf{A} \cdot \mathsf{M} \cdot \mathsf{A}^t = \mathsf{M}, \tag{2}$$

which implies that a vector u and its transform $\mathsf{A} \cdot \mathsf{u}$ possess the same squared modulus. This can be seen from $(\mathsf{A} \cdot \mathsf{u})^t \cdot \mathsf{M} \cdot (\mathsf{A} \cdot \mathsf{u}) = \mathsf{u}^t \cdot \mathsf{A}^t \cdot \mathsf{M} \cdot \mathsf{A} \cdot \mathsf{u} = \mathsf{u}^t \cdot \mathsf{M} \cdot \mathsf{u}$, where the last equality follows from (2). An alternative is obtained by multiplying (2) from the right by the inverse A^{-1}, and from the left by M, and observing that $\mathsf{M}^2 = \mathbf{1}$, where $\mathbf{1}$ is the 4×4 unit matrix. Hence

$$\mathsf{M} \cdot \mathsf{A}^t \cdot \mathsf{M} = \mathsf{A}^{-1}. \tag{3}$$

Note that this differs from the condition for orthogonal matrices, $\mathsf{A}^t = \mathsf{A}^{-1}$. While transposition can be viewed as mirroring the matrix elements on the diagonal, the operation on the left-hand side of (3) corresponds to mirroring the matrix elements on the counter-diagonal.

2.2. *Inner rotations and boosts as isometries*

Let us formulate the linear isometries, i.e. the automorphisms A that obey (2), by choosing appropriate generators X for each different type of transform, where X is a 4×4 matrix. The transformation matrices A are then obtained by (matrix) exponentiation. In order to see this, consider that the expression $\mathbf{1} + \mathsf{X}\,\mathrm{d}\tau$ can be viewed as an infinitesimal transform of differential magnitude $\mathrm{d}\tau$. A transform by a finite amount τ can then be obtained in the continuum limit of N-fold application of the infinitesimal transform, where each step is taken to be of magnitude τ/N. This amounts to $\lim_{N\to\infty}(\mathbf{1} + \tau\mathsf{X}/N)^N = \exp(\tau\mathsf{X}) \equiv \mathsf{A}$, where the result depends parametrically on τ and the form of A is specific to that of X. Here the exponential of a matrix is defined by its power series $\exp(\tau\mathsf{X}) = \sum_{m=0}^{\infty}(\tau^m/m!)\mathsf{X}^m$. In the following, we allow the transformation parameter τ to be dimensional, i.e. to carry a non-vanishing power of length scale.

In order to allow for meaningful matrix multiplication (as is necessary for matrix exponentiation) the generators need to possess matrix components with suitable dimensionalities. This implies that the product of the transformation parameter and

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a matrix entry, $\tau \mathsf{X}_{\mu\nu}$, where μ enumerates the rows and ν enumerates the columns, with both indices running from 0 to 3, must be of unit $(\text{length})^{\mu-\nu}$. Taking matrix powers then preserves the ordering of dimensions, i.e. the $\mu\nu$ component of the mth matrix power, $(\tau^m \mathsf{X}^m)_{\mu\nu}$, has the same dimensionality as $\tau \mathsf{X}_{\mu\nu}$ itself. Hence we can exponentiate the generators and obtain finite transforms. Besides letting τ be a dimensional object, in the following the only further dependence on length scale shall be via q^2, the squared argument in Fourier space. This corresponds to the (negative) Laplacian in the corresponding real three-dimensional space.

From general arguments for four-dimensional spaces, we expect the isometry group to be six-dimensional, i.e. to possess six linearly independent generators (see the cases of Euclidian space and Minkowski spacetime of special relativity mentioned above). Given a set of such generators, $\{\mathsf{X}_\alpha\}$, enumerated by index α, a general transform is obtained as $\exp(\sum_\alpha \tau_\alpha \mathsf{X}_\alpha)$, where τ_α is the magnitude of the αth transform. In principle, the different contributions to the total transform can be disentangled via the Baker–Campbell–Hausdorff formula. This requires knowledge of the algebraic group structure, which is encoded in commutator relations between the different generators, as laid out below.

Here we discriminate between four generators for boosts, B_α, and two generators for rotations, D_α. The subscript indicates the dimensionality; the $\mu\nu$ element of a given generator matrix possesses units of $(\text{length})^{\mu-\nu-\alpha}$. As laid out above, all elements along a given diagonal possess the same dimensionality; the dimensionality then decreases (increases) by one power of length scale when moving up (down) to the next diagonal. We call boosts those generators that satisfy $\mathsf{B}_\alpha \cdot \mathsf{B}_\alpha = q^{2\alpha}\mathbf{1}$. Generators of rotations are those that satisfy $\mathsf{D}_\alpha \cdot \mathsf{D}_\alpha = -q^{2\alpha}\mathbf{1}$. The generators are not unique; one can always build linear combinations to obtain a different formulation. Here we choose the following set of generators:

$$\mathsf{B}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \mathsf{B}_2 = \begin{pmatrix} 0 & 0 & -q^4 & 0 \\ 0 & 0 & 0 & q^4 \\ -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$
$$\mathsf{D}_2 = \begin{pmatrix} 0 & 0 & -q^4 & 0 \\ 0 & 0 & 0 & q^4 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}, \tag{4}$$

Table 1. Table for commutator relationships $[\mathsf{X}, \mathsf{Y}]/2$ for the generators of boosts, B_ν, and rotations, D_ν. X denotes a matrix of the leftmost column, Y one of the top row.

$[\mathsf{X}, \mathsf{Y}]/2$	B_0	B_2	D_2	$\mathsf{B}_{0'}$	B_1	D_1
B_0	0	D_2	B_2	0	0	0
B_2	$-\mathsf{D}_2$	0	$q^4\mathsf{B}_0$	0	0	0
D_2	$-\mathsf{B}_2$	$-q^4\mathsf{B}_0$	0	0	0	0
$\mathsf{B}_{0'}$	0	0	0	0	D_1	B_1
B_1	0	0	0	$-\mathsf{D}_1$	0	$q^2\mathsf{B}_{0'}$
D_1	0	0	0	$-\mathsf{B}_1$	$-q^2\mathsf{B}_{0'}$	0

$$\mathsf{B}_{0'} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \mathsf{B}_1 = \begin{pmatrix} 0 & -q^2 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & q^2 \\ 0 & 0 & 1 & 0 \end{pmatrix},$$
$$\mathsf{D}_1 = \begin{pmatrix} 0 & -q^2 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & q^2 \\ 0 & 0 & -1 & 0 \end{pmatrix}. \tag{5}$$

We have grouped the generators into two families, each consisting of two boosts and one rotation. The first consists of B_0, B_2, D_2 and is given in (4), and the second consists of $\mathsf{B}_{0'}$, B_1, D_1 and is given in (5). Both families form closed Lie algebras, constituted by the commutator relations

$$[\mathsf{B}_0, \mathsf{B}_2] = 2\mathsf{D}_2, \quad [\mathsf{B}_0, \mathsf{D}_2] = 2\mathsf{B}_2, \quad [\mathsf{B}_2, \mathsf{D}_2] = 2q^4\mathsf{B}_0, \tag{6}$$

$$[\mathsf{B}_{0'}, \mathsf{B}_1] = 2\mathsf{D}_1, \quad [\mathsf{B}_{0'}, \mathsf{D}_1] = 2\mathsf{B}_1, \quad [\mathsf{B}_1, \mathsf{D}_1] = 2q^2\mathsf{B}_{0'}, \tag{7}$$

where the commutator between two matrices X and Y is defined as $[\mathsf{X}, \mathsf{Y}] = \mathsf{X}\cdot\mathsf{Y} - \mathsf{Y}\cdot\mathsf{X}$. Members of different families commute; these are pairs of boosts: $[\mathsf{B}_0, \mathsf{B}_{0'}] = [\mathsf{B}_0, \mathsf{B}_1] = [\mathsf{B}_{0'}, \mathsf{B}_2] = [\mathsf{B}_1, \mathsf{B}_2] = 0$, the (only) pair of rotations: $[\mathsf{D}_1, \mathsf{D}_2] = 0$, and the four mixed pairs of a rotation and a boost: $[\mathsf{B}_0, \mathsf{D}_1] = [\mathsf{B}_1, \mathsf{D}_2] = [\mathsf{B}_2, \mathsf{D}_1] = [\mathsf{B}_{0'}, \mathsf{D}_2] = 0$. Table 1 gives an overview of the group structure in table format. All relationships can be obtained by straightforward matrix algebra. We give a full multiplication table in Table 2; anti-commutator relations are included for completeness. Note that, in each family, already the bare products (not commutators) give the result of the commutators up to a factor of 2. As a consequence, the anti-commutators within each sub-algebra vanish (see Table 1). Although commutators between members of different sub-algebras vanish, their plain

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products do not (see Table 2). The nine matrices that result from the products (as referred to in the off-diagonal blocks in Table 2) will be used below in order to define further, metamorphic, operations on the fundamental measures.

It is now straightforward to calculate finite transforms via exponentiation of the respective generators multiplied by its transformation parameter. Recall that the latter is a dimensional object, and that the most general finite transform is given by $\exp(\sum_\nu \tau_\nu \mathsf{X}_\nu)$, where τ_ν possess dimensions of $(\text{length})^\nu$. Here we give only the results for the case where all parameters bar one vanish. These are the following expressions for finite transformations corresponding to (4):

$$\exp(\tau_0\mathsf{B}_0) = \begin{pmatrix} e^{\tau_0} & 0 & 0 & 0 \\ 0 & e^{\tau_0} & 0 & 0 \\ 0 & 0 & e^{-\tau_0} & 0 \\ 0 & 0 & 0 & e^{-\tau_0} \end{pmatrix}, \tag{8}$$

$$\exp(\tau_2\mathsf{B}_2) = \begin{pmatrix} \cosh(\tau_2 q^2) & 0 & -q^2\sinh(\tau_2 q^2) & 0 \\ 0 & \cosh(\tau_2 q^2) & 0 & q^2\sinh(\tau_2 q^2) \\ -q^{-2}\sinh(\tau_2 q^2) & 0 & \cosh(\tau_2 q^2) & 0 \\ 0 & q^2\sinh(\tau_2 q^2) & 0 & \cosh(\tau_2 q^2) \end{pmatrix}, \tag{9}$$

$$\exp(\tau_2\mathsf{D}_2) = \begin{pmatrix} \cos(\tau_2 q^2) & 0 & -q^2\sin(\tau_2 q^2) & 0 \\ 0 & \cos(\tau_2 q^2) & 0 & q^2\sin(\tau_2 q^2) \\ q^{-2}\sin(\tau_2 q^2) & 0 & \cos(\tau_2 q^2) & 0 \\ 0 & -q^{-2}\sin(\tau_2 q^2) & 0 & \cos(\tau_2 q^2) \end{pmatrix}. \tag{10}$$

When applied to a vector u, (8) describes a multiplication of the components u_0 and u_1 by e^{τ_0}, and division of u_2 and u_3 by the same constant. Trivially, the (pseudo) squared modulus $2(u_1u_2+u_0u_3)$ is left unchanged. Equation (9) is reminiscent of a hyperbolic rotation, and (10) of an ordinary rotation. Note the difference in occurrence of the minus signs in (9) and (10).

For the generators (5) we obtain the following finite transforms:

$$\exp(\tau_0\mathsf{B}_{0'}) = \begin{pmatrix} e^{\tau_0} & 0 & 0 & 0 \\ 0 & e^{-\tau_0} & 0 & 0 \\ 0 & 0 & e^{\tau_0} & 0 \\ 0 & 0 & 0 & e^{-\tau_0} \end{pmatrix}, \tag{11}$$

$$\exp(\tau_1\mathsf{B}_1) = \begin{pmatrix} \cosh(\tau_1 q) & -q\sinh(\tau_1 q) & 0 & 0 \\ -q^{-1}\sinh(\tau_1 q) & \cosh(\tau_1 q) & 0 & 0 \\ 0 & 0 & \cosh(\tau_1 q) & q\sinh(\tau_1 q) \\ 0 & 0 & q^{-1}\sinh(\tau_1 q) & \cosh(\tau_1 q) \end{pmatrix}, \tag{12}$$

$$\exp(\tau_1\mathsf{D}_1) = \begin{pmatrix} \cos(\tau_1 q) & -q\sin(\tau_1 q) & 0 & 0 \\ q^{-1}\sin(\tau_1 q) & \cos(\tau_1 q) & 0 & 0 \\ 0 & 0 & \cos(\tau_1 q) & q\sin(\tau_1 q) \\ 0 & 0 & -q^{-1}\sin(\tau_1 q) & \cos(\tau_1 q) \end{pmatrix}. \tag{13}$$

Again, (11) induces a straightforward scaling of vector components, (12) is a hyperbolic rotation and (13) is an ordinary rotation. Recall that hyperbolic rotation can be viewed as Lorentz transforms (and *vice versa*).

As a summary, we have identified six real matrices $\mathsf{B}_0, \mathsf{B}_{0'}, \mathsf{B}_1, \mathsf{B}_2, \mathsf{D}_1$, and D_2, that posses the algebraic structure shown in Table 2. The general (real) linear group, i.e. that of all real 4×4 matrices, is $4^2=16$ dimensional. Besides the unit matrix, this leaves nine matrices to be considered. In the following we will use the matrices obtained as products of two isometric generators (see Table 2). We find it interesting to investigate their action, when viewed as infinitesimal transformations, on the space of fundamental measures. Clearly, they cannot generate isometries – we have exhausted these already. Hence we expect that the metric will not be conserved under the application of these further transformations, and we will henceforth refer to these transformations as metamorphic, as they change the underlying geometry in a fundamental way.

The difference between automorphism and metamorphisms is reflected in the symmetry properties of their generators. The isometric generators (4) and (5)

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Table 2. Left: Multiplication table $\mathsf{X}\cdot\mathsf{Y}$ for products of the generators of boosts and rotations. Right: Table of anti-commutator relationships $\{\mathsf{X},\mathsf{Y}\}/2$ for the generators of boosts and rotations. In both tables, X denotes a matrix of the leftmost column, Y one of the top row.

$\mathsf{X}\cdot\mathsf{Y}$	B_0	B_2	D_2	$\mathsf{B}_{0'}$	B_1	D_1
B_0	$\mathbf{1}$	D_2	B_2	P_0	H_1	F_1
B_2	$-\mathsf{D}_2$	$q^4\mathbf{1}$	$q^4\mathsf{B}_0$	H_2	F_3	P_3
D_2	$-\mathsf{B}_2$	$-q^4\mathsf{B}_0$	$-q^4\mathbf{1}$	F_2	$\mathsf{P}_{3'}$	$\mathsf{F}_{3'}$
$\mathsf{B}_{0'}$	P_0	H_2	F_2	$\mathbf{1}$	D_1	B_1
B_1	H_1	F_3	$\mathsf{P}_{3'}$	$-\mathsf{D}_1$	$q^2\mathbf{1}$	$q^2\mathsf{B}_{0'}$
D_1	F_1	P_3	$\mathsf{F}_{3'}$	$-\mathsf{B}_1$	$-q^2\mathsf{B}_{0'}$	$-q_2\mathbf{1}$

$\{\mathsf{X},\mathsf{Y}\}/2$	B_0	B_2	D_2	$\mathsf{B}_{0'}$	B_1	D_1
B_0	$\mathbf{1}$	0	0	P_0	H_1	F_1
B_2	0	$q^4\mathbf{1}$	0	H_2	F_3	P_3
D_2	0	0	$-q^4\mathbf{1}$	F_2	P_3	$\mathsf{F}_{3'}$
$\mathsf{B}_{0'}$	P_0	H_2	F_2	$\mathbf{1}$	0	0
B_1	H_1	F_3	$\mathsf{P}_{3'}$	0	$q^2\mathbf{1}$	0
D_1	F_1	P_3	$\mathsf{F}_{3'}$	0	0	$-q^2\mathbf{1}$

are anti-symmetric with respect to mirroring on the counter-diagonal, i.e. each generator X satisfies

$$\mathsf{M}\cdot\mathsf{X}^{\mathsf{t}}\cdot\mathsf{M} = -\mathsf{X}. \tag{14}$$

This can be seen by inserting the infinitesimal versions $\mathsf{A} = 1 + \mathsf{X}\,\mathrm{d}\tau$ and $\mathsf{A}^{-1} = 1 - \mathsf{X}\,\mathrm{d}\tau$ into (3). Note that the symmetry (14) leaves six parameters free, which is consistent with the dimensionality of the corresponding group of transformations (and hence the number of generators). Correspondingly, metamorphic generators are symmetric under mirroring on the counter-diagonal, i.e. they satisfy

$$\mathsf{M}\cdot\mathsf{X}^{\mathsf{t}}\cdot\mathsf{M} = \mathsf{X}, \tag{15}$$

as we will see in the following. Note that the symmetry (15) leaves 10 parameters undetermined.

2.3. *Metamorphic transformations*

We start by giving the explicit expressions for the matrices that we choose as generators of the metamorphic operations. As above, the index ν of a given generator X_ν indicates its dimensionality. Explicit expressions for the nine different generators are as follows:

$$\mathsf{F}_1 = \begin{pmatrix} 0 & -q^2 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -q^2 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathsf{F}_2 = \begin{pmatrix} 0 & 0 & -q^4 & 0 \\ 0 & 0 & 0 & -q^4 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix},$$

$$\mathsf{F}_3 = \begin{pmatrix} 0 & 0 & 0 & -q^6 \\ 0 & 0 & q^4 & 0 \\ 0 & q^2 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \tag{16}$$

$$\mathsf{H}_1 = \begin{pmatrix} 0 & -q^2 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -q^2 \\ 0 & 0 & -1 & 0 \end{pmatrix},$$

$$\mathsf{H}_2 = \begin{pmatrix} 0 & 0 & -q^4 & 0 \\ 0 & 0 & 0 & -q^4 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix},$$

$$\mathsf{F}_{3'} = \begin{pmatrix} 0 & 0 & 0 & -q^6 \\ 0 & 0 & -q^4 & 0 \\ 0 & -q^2 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \tag{17}$$

$$\mathsf{P}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \mathsf{P}_3 = \begin{pmatrix} 0 & 0 & 0 & -q^6 \\ 0 & 0 & -q^4 & 0 \\ 0 & q^2 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix},$$

$$\mathsf{P}_{3'} = \begin{pmatrix} 0 & 0 & 0 & -q^6 \\ 0 & 0 & q^4 & 0 \\ 0 & -q^2 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \tag{18}$$

Here we have grouped the nine generators into three Abelian subgroups, given in (16), (17), and (18), respectively. Any pair of matrices from one of these subgroups satisfies $[\mathsf{X}_\mu, \mathsf{Y}_\nu] = 0$. In general, the commutator between matrices from different subgroups is (up to a minus sign) a multiple of q^2 times an isometric

Table 3. Commutator relations $[\mathsf{X}, \mathsf{Y}]/2$ for the generators of metamorphic and isometric operations. X denotes a matrix of the leftmost column, Y one of the top row. The upper block of nine rows give the commutator between pairs of metamorphic generators. The lower block with six rows gives the commutators between one isometric and one metamorphic generator.

$[\mathsf{X}, \mathsf{Y}]/2$	F_1	F_2	F_3	H_1	H_2	$\mathsf{F}_{3'}$	P_0	P_3	$\mathsf{P}_{3'}$
F_1	0	0	0	$q^2\mathsf{B}_{0'}$	0	$-q^2\mathsf{B}_2$	$-\mathsf{B}_1$	$-q^2\mathsf{D}_2$	0
F_2	0	0	0	0	$q^4\mathsf{B}_0$	$-q^4\mathsf{B}_1$	$-\mathsf{B}_2$	0	$-q^4\mathsf{D}_1$
F_3	0	0	0	$-q^2\mathsf{D}_2$	$-q^4\mathsf{D}_1$	0	0	$-q^6\mathsf{B}_{0'}$	$-q^6\mathsf{B}_0$
H_1	$-q^2\mathsf{B}_{0'}$	0	$q^2\mathsf{D}_2$	0	0	0	$-\mathsf{D}_1$	0	$q^2\mathsf{B}_2$
H_2	0	$-q^4\mathsf{B}_0$	$q^4\mathsf{D}_1$	0	0	0	$-\mathsf{D}_2$	$q^4\mathsf{B}_1$	0
$\mathsf{F}_{3'}$	$q^2\mathsf{B}_2$	$q^4\mathsf{B}_1$	0	0	0	0	0	$-q^6\mathsf{B}_0$	$-q^6\mathsf{B}_{0'}$
P_0	B_1	B_2	0	D_1	D_2	0	0	0	0
P_3	$q^2\mathsf{D}_2$	0	$q^6\mathsf{B}_{0'}$	0	$-q^4\mathsf{B}_1$	$q^6\mathsf{B}_0$	0	0	0
$\mathsf{P}_{3'}$	0	$q^4\mathsf{D}_1$	$q^6\mathsf{B}_0$	$-q^2\mathsf{B}_2$	0	$q^6\mathsf{B}_{0'}$	0	0	0
B_0	0	H_2	P'_3	0	F_2	P_3	0	F'_3	F_3
B_2	$-\mathsf{F}'_3$	$-\mathsf{P}_0q^4$	0	$-\mathsf{P}'_3$	0	$-\mathsf{F}_1q^4$	$-\mathsf{F}_2$	0	$-\mathsf{H}_1q^4$
D_2	$-\mathsf{P}_3$	0	H_1q^4	$-\mathsf{F}_3$	P_0q^4	0	$-\mathsf{H}_2$	F_1q^4	0
B'_0	H_1	0	P_3	F_1	0	P'_3	0	F_3	F'_3
B_1	$-\mathsf{P}_0q^2$	$-\mathsf{F}'_3$	0	0	$-\mathsf{P}_3$	$-\mathsf{F}_2q^2$	$-\mathsf{F}_1$	$-\mathsf{H}_2q^2$	0
D_1	0	$-\mathsf{P}'_3$	H_2q^2	P_0q^2	$-\mathsf{F}_3$	0	$-\mathsf{H}_1$	0	F_2q^2

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generator. Some of these pairs commute. The complete algebra of commutator relationships between the metamorphic generators is summarized in Table 3. Remarkably, the commutator between any two pairs of these matrices either vanishes or is a multiple of one of the isometric generators of Section 2.2. Inevitably, some of the quite compact structure of the previous subsection is lost, due to the sheer number of possible pairs. Nevertheless, note that, indeed, members of the same triplet $\{\mathsf{F}_1, \mathsf{F}_2, \mathsf{F}_3\}$, $\{\mathsf{H}_1, \mathsf{H}_2, \mathsf{F}_{3'}\}$ and $\{\mathsf{P}_0, \mathsf{P}_3, \mathsf{P}_{3'}\}$ commute with each other. We defer multiplication and anti-commutator tables to the appendix. Clearly, the nine generators are not unique. In the following section we will relate a previously obtained third-rank tensor to a linear combination of these generators. Before doing so we give explicit expressions for the finite metamorphic transformations.

For the first triplet of generators, these are

$$\exp(\tau_1\mathsf{F}_1) = \begin{pmatrix} \cos(\tau_1 q) & -q\sin(\tau_1 q) & 0 & 0 \\ q^{-1}\sin(\tau_1 q) & \cos(\tau_1 q) & 0 & 0 \\ 0 & 0 & \cos(\tau_1 q) & -q\sin(\tau_1 q) \\ 0 & 0 & q^{-1}\sin(\tau_1 q) & \cos(\tau_1 q) \end{pmatrix}, \tag{19}$$

$$\exp(\tau_2\mathsf{F}_2) = \begin{pmatrix} \cos(\tau_2 q^2) & 0 & -q^2\sin(\tau_2 q^2) & 0 \\ 0 & \cos(\tau_2 q^2) & 0 & -q^2\sin(\tau_2 q^2) \\ q^{-2}\sin(\tau_2 q^2) & 0 & \cos(\tau_2 q^2) & 0 \\ 0 & q^{-2}\sin(\tau_2 q^2) & 0 & \cos(\tau_2 q^2) \end{pmatrix}, \tag{20}$$

$$\exp(\tau_3\mathsf{F}_3) = \begin{pmatrix} \cosh(\tau_3 q^3) & 0 & 0 & -q^3\sinh(\tau_3 q^3) \\ 0 & \cosh(\tau_3 q^3) & q\sinh(\tau_3 q^3) & 0 \\ 0 & q^{-1}\sinh(\tau_3 q^3) & \cosh(\tau_3 q^3) & 0 \\ -q^{-3}\sinh(\tau_3 q^3) & 0 & 0 & \cosh(\tau_3 q^3) \end{pmatrix}. \tag{21}$$

The second group of finite metamorphic operations is

$$\exp(\tau_1 \mathsf{H}_1) = \begin{pmatrix} \cosh(\tau_1 q) & -q\sinh(\tau_1 q) & 0 & 0 \\ -q^{-1}\sinh(\tau_1 q) & \cosh(\tau_1 q) & 0 & 0 \\ 0 & 0 & \cosh(\tau_1 q) & -q\sinh(\tau_1 q) \\ 0 & 0 & -q^{-1}\sinh(\tau_1 q) & \cosh(\tau_1 q) \end{pmatrix}, \tag{22}$$

$$\exp(\tau_2 \mathsf{H}_2) = \begin{pmatrix} \cosh(\tau_2 q^2) & 0 & -q^2\sinh(\tau_2 q^2) & 0 \\ 0 & \cosh(\tau_2 q^2) & 0 & -q^2\sinh(\tau_2 q^2) \\ -q^{-2}\sinh(\tau_2 q^2) & 0 & \cosh(\tau_2 q^2) & 0 \\ 0 & -q^{-2}\sinh(\tau_2 q^2) & 0 & \cosh(\tau_2 q^2) \end{pmatrix}, \tag{23}$$

$$\exp(\tau_3 \mathsf{F}_{3'}) = \begin{pmatrix} \cosh(\tau_3 q^3) & 0 & 0 & -q^3\sinh(\tau_3 q^3) \\ 0 & \cosh(\tau_3 q^3) & -q\sinh(\tau_3 q^3) & 0 \\ 0 & -q^{-1}\sinh(\tau_3 q^3) & \cosh(\tau_3 q^3) & 0 \\ -q^{-3}\sinh(\tau_3 q^3) & 0 & 0 & \cosh(\tau_3 q^3) \end{pmatrix}. \tag{24}$$

And the third group of finite metamorphic operations is

$$\exp(\tau_0 \mathsf{P}_0) = \begin{pmatrix} e^{\tau_0} & 0 & 0 & 0 \\ 0 & e^{-\tau_0} & 0 & 0 \\ 0 & 0 & e^{-\tau_0} & 0 \\ 0 & 0 & 0 & e^{\tau_0} \end{pmatrix}, \tag{25}$$

$$\exp(\tau_3 \mathsf{P}_3) = \begin{pmatrix} \cos(\tau_3 q^3) & 0 & 0 & -q^3\sin(\tau_3 q^3) \\ 0 & \cos(\tau_3 q^3) & -q\sin(\tau_3 q^3) & 0 \\ 0 & q^{-1}\sin(\tau_3 q^3) & \cos(\tau_3 q^3) & 0 \\ q^{-3}\sin(\tau_3 q^3) & 0 & 0 & \cos(\tau_3 q^3) \end{pmatrix}, \tag{26}$$

$$\exp(\tau_3 \mathsf{P}_{3'}) = \begin{pmatrix} \cos(\tau_3 q^3) & 0 & 0 & -q^3\sin(\tau_3 q^3) \\ 0 & \cos(\tau_3 q^3) & q\sin(\tau_3 q^3) & 0 \\ 0 & -q^{-1}\sin(\tau_3 q^3) & \cos(\tau_3 q^3) & 0 \\ q^{-3}\sin(\tau_3 q^3) & 0 & 0 & \cos(\tau_3 q^3) \end{pmatrix}. \tag{27}$$

2.4. *Morphological shifting and Jeffrey's third-rank tensor*

Based on the mathematical structure of Ref. [15], in Ref. [16] a 'shifting operation' was investigated that changes the radius of a sphere by a given amount R. These operations build a one-dimensional Abelian group. The generator of the group, T_1 (referred to as $\tilde{\mathbf{G}}$ in [16]), generates the kernel K_R of Ref. [15] upon exponentiation, $\mathsf{K}_R = \exp(RG) \equiv \exp(R\mathsf{T}_1)$. The significance of the matrix K_R lies (i) in the algebraic structure: $\mathsf{K}_R \cdot \mathsf{K}_{R'} = \mathsf{K}_{R'} \cdot \mathsf{K}_R = \mathsf{K}_{R+R'}$, and (ii) in the fact that it contains the expressions for the four Kierlik–Rosinberg weight functions explicitly.

Jeffrey's third-rank tensor as a central object of Ref. [16] is given by the following set of four matrices:

$$\mathsf{T}_0 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\mathsf{T}_1 = \begin{pmatrix} 0 & 0 & 0 & -q^4/(8\pi) \\ 1 & 0 & -q^2/(4\pi) & 0 \\ 0 & 8\pi & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \tag{28}$$

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Table 4. Tables for commutator relationships [X, Y]/2 and for products X·Y for the generators of T_μ transformations.

[X, Y]/2	T_0	T_1	T_2	T_3
T_0	0	0	0	0
T_1	0	0	0	0
T_2	0	0	0	0
T_3	0	0	0	0

X·Y	T_0	T_1	T_2	T_3
T_0	T_0	T_1	T_2	T_3
T_1	T_1	$8\pi\,\mathsf{T}_2$	$-\frac{q^2}{4\pi}\mathsf{T}_1+\mathsf{T}_3$	$-\frac{q^4}{8\pi}\mathsf{T}_0$
T_2	T_2	$-\frac{q^2}{4\pi}\mathsf{T}_1+\mathsf{T}_3$	$-\frac{q^4}{64\pi^2}\mathsf{T}_0-\frac{q^2}{4\pi}\mathsf{T}_2$	$-\frac{q^4}{64\pi^2}\mathsf{T}_1$
T_3	T_3	$-\frac{q^4}{8\pi}\mathsf{T}_0$	$-\frac{q^4}{64\pi^2}\mathsf{T}_1$	$-\frac{q^6}{32\pi^2}\mathsf{T}_0-\frac{q^4}{8\pi}\mathsf{T}_2$

$$\mathsf{T}_2=\begin{pmatrix}0 & 0 & -q^4/(64\pi^2) & 0\\ 0 & -q^2/(4\pi) & 0 & -q^4/(64\pi^2)\\ 1 & 0 & -q^2/(4\pi) & 0\\ 0 & 1 & 0 & 0\end{pmatrix}, \tag{29}$$

$$\mathsf{T}_3=\begin{pmatrix}0 & -q^4/(8\pi) & 0 & -q^6/(32\pi^2)\\ 0 & 0 & -q^4/(64\pi^2) & 0\\ 0 & 0 & 0 & -q^4/(8\pi)\\ 1 & 0 & 0 & 0\end{pmatrix}, \tag{30}$$

where $\mathsf{T}_2=\mathsf{T}_1\cdot\mathsf{T}_1/(8\pi)$, $\mathsf{T}_3=-q^4(\mathsf{T}_1)^{-1}/(8\pi)$, and $(\mathsf{T}_1)^{-1}$ is the inverse of T_1. All T_μ commute with each other, $[\mathsf{T}_\mu,\mathsf{T}_\nu]=0$. Finite transformations are obtained via exponentiation as $\exp(\chi_\nu\,\mathsf{T}_\nu)$, where χ_ν is the transformation parameter. The finite transforms commute with each other and they obey $\exp(\sum_\nu\chi_\nu\mathsf{T}_\nu)\exp(\sum_\nu\chi'_\nu\mathsf{T}_\nu)=\exp(\sum_\nu\chi'_\nu\mathsf{T}_\nu)\exp(\sum_\nu\chi_\nu\mathsf{T}_\nu)=\exp(\sum_\nu(\chi_\nu+\chi'_\nu)\mathsf{T}_\nu)$ (Table 4).

Explicitly, the matrices for finite transformations are given by

where we have used the short-hand notation $s=\sin(q\chi_1)$, $c=\cos(q\chi_1)$, $g=\exp(-q^2\chi_2/(8\pi))$, $C=\cos(q^3\chi_3/(8\pi))$, $S=\sin(q^3\chi_3/(8\pi))$. Equation (32) describes K_R when setting $\chi_1=R$.

It is an interesting application of the theory outlined in the previous section to try to express the T_ν as linear combinations of the metamorphic generators. This can indeed be done with a little algebra, yielding the result

$$\mathsf{T}_0=\mathbf{1}, \tag{35}$$

$$\mathsf{T}_1=\frac{\mathsf{F}_1-\mathsf{H}_1}{2}+\frac{2\pi(\mathsf{P}_3-\mathsf{P}_{3'}+\mathsf{F}_3-\mathsf{F}_{3'})}{q^2}+\frac{3\mathsf{P}_3-\mathsf{P}_{3'}-\mathsf{F}_3+3\mathsf{F}_{3'}}{32\pi q^2}, \tag{36}$$

$$\mathsf{T}_2=\frac{q^2(\mathsf{P}_0-\mathbf{1})}{8\pi}+\frac{\mathsf{F}_2-\mathsf{H}_2}{2}+\frac{\mathsf{F}_2+\mathsf{H}_2}{128\pi^2}, \tag{37}$$

$$\exp(\chi_0\mathsf{T}_0)=\begin{pmatrix}e^{\chi_0} & 0 & 0 & 0\\ 0 & e^{\chi_0} & 0 & 0\\ 0 & 0 & e^{\chi_0} & 0\\ 0 & 0 & 0 & e^{\chi_0}\end{pmatrix}, \tag{31}$$

$$\exp(\chi_1\mathsf{T}_1)=\begin{pmatrix}c+qs\chi_1/2 & (cq^2\chi_1-qs)/2 & -q^3s\chi_1/(16\pi) & (cq^4\chi_1-3sq^3)/(16\pi)\\ (s+cq\chi_1)/(2q) & c-(qs\chi_1)/2 & -(3sq+cq^2\chi_1)/(16\pi) & -q^3s\chi_1/(16\pi)\\ 4\pi s\chi_1/q & 4\pi(s+cq\chi_1)/q & c-(qs\chi_1)/2 & (cq^2\chi_1-sq)/2\\ 4\pi(s-cq\chi_1)/q^3 & 4\pi s\chi_1/q & (s+cq\chi_1)/(2q) & c+(qs\chi_1)/2\end{pmatrix}, \tag{32}$$

$$\exp(\chi_2\mathsf{T}_2)=\begin{pmatrix}g+(gq^2\chi_2)/(8\pi) & 0 & -gq^4\chi_2/(64\pi^2) & 0\\ 0 & g-gq^2\chi_2/(8\pi) & 0 & -gq^4\chi_2/(64\pi^2)\\ g\chi_2 & 0 & g-(gq^2\chi_2)/(8\pi) & 0\\ 0 & g\chi_2 & 0 & g+(gq^2\chi_2)/(8\pi)\end{pmatrix}, \tag{33}$$

$$\exp(\chi_3\mathsf{T}_3)=\begin{pmatrix}C-(q^3S\chi_3)/(16\pi) & -(8\pi qS+Cq^4\chi_3)/(16\pi) & q^5S\chi_3/(128\pi^2) & -(24\pi q^3S+Cq^6\chi_3)/(128\pi^2)\\ S/(2q)-(Cq^2\chi_3)/(16\pi) & C+(q^3S\chi_3)/(16\pi) & (-24\pi qS+Cq^4\chi_3)/(128\pi^2) & q^5S\chi_3/(128\pi^2)\\ -qS\chi_3/2 & 4\pi S/q-(Cq^2\chi_3)/2 & C+(q^3S\chi_3)/(16\pi) & -(8\pi qS+Cq^4\chi_3)/(16\pi)\\ 4\pi S/q^3+C\chi_3/2 & -qS\chi_3/2 & S/(2q)-Cq^2\chi_3/(16\pi) & C-(q^3S\chi_3)/(16\pi)\end{pmatrix}, \tag{34}$$

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$$\mathsf{T}_3 = \frac{q^2(\mathsf{F}_1 + \mathsf{H}_1)}{16\pi} + \frac{\mathsf{P}_3 + \mathsf{P}_{3'} - \mathsf{F}_3 - \mathsf{F}_{3'}}{4} + \frac{3\mathsf{P}_3 + \mathsf{P}_{3'} + \mathsf{F}_3 + 3\mathsf{F}_{3'}}{256\pi^2}. \quad (38)$$

3. Conclusions

In conclusion we have presented a framework for manipulating four-dimensional vector fields u that are defined on an underlying three-dimensional Euclidian space. In real space, the relevant operations are application of the Laplace operator and building convolutions. These operations turn into multiplication by $-q^2$ and the product operation in Fourier space. We have analysed the symmetries that leave the metric (1) for the four-vectors invariant. This leads to operations that either leave the metric invariant (isometric transforms) or that change the metric and hence the morphology that the four vectors describe (metamorphic operations). We have kept the nature of the four vectors general, i.e. these can taken on arbitrary real values. This includes specific geometries (such as spheres considered in Ref. [16]), but is more general. Whether the transformations presented here help to construct novel DFT approximations is an interesting question for future work. It would also be interesting to explore possible connections to the integral geometric framework of Hansen-Goos and Mecke [19].

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Appendix A. Mixed commutator relations of isometric and metamorphic generators

Here we give further details about the algebra of commutator relations. Table A1 gives a multiplication table between metamorphic generators as well as anti-commutator relationships. Table A2 gives products and anti-commutators between mixed pairs of an isometric and a morphometric generator.

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Table A1. Top: Multiplication table $X{\cdot}Y$ for products of the generators of metamorphic operations. Bottom: Anti-commutator relations $\{X, Y\}/2 = (X{\cdot}Y + Y{\cdot}X)/2$ for generators of metamorphic transformations. X denotes a matrix of the centermost column, Y one of the top row.

$X{\cdot}Y$	F_1	F_2	F_3	H_1	H_2	$F_{3'}$	P_0	P_3	$P_{3'}$
F_1	$-q^2\mathbf{1}$	$-F_3$	q^2F_2	$q^2B_{0'}$	$-P_{3'}$	$-q^2B_2$	$-B_1$	$-q^2D_2$	q^2H_2
F_2	$-F_3$	$-q^4\mathbf{1}$	q^4F_1	$-P_3$	q^4B_0	$-q^4B_1$	$-B_2$	q^4H_1	$-q^4D_1$
F_3	q^2F_2	q^4F_1	$q^6\mathbf{1}$	$-q^2D_2$	$-q^4D_1$	q^6P_0	$F_{3'}$	$-q^6B_{0'}$	$-q^6B_0$
H_1	$-q^2B_{0'}$	$-P_3$	q^2D_2	$q^2\mathbf{1}$	$-F_{3'}$	$-q^2H_2$	$-D_1$	$-q^2F_2$	q^2B_2
H_2	$-P_{3'}$	$-q^4B_0$	q^4D_1	$-F_{3'}$	$q^4\mathbf{1}$	$-q^4H_1$	$-D_2$	q^4B_1	$-q^4F_1$
$F_{3'}$	q^2B_2	q^4B_1	q^6P_0	$-q^2H_2$	$-q^4H_1$	$q^6\mathbf{1}$	F_3	$-q^6B_0$	$-q^6B_{0'}$
P_0	B_1	B_2	$F_{3'}$	D_1	D_2	F_3	$\mathbf{1}$	$P_{3'}$	P_3
P_3	q^2D_2	q^4H_1	$q^6B_{0'}$	$-q^2F_2$	$-q^4B_1$	q^6B_0	$P_{3'}$	$-q^6\mathbf{1}$	$-q^6P_0$
$P_{3'}$	q^2H_2	q^4D_1	q^6B_0	$-q^2B_2$	$-q^4F_1$	$q^6B_{0'}$	P_3	$-q^6P_0$	$-q^6\mathbf{1}$
$\{X, Y\}/2$									
F_1	$-q^2\mathbf{1}$	$-F_3$	q^2F_2	0	$-P_{3'}$	0	0	0	q^2H_2
F_2	$-F_3$	$-q^4\mathbf{1}$	q^4F_1	$-P_3$	0	0	0	q^4H_1	0
F_3	q^2F_2	q^4F_1	$q^6\mathbf{1}$	0	0	q^6P_0	$F_{3'}$	0	0
H_1	0	$-P_3$	0	$q^2\mathbf{1}$	$-F_{3'}$	$-q^2H_2$	0	$-q^2F_2$	0
H_2	$-P_{3'}$	0	0	$-F_{3'}$	$q^4\mathbf{1}$	$-q^4H_1$	0	0	$-q^4F_1$
$F_{3'}$	0	0	q^6P_0	$-q^2H_2$	$-q^4H_1$	$q^6\mathbf{1}$	F_3	0	0
P_0	0	0	$F_{3'}$	0	0	F_3	$\mathbf{1}$	$P_{3'}$	P_3
P_3	0	q^4H_1	0	$-q^2F_2$	0	0	$P_{3'}$	$-q^6\mathbf{1}$	$-q^6P_0$
$P_{3'}$	q^2H_2	0	0	0	$-q^4F_1$	0	P_3	$-q^6P_0$	$-q^6\mathbf{1}$

Table A2. Top: Multiplication table between generators of isomorphisms, X, and generators of metamorphisms, Y. Middle: Reverse product order, $Y{\cdot}X$. Bottom: Anti-commutator relationships for the same pairs.

$X{\cdot}Y$	F_1	F_2	F_3	H_1	H_2	F'_3	P_0	P_3	P'_3
B_0	D_1	H_2	P'_3	B_1	F_2	P_3	B'_0	F'_3	F_3
B_2	$-F'_3$	$-P_0q^4$	B_1q^4	$-P'_3$	B'_0q^4	$-F_1q^4$	$-F_2$	D_1q^4	$-H_1q^4$
D_2	$-P_3$	$-B'_0q^4$	H_1q^4	$-F_3$	P_0q^4	$-D_1q^4$	$-H_2$	F_1q^4	$-B_1q^4$
B'_0	H_1	D_2	P_3	F_1	B_2	P'_3	B_0	F_3	F'_3
B_1	$-P_0q^2$	$-F'_3$	B_2q^2	B_0q^2	$-P_3$	$-F_2q^2$	$-F_1$	$-H_2q^2$	D_2q^2
D_1	$-B_0q^2$	$-P'_3$	H_2q^2	P_0q^2	$-F_3$	$-D_2q^2$	$-H_1$	$-B_2q^2$	F_2q^2
$Y{\cdot}X$									
B_0	D_1	$-H_2$	$-P'_3$	B_1	$-F_2$	$-P_3$	B'_0	$-F'_3$	$-F_3$
B_2	F'_3	P_0q^4	B_1q^4	P'_3	B'_0q^4	F_1q^4	F_2	D_1q^4	H_1q^4
D_2	P_3	$-B'_0q^4$	$-H_1q^4$	F_3	$-P_0q^4$	$-D_1q^4$	H_2	$-F_1q^4$	$-B_1q^4$
B'_0	$-H_1$	D_2	$-P_3$	$-F_1$	B_2	$-P'_3$	B_0	$-F_3$	$-F'_3$
B_1	P_0q^2	F'_3	B_2q^2	B_0q^2	P_3	F_2q^2	F_1	H_2q^2	D_2q^2
D_1	$-B_0q^2$	P'_3	$-H_2q^2$	$-P_0q^2$	F_3	$-D_2q^2$	H_1	$-B_2q^2$	$-F_2q^2$
$\{X,Y\}/2$									
B_0	D_1	0	0	B_1	0	0	B'_0	0	0
B_2	0	0	B_1q^4	0	B'_0q^4	0	0	D_1q^4	0
D_2	0	$-B'_0q^4$	0	0	0	$-D_1q^4$	0	0	$-B_1q^4$
B'_0	0	D_2	0	0	B_2	0	B_0	0	0
B_1	0	0	B_2q^2	B_0q^2	0	0	0	0	D_2q^2
D_1	$-B_0q^2$	0	0	0	0	$-D_2q^2$	0	$-B_2q^2$	0

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