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Peel or coat spheres by convolution, repeatedly

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A convolution transformation is presented that maps the four fundamental measures (Minkowski functionals) of a three-dimensional sphere to those of a sphere with a different radius. It is shown that the set of all these transformations, parametrized by the induced change in radius, forms an Abelian (commutative) group and hence constitutes a flexible framework for the manipulation of spheres. The corresponding one-dimensional case is laid out and the relationship to fundamental measure density functional theory is discussed briefly. © *2007 American Institute of Physics.* [DOI: 10.1063/1.2816259]

I. INTRODUCTION

The geometry of spheres is at the heart of fundamental measure theory (FMT), the density functional theory[1,2] that Rosenfeld established in his seminal 1989 paper[3] and that has become of widespread use in the study of inhomogeneous hard sphere fluids and related models. The theory possesses roots in scaled-particle theory and Percus-Yevick theory, as well as in one-dimensional exact solutions.[4,5] Its relation to geometry arises through the use of Minkowski functionals[6,7] (fundamental measures) and the Gauss-Bonnet theorem. The relevant geometrical objects are local weight functions that are characteristic of the volume, surface, integral mean curvature, and Euler characteristic of the sphere. In FMT they are used to build weighted densities via convolution with the bare one-body density profiles of the system. Rosenfeld's original theory relies on scalar and vectorial weight functions; in Kierlik and Rosinberg's equivalent reformulation solely scalar weight functions appear.[8,9] Much light was shed on the significance of the weight functions by Lafuente and Cuesta's lattice version of FMT that applies to discrete lattice gases: Deep connections to zero-dimensional cavities were established and exploited to construct DFTs for such models. The continuum version of FMT has seen several extensions[10,11] as well as generalizations to further models, such as that by Tutschka and Kahl to adhesive hard spheres.[12] The recent FMT for non-additive hard spheres[13] has introduced major alterations of the structure of the functional as compared to the Rosenfeld functional for additive hard sphere mixtures:[3] The way the weight functions relate to the Mayer bond differs significantly from the additive case in that two convolutions (rather than a single one) are used to express the Mayer bond of the cross interaction between particles of unlike species. For hard core particles, the Mayer bond equals -1 if two particles overlap and is zero otherwise. Hence for hard spheres it represents a sphere when the distance vector between the two particle centers is taken as the spatial coordinate.

The present paper delves deeper into the spherical geometry involved. It is shown that the weight functions of Ref. 13 form flexible tools to express and manipulate the geometry of three-dimensional spheres via convolution, in particular, to decrease (peel) or increase (coat) the size of a given sphere. These operations can be repeated (chained) and inverted, and hence possess an (Abelian) group structure. This is established by considering the four measures of a sphere as an element of an abstract four-dimensional vector space on which the operations act as linear transformations. Besides the intrinsic interest in the geometry involved, this formalized framework might constitute a valuable resource for future developments in FMT.

This paper is organized as follows. In Sec. II a summary of the geometrical weight functions as introduced in Refs. 3, 8, and 9 is given, and it is shown that the set of weight functions of a sphere with a given radius can be viewed as an element of a vector space. In Sec. III linear transformations that act on elements of this vector space are introduced, and shown to possess an Abelian (commutative) group structure. The central result is that the matrices defined via Eqs. (27) and (28) fulfill the remarkable set of properties (18)–(23). Furthermore a third-rank tensor representation is given and discussed in detail. Section 4 presents a similar analysis in one dimension, as is relevant for the geometry of line segments in one dimension (which relates to a one-dimensional hard core model[14]), and we conclude in Sec. V.

II. VECTORS OF WEIGHT FUNCTIONS AND AN INNER PRODUCT

We consider "weight" functions $w_\nu(r,R)$ that express the geometry of a sphere of radius R, where $r=|\mathbf{r}|$ and $\mathbf{r}$ is the three-dimensional space coordinate; the index ν labels the type of weight function and indicates that $w_\nu(r,R)$ possesses the dimension $(\text{length})^{\nu-3}$. The weight functions in the (fully scalar) Kierlik-Rosinberg form[8,9] are given by

$$w_3(r,R) = \text{sgn}(R)\Theta(|R|-r), \tag{1}$$

$$w_2(r,R) = \delta(|R|-r), \tag{2}$$

$$w_1(r,R) = \text{sgn}(R)\,\delta'(|R|-r)/(8\pi), \tag{3}$$

$$w_0(r,R) = \delta'(|R|-r)/(2\pi r) - \delta''(|R|-r)/(8\pi), \tag{4}$$

where sgn(·) is the sign function, Θ(·) is the Heaviside (unit step) function, δ(·) is the Dirac distribution, and the prime denotes the derivative with respect to the argument. In Fourier space the weight functions are obtained as $\tilde{w}_\nu(q,R)=4\pi\int_0^\infty dr w_\nu(r,R)\sin(qr)r/q$ and are given explicitly as

$$\tilde{w}_3(q,R) = 4\pi[\sin(qR) - qR\cos(qR)]/q^3, \tag{5}$$

$$\tilde{w}_2(q,R) = 4\pi R\sin(qR)/q, \tag{6}$$

$$\tilde{w}_1(q,R) = [qR\cos(qR) + \sin(qR)]/(2q), \tag{7}$$

$$\tilde{w}_0(q,R) = \cos(qR) + [qR\sin(qR)/2]. \tag{8}$$

The fundamental measures ξ_ν are related to the weight functions through $\xi_\nu=\int d\mathbf{r} w_\nu(|\mathbf{r}|,R) =\tilde{w}(q\to 0,R)$, and correspond to the volume, surface, integral mean curvature, and Euler characteristic of a sphere, given by $\xi_3=4\pi R^3/3$, $\xi_2=4\pi R^2$, $\xi_1=R$, and $\xi_0=1$, respectively. Here and in the following we allow R to be negative. While this seems unusual for a single sphere, as considered here, it has a very natural interpretation of peeling a layer of thickness R from a sphere of a larger radius; such situations will be considered below.

We treat a set of four weight functions as a vector, either in real space or in Fourier space, defined as[15]

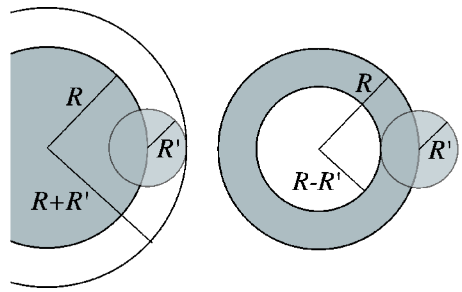

FIG. 1. Illustration of the length scales relevant for the convolution of two spheres. The sphere of radius R (dark gray) is convolved with a sphere of radius R' (light gray) to form a sphere of radius $R+R'$ (white, left) or of radius $R-R'$ (white, right).

$$\mathbf{w}_R = \begin{pmatrix} w_0(r,R) \\ w_1(r,R) \\ w_2(r,R) \\ w_3(r,R) \end{pmatrix}, \quad \tilde{\mathbf{w}}_R = \begin{pmatrix} \tilde{w}_0(q,R) \\ \tilde{w}_1(q,R) \\ \tilde{w}_2(q,R) \\ \tilde{w}_3(q,R) \end{pmatrix}, \tag{9}$$

respectively. The operations that define the vector space are trivial: Two vectors are added componentwise and a vector is multiplied by a (possibly complex) scalar by multiplying each component of the vector with the scalar. In the tensor notation used below we refer to $\tilde{\mathbf{w}}_R$ as $\tilde{w}_\mu(q,R)$, where $\mu=0,1,2,3$ enumerates the components.

We next seek to define an inner product. As the weight functions are dimensional quantities, the Cartesian dot product, represented by the 4×4 identity matrix $\mathbf{1}$, is inappropriate as it attempts to sum over terms of differing dimensionality when used as $\tilde{\mathbf{w}}_R^{\mathsf{t}}\mathbf{1}\tilde{\mathbf{w}}_{R'}$; the superscript t indicates transposition, i.e., $\tilde{\mathbf{w}}_{R'}^{\mathsf{t}}$ is a row vector. This dimensionality problem does not occur when defining an inner product using

$$\mathbf{M} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \tag{10}$$

which we refer to as $M_{\mu\nu}$ (componentwise equal to its inverse $M^{\mu\nu}$) in tensor notation; indices of tensors are taken to run from 0 to 3, as do those of vectors. $M_{\mu\nu}$ possesses $(++--)$ signature. Recall that the signature is the set of signs of all eigenvalues; hence the present case is distinct both from the Euclidean case $(++++)$ and from the Minkowski case $(+---)$ of special relativity.

The inner product of two vectors $\tilde{\mathbf{w}}_R$ and $\tilde{\mathbf{w}}_{R'}$ is obtained as the contraction

$$\tilde{\mathbf{w}}_R^{\mathsf{t}}\mathbf{M}\tilde{\mathbf{w}}_{R'} = \tilde{w}_\mu(q,R)M^{\mu\nu}w_\nu(q,R') = \tilde{w}_3(q,R+R'), \tag{11}$$

where (here and throughout) we use the Einstein sum convention, such that summation is implied over (Greek) indices that appear twice, as an upper and as a lower index, from 0 to 3. The second equality in (11) can be obtained with straightforward algebra using trigonometric identities from (5)–(8) and represents the celebrated "deconvolution of the hard sphere Mayer bond"[3,8] when read from right to left; this can be viewed as a special case of the Gauss-Bonnet theorem.[16,17] Note that the Mayer bond, which is crucial for the low-density expansion of the properties of a fluid, for particles interacting with a hard sphere pair potential of range $R+R'$ equals $-\Theta(R+R'-|\mathbf{r}|)$, where $\mathbf{r}$ is the distance vector between the two particle centers; this in turn is equal (up to a minus sign) to $w_3(|\mathbf{r}|,R+R')$, the measure characteristic of the sphere volume. Figure 1 displays an illustration of the geometrical situation. The relationship of the four fundamental measures of the two initial spheres (with radius R and R') to one of the measures (volume) of the resulting sphere (with radius $R+R'$) provides the *a posteriori* motivation for the use of the metric (10). Note that we carry out products of weight functions only in Fourier space; the corresponding operation in real space is the (three-dimensional) convolution. We use the Fourier representation for mere notational convenience in order to address the underlying geometric (real space) problem.

The remainder of the paper seeks to remedy an apparent loss: Only one of the four measures of a sphere of radius $R+R'$, namely, $w_3(r,R+R')$, is obtained via (11). How the remaining three measures, corresponding to the surface, integral mean curvature, and Euler characteristic, Eqs. (6)–(8) respectively, can be restored will be addressed in the following section.

Before doing so, let us explicitly introduce a dual vector

$$\tilde{\mathbf{w}}_R^{\dagger}\mathbf{M} = (\tilde{w}_3(q,R),\tilde{w}_2(q,R),\tilde{w}_1(q,R),\tilde{w}_0(q,R)), \tag{12}$$

that satisfies $\tilde{w}^{\mu}(q,R)=M^{\mu\nu}\tilde{w}_{\nu}(q,R)$. Note the descending order of subscripts which contrasts that of vectors, Eq. (9); those possess ascending order of indices. The difference is a necessary consequence of the structure of (10) and for each component $\mu=0,1,2,3$ the identity $\tilde{w}^{\mu}(q,R)=\tilde{w}_{3-\mu}(q,R)$ holds.

III. THE SPHERICAL SHIFTING GROUP

In order to introduce (linear) transformations between vectors of weight functions, we consider the following matrix:

$$\mathbf{K}_R = \begin{pmatrix} w_0(r,R) & w_{-1}(r,R) & w_{-2}(r,R) & w_{-3}(r,R) \\ w_1(r,R) & w_0^{\dagger}(r,R) & w_{-1}^{\dagger}(r,R) & w_{-2}(r,R) \\ w_2(r,R) & w_1^{\dagger}(r,R) & w_0^{\dagger}(r,R) & w_{-1}(r,R) \\ w_3(r,R) & w_2(r,R) & w_1(r,R) & w_0(r,R) \end{pmatrix}, \tag{13}$$

where † is used to discriminate an element from the corresponding element without this symbol. The elements in the first column and those in the last row are defined through (1)–(4); the remaining ones[18] are given by

$$\begin{aligned} w_1^{\dagger}(r,R) &= \mathrm{sgn}(R)\,\delta'(|R|-r), \\ w_0^{\dagger}(r,R) &= \delta''(|R|-r)/(8\pi), \\ w_{-1}^{\dagger}(r,R) &= \mathrm{sgn}(R)\,\delta^{(3)}(|R|-r)/(64\pi^2), \\ w_{-1}(r,R) &= \mathrm{sgn}(R)[\delta''(|R|-r)/(2\pi r) - \delta^{(3)}(|R|-r)/(8\pi)], \\ w_{-2}(r,R) &= \delta^{(3)}(|R|-r)/(16\pi^2 r) - \delta^{(4)}(|R|-r)/(64\pi^2), \\ w_{-3}(r,R) &= \mathrm{sgn}(R)[-\delta^{(4)}(|R|-r)/(8\pi^2 r) + \delta^{(5)}(|R|-r)/(64\pi^2)], \end{aligned} \tag{14}$$

with the derivatives of the Dirac distribution $\delta^{(\gamma)}(x)=d^{\gamma}\delta(x)/dx^{\gamma}$ for $\gamma=3,4,5$. In Fourier space we have

$$\widetilde{\mathbf{K}}_R = \begin{pmatrix} \widetilde{w}_0(q,R) & \widetilde{w}_{-1}(q,R) & \widetilde{w}_{-2}(q,R) & \widetilde{w}_{-3}(q,R) \\ \widetilde{w}_1(q,R) & \widetilde{w}_0^\dagger(q,R) & \widetilde{w}_{-1}^\dagger(q,R) & \widetilde{w}_{-2}(q,R) \\ \widetilde{w}_2(q,R) & \widetilde{w}_1^\dagger(q,R) & \widetilde{w}_0^\dagger(q,R) & \widetilde{w}_{-1}(q,R) \\ \widetilde{w}_3(q,R) & \widetilde{w}_2(q,R) & \widetilde{w}_1(q,R) & \widetilde{w}_0(q,R) \end{pmatrix}, \tag{15}$$

which we refer to as $\widetilde{K}_\mu{}^\nu(q,R)$ in tensor notation, where μ selects a row and ν selects a column. Note that the index-raised $\widetilde{K}^{\mu\nu}(q,R)=M^{\mu\lambda}\widetilde{K}_\lambda{}^\nu(q,R)$ and index-lowered forms $\widetilde{K}_{\mu\nu}(q,R)=\widetilde{K}_\mu{}^\lambda(q,R)M_{\lambda\nu}$ are symmetric under exchange of indices: $\widetilde{K}_{\mu\nu}(q,R)=\widetilde{K}_{\nu\mu}(q,R)$ and $\widetilde{K}^{\mu\nu}(q,R)=\widetilde{K}^{\nu\mu}(q,R)$; the latter operation corresponds to matrix transposition, and the two equalities reflect the mirror symmetry of (15) against the counterdiagonal.[19]

The Fourier representation of (14) reads

$$\begin{aligned} \widetilde{w}_1^\dagger(q,R) &= 4\pi[qR\cos(qR)+\sin(qR)]/q, \\ \widetilde{w}_0^\dagger(q,R) &= \cos(qR)-[qR\sin(qR)/2], \\ \widetilde{w}_{-1}^\dagger(q,R) &= -[q^2R\cos(qR)+3q\sin(qR)]/(16\pi), \\ \widetilde{w}_{-1}(q,R) &= [q^2R\cos(qR)-q\sin(qR)]/2, \\ \widetilde{w}_{-2}(q,R) &= -q^3R\sin(qR)/(16\pi), \\ \widetilde{w}_{-3}(q,R) &= [q^4R\cos(qR)-3q^3\sin(qR)]/(16\pi), \end{aligned} \tag{16}$$

and summarizing, $\widetilde{\mathbf{K}}_R$ is given explicitly by

$$\begin{pmatrix} c+(qRs/2) & (q^2Rc-qs)/2 & -q^3Rs/(16\pi) & (q^4Rc-3q^3s)/(16\pi) \\ (qRc+s)/(2q) & c-(qRs/2) & -(q^2Rc+3qs)/(16\pi) & -q^3Rs/(16\pi) \\ 4\pi Rs/q & 4\pi(qRc+s)/q & c-(qRs/2) & (q^2Rc-qs)/2 \\ 4\pi(s-qRc)/q^3 & 4\pi Rs/q & (qRc+s)/(2q) & c+(qRs/2) \end{pmatrix}, \tag{17}$$

where $s=\sin(qR)$ and $c=\cos(qR)$.

There is a variety of relationships that possess remarkable simplicity given the considerable complexity of (17). Among those relationships are the following:

$$\widetilde{\mathbf{K}}_R\widetilde{\mathbf{K}}_{R'} = \widetilde{\mathbf{K}}_{R'}\widetilde{\mathbf{K}}_R = \widetilde{\mathbf{K}}_{R+R'}, \tag{18}$$

$$\widetilde{\mathbf{K}}_R\widetilde{\mathbf{K}}_{-R'} = \widetilde{\mathbf{K}}_{-R'}\widetilde{\mathbf{K}}_R = \widetilde{\mathbf{K}}_{R-R'}, \tag{19}$$

$$(\widetilde{\mathbf{K}}_R)^{-1} = \widetilde{\mathbf{K}}_{-R} \quad \text{or } (\widetilde{\mathbf{K}}_R\widetilde{\mathbf{K}}_{-R} = \mathbf{1}), \tag{20}$$

$$\widetilde{\mathbf{K}}_0 = \mathbf{1}, \tag{21}$$

$$(\widetilde{\mathbf{K}}_R)^n = \widetilde{\mathbf{K}}_{nR}, \tag{22}$$

$$\det \tilde{\mathbf{K}}_R = 1, \tag{23}$$

all of which can be obtained with straightforward algebra using trigonometric identities. These relationships establish that $\{\tilde{\mathbf{K}}_R, R \in \mathbb{R}\}$ forms an Abelian group with respect to matrix multiplication. The group is isomorphic (via the radius R) to the real numbers under addition. As the first column of $\tilde{\mathbf{K}}_R$ equals the vector of weight functions $\tilde{\mathbf{w}}_R$, i.e., $\tilde{w}_\mu(q,R) = \tilde{K}_\mu{}^1(q,R)$, the above properties imply operations on vectors; the essence can be condensed into

$$\tilde{\mathbf{K}}_{R'}\tilde{\mathbf{w}}_R = \tilde{\mathbf{w}}_{R+R'} \quad (\text{and } \tilde{\mathbf{K}}_{-R'}\tilde{\mathbf{w}}_R = \tilde{\mathbf{w}}_{R-R'}), \tag{24}$$

which corresponds to the real space form $\mathbf{K}_{R'} * \mathbf{w}_R = \mathbf{w}_{R+R'}$, where $*$ denotes the three-dimensional convolution. This constitutes the operation that we had sought: Starting from a sphere of radius R and represented by its four measures contained in $\mathbf{w}_R$, we transform to a sphere of radius $R+R'$ (coating by a layer with thickness R') or $R-R'$ (peeling by a shell with thickness R'). The new sphere is again represented by its four measures. This represents a shift (rather than a stretch) of the radius and hence one could term the set of the transformations $\tilde{\mathbf{K}}_R$ the *spherical shifting group*. When viewed componentwise as four independent equalities, (24) augments the deconvolution equation (11) to the full set of four geometric measures; the first one being identical to the deconvolution equation. Note, however, that the more general case is constituted by (18). Taking the risk of obfuscating terminology, one could refer to (18) as the *deconvolution of the fundamental measures*. The remarkable qualitative feature that discriminates this relationship from the deconvolution of the volume weight (11) is that the complete matrix of weight functions is recovered without any loss. Note that this structure has not been obvious at all from the outset. Further deconvolving the left hand side of (11) into shorter ranged weight functions could have potentially led to an increased level of complexity (as measured by an increase in tensor rank and/or by the appearance of additional weight functions). This is not the case. Given a set of radii R_i that fulfill $R = \Sigma_{i=1}^n R_i$, we can use (11) and repeatedly apply (18) in order to express the volume weight as

$$\tilde{w}_3(q,R) = \tilde{\mathbf{w}}_{R_1}^{\mathrm{t}} \mathbf{M} \tilde{\mathbf{K}}_{R_2}, \ldots, \tilde{\mathbf{K}}_{R_{n-1}} \tilde{\mathbf{w}}_{R_n}. \tag{25}$$

This can be viewed as the 30-element of the slightly more compact "onion" relationship

$$\tilde{\mathbf{K}}_R = \tilde{\mathbf{K}}_{R_1} \tilde{\mathbf{K}}_{R_2}, \ldots, \tilde{\mathbf{K}}_{R_n}, \tag{26}$$

which follows by inference from (18). For completeness a discussion of the eigensystem of $\tilde{\mathbf{K}}_R$ is given in the Appendix.

We next seek an infinitesimal shifting operation, $\tilde{\mathbf{G}}$, such that

$$\tilde{\mathbf{K}}_R = \exp(R\tilde{\mathbf{G}}), \tag{27}$$

where the argument of the exponential is the product of the scalar R and a matrix $\tilde{\mathbf{G}}$ that acts as a generator for the group; the exponential of a matrix $\mathbf{A}$ is defined via its power series, $\exp(\mathbf{A}) = \Sigma_{m=0}^{\infty} \mathbf{A}^m / n!$ with $\mathbf{A}^0 = \mathbf{1}$. Via expanding (17) in R and isolating the linear contribution one finds that

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

which has an obvious real space interpretation via the correspondence of multiplication by $-q^2$ in Fourier space with applying the Laplace operator ∇^2 in direct space. The matrix $\tilde{\mathbf{G}}$ possesses a variety of interesting properties among which are $\det \tilde{\mathbf{G}} = q^4$ and that it obeys the simple quartic equation

$$(\tilde{\mathbf{G}} + q^2\mathbf{1})^2 = 0. \tag{29}$$

The latter can be used to obtain by inference a recurrence relation $\tilde{\mathbf{G}}^{2n} = (\mathbf{1} - n(\mathbf{1} + \tilde{\mathbf{G}}^2/q^2))(iq)^{2n}$ that helps to verify the relationship of $\tilde{\mathbf{G}}$ to $\tilde{\mathbf{K}}_R$, Eq. (27), explicitly.

There is yet more structure to be revealed by introducing a third-rank tensor

$$\tilde{\mathbf{T}} = (\mathbf{M}, \mathbf{M}\tilde{\mathbf{G}}, \mathbf{M}\tilde{\mathbf{G}}^2/(8\pi), \mathbf{M}(2q^2\tilde{\mathbf{G}} + \tilde{\mathbf{G}}^3)/(8\pi))$$
$$= \left(\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 8\pi & 0 & 0 \\ 1 & 0 & \frac{-q^2}{4\pi} & 0 \\ 0 & 0 & 0 & \frac{-q^4}{8\pi} \end{pmatrix}, \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & \frac{-q^2}{4\pi} & 0 \\ 0 & \frac{-q^2}{4\pi} & 0 & \frac{-q^4}{64\pi^2} \\ 0 & 0 & \frac{-q^4}{64\pi^2} & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{-q^4}{8\pi} \\ 0 & 0 & \frac{-q^4}{64\pi^2} & 0 \\ 0 & \frac{-q^4}{8\pi} & 0 & \frac{-q^6}{32\pi^2} \end{pmatrix} \right), \tag{30}$$

where the components of $\tilde{\mathbf{T}}$ are $\tilde{T}^{\mu\nu\tau}(q)$ with indexing such that the first index (μ) selects a 4×4-matrix from the 4-tuple of matrices in (30), the second index (ν) selects a row, and the third index (τ) selects a column from this 4×4-matrix; again all indices run from 0 to 3. Having made this explicit, note though that $\tilde{\mathbf{T}}$ is fully symmetric under permutations of all its three indices in the form with all indices raised: $\tilde{T}^{\mu\nu\tau}(q) = \tilde{T}^{\nu\mu\tau}(q) = \tilde{T}^{\mu\tau\nu}(q) = \tilde{T}^{\tau\nu\mu}(q)$, as well as with all indices lowered: $\tilde{T}_{\mu\nu\tau}(q) = \tilde{T}_{\nu\mu\tau}(q) = \tilde{T}_{\mu\tau\nu}(q) = \tilde{T}_{\tau\nu\mu}(q)$, where $\tilde{T}_{\mu\nu\tau}(q) = M_{\mu\mu'}M_{\nu\nu'}M_{\tau\tau'}\tilde{T}^{\mu'\nu'\tau'}(q)$. More generally, the symmetry applies to exchange between pairs of either lower or upper indices. Alternatively to (30) all nonvanishing elements can be defined via $\tilde{T}^{003} = \tilde{T}^{012} = 1$, $\tilde{T}^{111} = 8\pi$, $\tilde{T}^{122} = -q^2/(4\pi)$, $\tilde{T}^{133} = -q^4/(8\pi)$, $\tilde{T}^{223} = -q^4/(64\pi^2)$, and $\tilde{T}^{333} = -q^6/(32\pi^2)$ and using the symmetry under pairwise exchange of indices. Figure 2 illustrates the symmetry properties of $\tilde{\mathbf{T}}$ graphically. Note furthermore that $\tilde{\mathbf{T}}$ is *free* of the length scale R. It hence cannot be associated with a given sphere and thus constitutes, in this sense, a more general object than $\tilde{\mathbf{K}}_R$.

Several important properties follow. One can use $\tilde{\mathbf{T}}$ to express $\tilde{\mathbf{K}}_R$ via contraction with a vector of weight functions

$$\tilde{\mathbf{K}}_R = \mathbf{M}\tilde{\mathbf{T}}\tilde{\mathbf{w}}_R, \tag{31}$$

which is in tensor notation $\tilde{K}_\mu{}^\nu(q,R) = \tilde{T}_\mu{}^{\nu\tau}(q)\tilde{w}_\tau(q,R)$. Remarkably only the four "original" Kierlik-Rosinberg weight functions (1)–(4) appear on the right hand side of this identity, but not the additional ones (14) that define $\tilde{\mathbf{K}}_R$ in (15); these are "generated" in (31) by the action of $\tilde{\mathbf{T}}$. It follows that we can rewrite (24) as[20]

$$\tilde{\mathbf{w}}_{R+R'} = (\mathbf{M}\tilde{\mathbf{T}}\tilde{\mathbf{w}}_R)\tilde{\mathbf{w}}_{R'}, \tag{32}$$

corresponding to the real space form $\mathbf{w}_{R+R'} = (\mathbf{M}\mathbf{T}\mathbf{w}_R) * \mathbf{w}_{\mathbf{R}'}$, where $\mathbf{T}$ is obtained from $\tilde{\mathbf{T}}$ via replacing q^{2n} with $(-1)^n\nabla^{2n}$ for $n=1,2,3$. In tensor notation (32) reads as

$$\tilde{w}_\mu(q,R+R') = \tilde{T}_\mu{}^{\nu\tau}(q)\tilde{w}_\nu(q,R')\tilde{w}_\tau(q,R), \tag{33}$$

where $\tilde{T}_\mu{}^{\nu\tau}(q) = M_{\mu\lambda}\tilde{T}^{\lambda\nu\tau}(q)$. Yet more explicitly, componentwise,

$$\tilde{w}_3(q,R+R') = \tilde{\mathbf{w}}_R^{\mathrm{t}}\mathbf{M}\tilde{\mathbf{w}}_{R'} = \tilde{w}_0(R)\tilde{w}_3(R') + \tilde{w}_1(R)\tilde{w}_2(R') + \tilde{w}_2(R)\tilde{w}_1(R') + \tilde{w}_3(R)\tilde{w}_0(R') \tag{34}$$

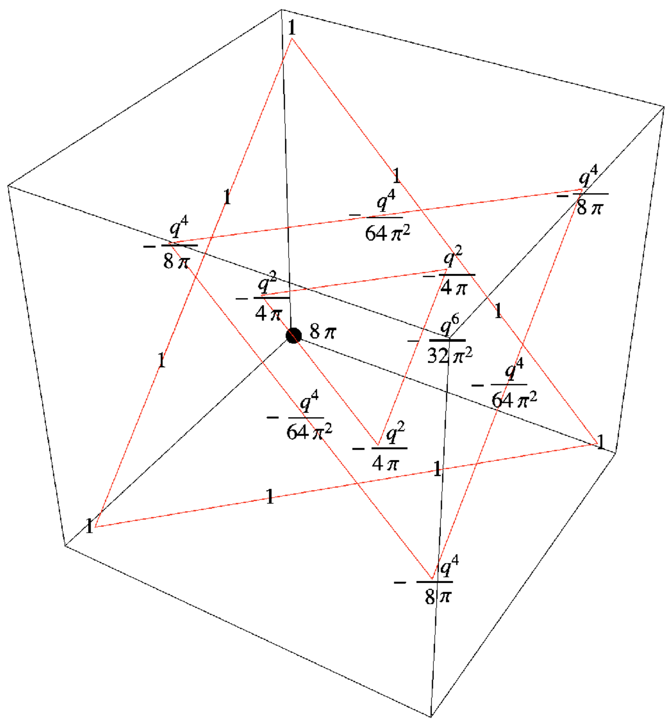

FIG. 2. (Color online) Illustration of $\widetilde{\mathbf{T}}$. The three spatial dimensions correspond to the three indices; the origin (black dot) corresponds to 000. The triangles mark entries with common dimensionalities (8π lies in the plane spanned by the 1 entries). Note the symmetry under exchange of any two axes and under rotations by 120° around the space diagonal.

$$\widetilde{w}_2(q,R+R') = \widetilde{\mathbf{w}}_R^{\mathrm{t}}\mathbf{M}\widetilde{\mathbf{G}}\widetilde{\mathbf{w}}_{R'} = \widetilde{w}_0(R)\widetilde{w}_2(R') + 8\pi\widetilde{w}_1(R)\widetilde{w}_1(R') + \widetilde{w}_2(R)\widetilde{w}_0(R') - \frac{q^2}{4\pi}\widetilde{w}_2(R)\widetilde{w}_2(R') - \frac{q^4}{8\pi}\widetilde{w}_3(R)\widetilde{w}_3(R') \tag{35}$$

$$\widetilde{w}_1(q,R+R') = \widetilde{\mathbf{w}}_R^{\mathrm{t}}\mathbf{M}\widetilde{\mathbf{G}}^2\widetilde{\mathbf{w}}_{R'}/(8\pi) = \widetilde{w}_0(R)\widetilde{w}_1(R') + \widetilde{w}_1(R)\widetilde{w}_0(R') - \frac{q^2}{4\pi}(\widetilde{w}_1(R)\widetilde{w}_2(R') + \widetilde{w}_2(R)\widetilde{w}_1(R')) - \frac{q^4}{64\pi^2}(\widetilde{w}_2(R)\widetilde{w}_3(R') + \widetilde{w}_3(R)\widetilde{w}_2(R')) \tag{36}$$

$$\begin{aligned}\widetilde{w}_0(q,R+R') &= \widetilde{\mathbf{w}}_R^{\mathrm{t}}\mathbf{M}(\widetilde{\mathbf{G}}^3 + 2q^2\widetilde{\mathbf{G}})\widetilde{\mathbf{w}}_{R'}/(8\pi)\\ &= \widetilde{w}_0(R)\widetilde{w}_0(R') - \frac{q^4}{8\pi}\left(\widetilde{w}_1(R)\widetilde{w}_3(R') + \frac{1}{8\pi}\widetilde{w}_2(R)\widetilde{w}_2(R') + \widetilde{w}_3(R)\widetilde{w}_1(R')\right)\\ &\quad - \frac{q^6}{32\pi^2}\widetilde{w}_3(R)\widetilde{w}_3(R'),\end{aligned} \tag{37}$$

where the argument q was omitted in $\widetilde{w}_\mu(q,R)$ on the right hand sides to unclutter the notation. This presents the generalization of the deconvolution of the volume measure (11) to *all four* fundamental measures, $\mu=0,1,2,3$ [the case $\mu=3$ being recovered in (34)], where in contrast to (24) *two* vectors of weight functions (of radii R and R') are mapped onto one vector of weight functions (of radius $R+R'$). An important distinction between (34) on the one hand and (35)–(37)

on the other hand is that the tensor $\widetilde{\mathbf{T}}$ contributes (even) powers of q on the right hand sides of (35)–(37), whereas this is not the case for the volume deconvolution (34). The remarkable fact is that $\widetilde{\mathbf{T}}$ is free of the possible length scales R and R' and hence expressions including these radii are algebraically separated in the general tensor product (33). Given the requirement that $\widetilde{\mathbf{T}}$ is free of both R and R' its form is uniquely determined.

From the above we conclude that a group structure is imposed on $\{\widetilde{\mathbf{w}}_R, R \in \mathbb{R}\}$, with $(\mathbf{M}\widetilde{\mathbf{T}}\cdot)\cdot$ as the multiplication operation. The inverse of $\widetilde{\mathbf{w}}_R$ is $\widetilde{\mathbf{w}}_{-R}$, the neutral element is $\widetilde{\mathbf{w}}_0 = (1,0,0,0)^{\mathrm{t}}$, and again the group is commutative.

Furthermore, an operation akin to a triple vector product is

$$\widetilde{w}_3(q,R+R'+R'') = ((\widetilde{\mathbf{T}}\widetilde{\mathbf{w}}_R)\widetilde{\mathbf{w}}_{R'})\widetilde{\mathbf{w}}_{R''} = \widetilde{T}^{\mu\nu\tau}(q)\widetilde{w}_\mu(q,R)\widetilde{w}_\nu(q,R')\widetilde{w}_\tau(q,R''), \tag{38}$$

and again chaining is possible, similar to (26),

$$\widetilde{\mathbf{w}}_R = (\mathbf{M}\widetilde{\mathbf{T}}\widetilde{\mathbf{w}}_{R_1})(\mathbf{M}\widetilde{\mathbf{T}}\widetilde{\mathbf{w}}_{R_2}), \ldots, (\mathbf{M}\widetilde{\mathbf{T}}\widetilde{\mathbf{w}}_{R_{n-1}})\widetilde{\mathbf{w}}_{R_n}, \tag{39}$$

$$\widetilde{w}_{\nu_n}(q,R) = \widetilde{w}^{\nu_1}(q,R_n)\prod_{i=1}^{n-1}\widetilde{T}_{\nu_i}{}^{\nu_{i+1}\tau_i}\widetilde{w}_{\tau_i}(q,R_i), \tag{40}$$

where $R=\Sigma_{i=1}^{n}R_i$.

IV. THE ONE-DIMENSIONAL CASE

In the following we investigate the geometry of line segments of length $2R$ (intervals) on a one-dimensional line. This shares many features with the three-dimensional considerations above, but offers the advantage of reduced complexity of the analytical expressions involved. We keep the discussion to a minimum, as the structure is very similar to that in three dimensions. The relevant weight functions are

$$w_1(x,R) = \mathrm{sgn}(R)\Theta(|R|-|x|), \tag{41}$$

$$w_0(x,R) = \delta(|R|-|x|)/2, \tag{42}$$

$$w_{-1}(x,R) = \mathrm{sgn}(R)\delta'(|R|-|x|)/4, \tag{43}$$

which in Fourier space, where $\widetilde{w}_\nu(q,R) = \int_{-\infty}^{\infty}dx\,\exp(iqx)w_\nu(x,R)$, corresponds to

$$\widetilde{w}_1(q,R) = 2\sin(qR)/q, \tag{44}$$

$$\widetilde{w}_0(q,R) = \cos(qR), \tag{45}$$

$$\widetilde{w}_{-1}(q,R) = -q\sin(qR)/2. \tag{46}$$

We define vectors of weight functions as

$$\mathbf{w}_R = (w_0(r,R), w_1(r,R)) = (\delta(R-|x|)/2, \Theta(R-|x|)), \tag{47}$$

$$\widetilde{\mathbf{w}}_R = (\widetilde{w}_0(q,R), \widetilde{w}_1(q,R)) = (\cos(qR), 2\sin(qR)/q). \tag{48}$$

Using the matrix

$$\mathbf{M} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{49}$$

one can express the inner product of two vectors of weight functions

$$\tilde{\mathbf{w}}_R^{\mathrm{t}} \mathbf{M} \tilde{\mathbf{w}}_{R'} = \tilde{w}_\mu(q,R) M^{\mu\nu} \tilde{w}_\nu(q,R') \tag{50}$$

$$= \tilde{w}_0(q,R)\tilde{w}_1(q,R') + \tilde{w}_0(q,R')\tilde{w}_1(q,R) \tag{51}$$

$$= w_1(q,R+R'), \tag{52}$$

where sums run over 0 and 1, and, similar to the three-dimensional case, the last equality represents the deconvolution of the "volume" weight (of dimension length). The (linear) shifting transformation is represented by

$$\mathbf{K}_R = \begin{pmatrix} w_0(x,R) & w_{-1}(x,R) \\ w_1(x,R) & w_0(x,R) \end{pmatrix} \tag{53}$$

$$= \begin{pmatrix} \delta(|x|-R)/2 & \delta'(|x|-R)/4 \\ \Theta(|x|-R) & \delta(|x|-R)/2 \end{pmatrix}, \tag{54}$$

and in Fourier space by

$$\tilde{\mathbf{K}}_R = \begin{pmatrix} \tilde{w}_0(q,R) & \tilde{w}_{-1}(q,R) \\ \tilde{w}_1(q,R) & \tilde{w}_0(q,R) \end{pmatrix} \tag{55}$$

$$= \begin{pmatrix} \cos(qR) & -q\sin(qR)/2 \\ 2\sin(qR)/q & \cos(qR) \end{pmatrix}. \tag{56}$$

This can be rewritten using a generator $\tilde{\mathbf{G}}$ such that

$$\tilde{\mathbf{K}}_R = \exp(2R\tilde{\mathbf{G}}), \tag{57}$$

$$\tilde{\mathbf{G}} = \begin{pmatrix} 0 & -q^2/4 \\ 1 & 0 \end{pmatrix}, \tag{58}$$

with $\det \tilde{\mathbf{G}} = q^2$. The third-rank tensor is given by

$$\tilde{\mathbf{T}} = (\mathbf{M}, \mathbf{M}\tilde{\mathbf{G}}) \tag{59}$$

$$= \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & -q^2/4 \end{pmatrix} \right). \tag{60}$$

Most of the properties of $\tilde{\mathbf{K}}_R$ and $\tilde{\mathbf{T}}$ as discussed above in the three-dimensional case apply here, as can be (more easily than in three dimensions) derived by explicit algebra.

Note that the present one-dimensional case is also of significance for the geometry of d-dimensional parallel (hyper)cubes (or cuboids when considering different sizes) via building direct products of the one-dimensional quantities characteristic for each of the d Cartesian dimensions (see, e.g., Refs. 21 and 22).

V. CONCLUSIONS

We have shown that the weight functions used in Ref. 13 form a complete and closed framework for the manipulation of the size of spheres via convolution in that the geometry of a sphere can be represented by an arbitrary number of convolutions of spheres. The transformations that perform such a shift of length scales can be chained and reversed and hence form an Abelian group. We have investigated in detail the linear algebra of the convolution transformation involved including second- and third-rank representations. Our findings might prove useful in the further development of geometry-based density functional theories.

Some of the more recent developments in FMT are based on the requirement to regularize the free energy density functional for delta-function density distributions.[11,23,24] This is achieved using tensorial weight functions (which can be viewed as an extension of Rosenfeld's vectorial weight functions). Elucidating the precise relationship of these objects to the framework presented here deserves further study.

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APPENDIX: EIGENSYSTEMS IN THE THREE-DIMENSIONAL CASE

For completeness we investigate the two eigensystems of $\widetilde{\mathbf{K}}_R$. The right eigensystem consists of a pair of doubly degenerate eigenvectors $\mathbf{v}$ and $\mathbf{v}^*$ that are complex conjugate to each other (indicated by the superscript asterisk) and correspond to doubly degenerate eigenvalues λ and λ^* given by

$$\mathbf{v} = (1, -i/q, 8\pi/q^2, 8\pi i/q^3), \quad \lambda = \mathrm{e}^{-iqR}. \tag{A1}$$

The left eigensystem possesses similar features. The two eigenvectors are each doubly degenerate and form a pair of complex conjugates $\mathbf{u}$ and $\mathbf{u}^*$ with the same eigenvalues λ and λ^* as given above for the right eigensystem and

$$\mathbf{u} = (1, -iq, -q^2/(8\pi), -iq^3/(8\pi)). \tag{A2}$$

Again the simplicity of these expressions might seem striking given the complexity of $\widetilde{\mathbf{K}}_R$. Note, in particular, that $\mathbf{v}$ and $\mathbf{u}$ are scale-free objects in that they *do not* contain the length scale R; the latter appears solely in the corresponding eigenvalue, where it plays the role of tuning the phase in a complex exponential. It is worth noting that all possible inner products vanish:

$$\mathbf{v}^{\mathrm{t}}\mathbf{M}\mathbf{v} = \mathbf{v}^{\mathrm{t}}\mathbf{M}\mathbf{v}^* = \mathbf{v}^{\mathrm{t}*}\mathbf{M}\mathbf{v}^* = 0, \tag{A3}$$

$$\mathbf{u}^{\mathrm{t}}\mathbf{M}\mathbf{u} = \mathbf{u}^{\mathrm{t}}\mathbf{M}\mathbf{u}^* = \mathbf{u}^{\mathrm{t}*}\mathbf{M}\mathbf{u}^* = 0, \tag{A4}$$

$$\mathbf{u} \cdot \mathbf{v} = \mathbf{u} \cdot \mathbf{v}^* = \mathbf{u}^* \cdot \mathbf{v} = \mathbf{u}^* \cdot \mathbf{v}^* = 0. \tag{A5}$$

In particular, the first line is striking: When viewed as a vector of weight functions, $\mathbf{v}$ (and its complex conjugate $\mathbf{v}^*$) serves to deconvolve naught. Note that all corresponding fundamental measures (obtained in the limit $q \to 0$) diverge, except for the Euler characteristic, which is well behaved and equals unity. Furthermore Eqs. (A3) and (A4) also hold when $\mathbf{M}$ is replaced by either of the following matrices: $\mathbf{M}\widetilde{\mathbf{G}}$, $\mathbf{M}\widetilde{\mathbf{G}}^2$, or $\mathbf{M}(\widetilde{\mathbf{G}}^3 + 2q^2\widetilde{\mathbf{G}})$, which together form the third-rank tensor $\widetilde{\mathbf{T}}$. Hence, in summary, rewriting the first equality of (A3) as

$$\tilde{T}_{\mu}{}^{\nu\tau}v_{\nu}v_{\tau}=0, \quad \mu=0,1,2,3 \tag{A6}$$

holds accordingly for the other cases involving $\mathbf{v}^*$, $\mathbf{u}$, and $\mathbf{u}^*$.

The above eigenvectors can be augmented to form a matrix

$$\tilde{\mathbf{S}}=\begin{pmatrix} 1 & -iq & -q^2/(8\pi) & -iq^3/(8\pi) \\ -i/q & -1 & iq/(8\pi) & -q^2/(8\pi) \\ 8\pi/q^2 & -8\pi i/q & -1 & -iq \\ 8\pi i/q^3 & 8\pi/q^2 & -i/q & 1 \end{pmatrix}, \tag{A7}$$

with $\det\tilde{\mathbf{S}}=0$ and the properties $\tilde{\mathbf{S}}\tilde{\mathbf{S}}=\tilde{\mathbf{S}}\tilde{\mathbf{S}}^*=\tilde{\mathbf{S}}^*\tilde{\mathbf{S}}=\tilde{\mathbf{S}}^*\tilde{\mathbf{S}}^*=0$, $\tilde{\mathbf{K}}_R\tilde{\mathbf{S}}=\tilde{\mathbf{S}}\tilde{\mathbf{K}}_R=\mathrm{e}^{-iqR}\tilde{\mathbf{S}}$, and $\tilde{\mathbf{K}}_R\tilde{\mathbf{S}}^*=\tilde{\mathbf{S}}^*\tilde{\mathbf{K}}_R=\mathrm{e}^{iqR}\tilde{\mathbf{S}}^*$.

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