Explicit excluded volume of cylindrically symmetric convex bodies

Marco Piastra
Dipartimento di Ingegneria Industriale e dell'Informazione, Università di Pavia, via Ferrata 1, I-27100 Pavia, Italy

Epifanio G. Virga
Dipartimento di Matematica, Università di Pavia, Via Ferrata 5, I-27100 Pavia, Italy

(Dated: March 17, 2015)

We represent explicitly the excluded volume $V_e\{B_1, B_2\}$ of two generic cylindrically symmetric, convex rigid bodies, $B_1$ and $B_2$, in terms of a family of shape functionals evaluated separately on $B_1$ and $B_2$. We show that $V_e\{B_1, B_2\}$ fails systematically to feature a dipolar component, thus making illusory the assignment of any shape dipole to a tapered body in this class. The method proposed here is applied to cones and validated by a shape-reconstruction algorithm.

PACS numbers: 61.30.-v; 61.30.Cz; 47.57.J-
Keywords: Excluded volume; Second virial coefficient; Hard-body interactions; Brunn-Minkowski theory; Minkowski functionals; Colloids.

* e-mail: marco.piastra@unipv.it
† e-mail: eg.virga@unipv.it
I. INTRODUCTION

Onsager’s celebrated paper [1] on the effect of shape on the interaction between hard particles has perhaps been the most influential contribution to colloidal sciences of the last century [2]. There, entropic forces alone were first recognized as capable of inducing a structural ordering transition with no involvement of whatever cohesion force may be present. The typical prototype of such an ordering transition remains indeed the isotropic-to-nematic transition predicted in [1] for an assembly of slender hard rods as their number density is increased beyond a critical value (falling within a narrow gap of phase coexistence). As paradoxical as it may appear at a superficial glance, such an ordering transition is duly accompanied by an increase in entropy, since the loss in orientational disorder attached to the rods’ alignment is outbalanced by the gain in translational disorder made possible by the increase in the volume available for the particles’ centers of mass [2, 3]. The conjugated counterpart of this volume is the excluded volume.

The excluded volume of two rigid bodies is the volume in space that any one point in one body cannot access by the very presence of the other body. This definition is delusively simple as it conceals a formidable mathematical task which can seldom be accomplished in an exact analytic form.³ Of course, there are exceptions to this general statement, but they are very few.²

Despite its technical difficulties, the excluded volume remains a key ingredient of both Onsager’s original theory and its most recent extensions. In all of these, the per-particle free energy $F$ of an assembly of hard bodies (appropriately made dimensionless) is a functional of the single-body local density $\varrho$. A number of papers have interpreted Onsager’s original theory in the light of the modern density functional theories; here we refer the reader to the most recent review on the subject [7], which is mostly concerned with hard-body systems that exhibit liquid crystalline phases.³ $F[\varrho]$ differs from the free-energy functional for an ideal gas by the addition of an excess free energy $F_{\text{ex}}[\varrho]$, which characterizes the interactions of anisometric particles. In general, $F_{\text{ex}}[\varrho]$ is not known explicitly, but it can always be expressed as a power series in the total number density $\varrho_0$, which is often called the virial expansion. The first non-trivial term of such an expansion is $\varrho_0 B_2[\varrho]$, where the functional $B_2$ is the second virial coefficient, which is nothing but the ensemble average of the excluded volume,

$$B_2[\varrho] := \frac{1}{2} \int_{\Omega} V_e(\omega, \omega') \varrho(\omega) \varrho(\omega') d\omega d\omega'.$$

In (1), $\Omega$ is the orientational manifold, which describes all possible orientations of a particle in the system and $V_e(\omega, \omega')$ is the excluded volume of two particles with orientations $\omega$ and $\omega'$, respectively. Higher powers of $\varrho_0$ bear higher virial coefficients $B_n$, which however are even more difficult to compute than $B_2$.

Onsager [1] remarkably estimated that for rods sufficiently slender $B_2$ actually prevails over all other $B_n$’s. This makes Onsager’s theory virtually exact, as was also subsequently confirmed directly by numerical computations [9, 10]. Nevertheless, even when the second virial coefficient $B_2[\varrho]$ cannot be proved to be dominant, it remains a viable approximation to $F_{\text{ex}}[\varrho]$ in establishing, at least qualitatively, the variety of possible equilibrium phases in a hard-body system and the entropy-driven transitions between them. To this end, explicit formulas for the excluded volume of rigid bodies are to be especially treasured.

This is the motivation for our study. Our objective is to express $V_e\{B_1, B_2\}$, the excluded volume for two rigid bodies, $B_1$ and $B_2$, in terms of shape functionals depending solely on the individual bodies $B_1$ and $B_2$. We shall accomplish this task for bodies both convex and cylindrically symmetric, for which $V_e\{B_1, B_2\}$ can be given with no loss in generality as the sum of a series of Legendre polynomials $P_n$,

$$V_e\{B_1, B_2\} = \sum_{n=0}^{\infty} B_1 B_2 P_n (m_1 \cdot m_2),$$

where $m_1$ and $m_2$ are unit vectors along the symmetry axes of $B_1$ and $B_2$, respectively. The shape functionals involved in our explicit representation will be natural extensions of the classical functionals on which was largely based the celebrated Brunn-Minkowski theory of convex bodies.⁴ The major advantage of the method proposed here is the explicit computability of such extended Minkowski functionals, which makes our representation formula directly applicable to bodies $B_1$ and $B_2$ not necessarily congruent, possibly representing particles of different species.

---

1 We learn from [4] that Viellard-Baron, who took an early interest in this problem [5], “was reportedly greatly disturbed by the difficulties he encountered.”

2 We mention here the early exact calculation of the excluded volume of two hard spherocylinders [6] and the recent exact determination of the distance of closest approach between two hard ellipses in two space dimensions [4], which is strictly related to the excluded volume of two hard ellipses.

3 A general reference for simple liquids is still the classical book [8], now enriched by an addition on complex fluids.

4 Besides the original sources [11, 12], the general books [13, 14] are highly recommended. We also collected a number of relevant results phrased in the same mathematical language employed here in Appendix A to our earlier study on this subject [15]. Finally, a different but equivalent approach is presented in [16].
The paper is organized as follows. In Sec. II, we set the scene for our development by showing that the Legendre coefficients $B_n$ of the representation formula (2) can be expressed as appropriate anisotropic volume averages. Section III is devoted to the coefficient $B_1$ of the first Legendre polynomial $P_1(m_1 \cdot m_2) = m_1 \cdot m_2$ in (2). We attach a special meaning to this, as it represents the dipolar contribution to $V_\epsilon(\mathcal{B}_1, \mathcal{B}_2)$ which would possibly arise from tapered, cylindrically symmetric, convex bodies, if only one could unambiguously assign a shape dipole to them. The somewhat surprising conclusion will be that $B_1$ vanishes identically on this class of bodies, making the very notion of shape dipole void, despite its intuitive appeal. Section IV is concerned with the extended Minkowski functionals, in terms of which, once evaluated on the bodies $\mathcal{B}_1$ and $\mathcal{B}_2$, we can write in closed form all coefficients $B_n$ in (2). An explicit application of our method is illustrated in Sec. V, where we evaluate the extended Minkowski functionals for a generic circular cone and validate our evaluations through a direct computation of the coefficients $B_n$ made possible by an independent shape-reconstruction algorithm, appropriately modified to tackle efficiently the cone’s sharp ridge. In Sec. VI, we collect the main conclusions of our work, looking back a fresh to some of them, also in the light of possible future developments that they may suggest.

We shall endeavor to make our presentation as free as possible from unwanted technical details that might obscure both the outcomes of our study and the strategy adopted to obtain them. To provide, however, the interested reader with enough information to appreciate the mathematical infrastructure underlining this paper, we collect in two closing appendices the details of both the mathematical theory and the shape-reconstruction algorithm.

II. ANISOTROPIC VOLUME AVERAGES

It was proved by Mulder [17] that the excluded volume of $V_\epsilon(\mathcal{B}_1, \mathcal{B}_2)$ of two bodies, $\mathcal{B}_1$ and $\mathcal{B}_2$, be they convex or not, can be expressed as

$$V_\epsilon(\mathcal{B}_1, \mathcal{B}_2) = V[\mathcal{B}_1 + \mathcal{B}_2^*],$$  

(3)

where $V$ is the volume functional, $\mathcal{B}_2^*$ is the central inverse (relative to a specified origin $o$) of the body $\mathcal{B}_2$, and $+$ denotes the Minkowski addition (to the definition of which concurs the origin $o$).\(^5\) Letting both $\mathcal{B}_1$ and $\mathcal{B}_2$ be cylindrically symmetric bodies with axes $m_1$ and $m_2$, respectively, since $V_\epsilon(\mathcal{B}_1)$ is an isotropic scalar-valued function, by a theorem of Cauchy,\(^6\) we can say that $V_\epsilon(\mathcal{B}_1, \mathcal{B}_2)$ is a function (still denoted as) $V_\epsilon$ of the inner product $m_1 \cdot m_2$. Setting $m_1 \cdot m_2 = \cos \vartheta$, the function $V_\epsilon(\cos \vartheta)$ can be expanded as the sum of a series of Legendre polynomials (see, for example, Secs. 18.2 and 18.3 of [19]):

$$V_\epsilon(\cos \vartheta) = \sum_{n=0}^{\infty} B_n P_n(\cos \vartheta),$$  

(4)

where

$$B_n := \frac{2n + 1}{2} \int_{0}^{\pi} V_\epsilon(\cos \vartheta) P_n(\cos \vartheta) \sin \vartheta d\vartheta$$  

(5)

are the Legendre coefficients of $V_\epsilon$. We record for future use a few basic properties of the orthogonal polynomials $P_n$ (see, in particular, Secs. 18.6.1 of [19] and 8.917.1 of [20]):

$$P_n(-x) = (-1)^n P_n(x), \quad P_n(1) = 1, \quad |P_n(x)| \leq 1.$$  

(6)

There is another way of expressing the coefficients $B_n$, which we find illuminating. Consider the average

$$\langle P_n V_\epsilon \rangle [\mathcal{B}_1, \mathcal{B}_2] := \langle P_n(m_1 \cdot m_2) V_\epsilon(m_1 \cdot m_2) \rangle_{\mathcal{B}_2}$$  

(7)

computed for fixed $\mathcal{B}_1$ over all possible replicas of $\mathcal{B}_2$ obtained by rotating arbitrarily $\mathcal{B}_2$ in space. By the cylindrical symmetry of $\mathcal{B}_2$, the average (7) also acquires the equivalent form

$$\langle P_n V_\epsilon \rangle [\mathcal{B}_1, \mathcal{B}_2] = \langle P_n(m_1 \cdot m_2) V_\epsilon(m_1 \cdot m_2) \rangle_{m_2}.$$  

(8)

\(^5\) The reader is referred to the primer on the Brunn-Minkowski theory of convex bodies in Appendix A of [15]. A short recapitulation of this theory is also given in Appendix A 1 below to make our paper self-contained.

\(^6\) See, for example, Sec. 113.1 of [18].
where, for any function $f(e)$ defined on the unit sphere $S^2$,

$$\langle f \rangle_e := \frac{1}{4\pi} \int_{S^2} f(e) \, da(e)$$

(9)

and $da(e)$ denotes the area element with unit normal $e$. Representing $m_2$ in polar spherical coordinates with polar axis $m_1$ and combining (8) and (5), we readily arrive at

$$\langle P_n V \rangle [\mathcal{B}_1, \mathcal{B}_2] = \frac{1}{2} \int_{0}^{\pi} P_n(\cos \vartheta) V_n(\cos \vartheta) \sin \vartheta d\vartheta = \frac{1}{2n+1} B_n.$$  

(10)

Since both functions $V_n$ and $P_n$ are symmetric under the exchange of $m_1$ and $m_2$, the average $\langle P_n V \rangle [\mathcal{B}_1, \mathcal{B}_2]$ is also symmetric under the exchange of bodies $\mathcal{B}_1$ and $\mathcal{B}_2$:

$$\langle P_n V \rangle [\mathcal{B}_1, \mathcal{B}_2] = \langle P_n V \rangle [\mathcal{B}_2, \mathcal{B}_1].$$  

(11)

Equation (3) allows us to express the Legendre coefficients $B_n$ of the excluded volume of two cylindrically symmetric bodies in a way directly related to the anisotropic averages of the volume of a Minkowski sum. Combining (10), (7), and (3), we readily see that

$$B_n = (2n + 1) \langle P_n (m_1 \cdot m_2) V[\mathcal{B}_1 + \mathcal{B}_2] \rangle_{\mathcal{B}_2} = (2n + 1)^n \langle P_n (m_1 \cdot m_2^*) V[\mathcal{B}_1 + \mathcal{B}_2^*] \rangle_{\mathcal{B}_2},$$

(12)

where $m_2^* = -m_2$ is the symmetry axis of the central inverse $\mathcal{B}_2^*$ of $\mathcal{B}_2$ and use has been made of (6) and the fact that averaging over $\mathcal{B}_2$ is just the same as averaging over $\mathcal{B}_2^*$. Thus, to obtain all coefficients $B_n$ in (4), we need to learn how to compute the anisotropic volume averages

$$\langle P_n V \rangle [\mathcal{B}_1, \mathcal{B}_2] := \langle P_n V[\mathcal{B}_1 + \mathcal{B}_2] \rangle_{\mathcal{B}_2},$$

(13)

as then (12) would simply reduce to

$$B_n = (2n + 1)(-1)^n \langle P_n V \rangle [\mathcal{B}_1, \mathcal{B}_2^*],$$

(14)

which obeys the same symmetry relation as in (11). Equation (14) is the basic building block of our development.

Although (14) is as general as (3) for cylindrically symmetric bodies, this paper will solely be concerned with the excluded volume of convex cylindrically symmetric bodies. For $n = 0$, the average in (13) becomes isotropic as $P_0 \equiv 1$ and its expression has long been known for generic convex bodies:

$$\langle V \rangle [\mathcal{B}_1, \mathcal{B}_2] = V[\mathcal{B}_1] + V[\mathcal{B}_2] + \frac{1}{4\pi} (M[\mathcal{B}_1] S[\mathcal{B}_2] + M[\mathcal{B}_2] S[\mathcal{B}_1]),$$

(15)

where $M$ is the total mean curvature functional in (A12a) and $S$ is the surface area functional in (A12b). Since both $M[\mathcal{B}]$ and $S[\mathcal{B}]$ are invariant under central body inversion of $\mathcal{B}$, it follows from (14) and (15) that

$$B_0 = \langle V \rangle [\mathcal{B}_1, \mathcal{B}_2].$$

(16)

Here our challenge is to extend the neat classical formula (15) for the isotropic average of the volume of the Minkowski sum of convex bodies to the anisotropic averages needed in (14). This will be achieved in the two following sections with the aid of appropriate extensions of the classical Minkowski functionals $M$ and $S$. We anticipate that they are invariant under central body inversion like the classical Minkowski functionals, so that, in complete analogy with (15) and (16), we shall be able to express the excluded volume $V_n[\mathcal{B}_1, \mathcal{B}_2]$ of cylindrically symmetric bodies $\mathcal{B}_1$ and $\mathcal{B}_2$ in terms of functionals evaluated separately on $\mathcal{B}_1$ and $\mathcal{B}_2$.

As recalled in Appendix A, there is no loss in generality in limiting attention to the class $\mathcal{K}^+$ of convex bodies with smooth boundaries and strictly positive principal curvatures, as $\mathcal{K}^+$ is dense in the whole class $\mathcal{K}$ of convex bodies (see Appendix A1). Thus, our strategy will be to compute first the anisotropic volume averages in $\mathcal{K}^+$ and then extend them by continuity to the whole of $\mathcal{K}$. In the following section, we shall first accomplish our task for $\langle P_1 V \rangle [\mathcal{B}_1, \mathcal{B}_2]$: this will lead us to conclude that $B_1 \equiv 0$, a general result of some import. In Sec. IV, we shall compute $\langle P_n V \rangle [\mathcal{B}_1, \mathcal{B}_2]$ for all $n \geq 2$ and arrive at the expected general explicit formula for all $B_n$'s.

---

7 A derivation of (15) can be found in [16]. Moreover, Kihara [21, 22] credits Ishihara [23] and Ishihara and Hayashida [24, 25] for having proved (15), although he also seems aware that a proof had already been contained in the classical work of Minkowski [12].
III. NO SHAPE DIPOLES

Here our task is to compute $B_1$. To this end we remark that

$$
\langle P_n(m_1 \cdot m_2) \rangle \equiv \langle P_n(m_1 \cdot m_2) \rangle_{m_2} = 0, 
$$

(17a)

$$
\langle P_n(m_1 \cdot m_2)V[B_2]\rangle_{m_2} = V[B_2] \langle P_n(m_1 \cdot m_2) \rangle_{m_2} = 0, \ n \geq 1,
$$

(17b)

the former following from (9) and the orthogonality of Legendre polynomials, and the latter also from the invariance of the volume functional under rotations. Then we represent $m_2$ in a Cartesian frame ($e_x, e_y, e_z$) fixed in $B_1$. Letting $e_z = \nu$, where $\nu$ is the outer unit normal to $B_1$ at a selected point on $\partial B_1$, and choosing $e_y$ orthogonal to the plane $(m, \nu)$, we have that

$$
m_1 = \sin \vartheta_1 e_x + \cos \vartheta_1 \nu,
$$

(18a)

$$
m_2 = \cos \phi \sin \vartheta_1 e_x + \sin \phi \sin \vartheta_2 e_y + \cos \vartheta_2 \nu,
$$

(18b)

the latter of which represents all possible orientations of $m_2$, for given $\vartheta_1$ and $\vartheta_2$, the angles that $m_1$ and $m_2$ make with $\nu$ (see Fig. 1). An easy, but important consequence of (18) is that

FIG. 1. Sketch representing the unit vectors $\nu, m_1$, and $m_2$. With $\nu$ and $m_1$ fixed, $m_2$ as represented by (18b) describes a cone around $\nu$ in the first step of the averaging process described in the text.

$$
m_1 \cdot m_2 = \sin \vartheta_1 \sin \vartheta_2 \cos \phi + \cos \vartheta_1 \cos \vartheta_2
$$

$$
\quad = \sin \vartheta_1 \sin \vartheta_2 \cos \phi + (m_1 \cdot \nu)(m_2 \cdot \nu).
$$

(19)

Now, using also (17), we can derive from (A14) the following expression

$$
\langle P_1V \rangle \equiv [B_1, B_2] = \frac{1}{3} \left( \langle m_2 \cdot \nu \rangle \int_{\partial B_1} (\nu \cdot r_1)(\nu \cdot m_1) da(\nu) + (\nu \cdot r_2)(\nu \cdot m_2) \rangle \int_{\partial B_2} \frac{m_1 \cdot \nu}{K(\nu)} da(\nu) \right.
$$

$$
\quad + \frac{1}{6} \left( \langle m_2 \cdot \nu \rangle \left( \rho_1^{(2)} + \rho_2^{(2)} \right) \int_{\partial B_1} (\nu \cdot r_1)(\nu \cdot m_1) \left( \rho_1^{(1)} + \rho_2^{(1)} \right) da(\nu) \right.
$$

$$
\quad + \frac{1}{6} \left( \langle \nu \cdot r_2 \rangle (m_2 \cdot \nu) \left( \rho_1^{(2)} + \rho_2^{(2)} \right) \int_{\partial B_2} (m_1 \cdot \nu) \left( \rho_1^{(1)} + \rho_2^{(1)} \right) da(\nu), \right)
$$

(20)

which results from computing the average over $B_2$ in two separate steps: first averaging over the angle $\phi$ in (19) which ranges in $[0, 2\pi]$ and then averaging formally over $\nu$, meant as the outward unit normal to $B_2$, which ranges over $S^2$. If the former average is taken over the process in which, with $\nu$ and $m_1$ fixed, $m_2$ is seen to describe a cone around $\nu$ (see Fig. 1), the latter is nothing but the average over the independent process in which all different points of $\partial B_2$ come to be associated with one and the same fixed normal $\nu$. As in (A14), also in (20) $\rho_1^{(1)}$ and $\rho_2^{(1)}$ denote the principal radii of curvature of $\partial B_1$ and $\rho_1^{(2)}$ and $\rho_2^{(2)}$ denote the principal radii of curvature of $\partial B_2$; correspondingly, $K^{(1)} = \left( \rho_1^{(1)} \rho_2^{(1)} \right)^{-1}$ and $K^{(2)} = \left( \rho_1^{(2)} \rho_2^{(2)} \right)^{-1}$ are the Gaussian curvatures of $\partial B_1$ and $\partial B_2$ and $r_1$ and $r_2$ are the radial mappings of $\partial B_1$ and $\partial B_2$ (see Appendix A 1 for more details).

Now, with the aid of the theory recalled in Appendix A 1, we compute the new shape functionals featuring in (20). It readily follows from (A8) that for any body $B \in K^+$

$$
\int_{\partial B} \frac{m \cdot \nu}{K} da(\nu) = \int_{\partial B} m \cdot n da(n) = \int_{\partial B} \text{div} m dv = 0,
$$

(21)

where use has also been made of the classical divergence theorem (and the fact that $m$ can be extended to the whole space as a uniform field). Likewise, (A9) and (A8) imply that

$$
\int_{\partial B} (m \cdot \nu)(\rho_1 + \rho_2) da(\nu) = \int_{\partial B} (m \cdot \nu) \frac{1}{K} \text{div}_n n da(\nu)
$$

$$
= \int_{\partial B} (m \cdot n) \text{div}_n n da(n) = \int_{\partial B} \text{div}_n m da(n) = 0,
$$

(22)
where use has also been made of the surface divergence theorem recalled in (A11). Combining (21) and (22), we obtain from (20) that \( \langle P_1 V \rangle [B_1, B_2] \) vanishes identically for all \( B_1 \) and \( B_2 \), and so, by (14),

\[
B_1 = -3 \langle P_1 V \rangle [B_1, B_2^*] \equiv 0. \tag{23}
\]

Equation (23) says that for cylindrically symmetric bodies, \( B_1 \) and \( B_2 \), the excluded volume \( V_e \) in (4) does not contain any dipolar contribution, no matter how tethered \( B_1 \) and \( B_2 \) can be, suggesting that no shape dipole can be assigned to a body \( B \). Equation (23) shows that no matter how we endeavor to assign a shape dipole to \( B \) it plays no role in the hard-particle interactions governed by the excluded volume. Of course, polarity effects are also expected to be seen in these interactions. For example, it was proved in [26] that the excluded volume of two congruent cylindrically symmetric convex bodies is minimized when the bodies are in the antiparallel configuration, where \( m_2 = -m_1 \).

Such polar effects, however, cannot involve shape dipoles: as shown in [15], they start being manifested thorough the shape octupole that features in (4) through the coefficient \( B_3 \). This and all higher order Legendre coefficients will be computed in the following section.

### IV. EXTENDED MINKOWSKI FUNCTIONALS

Computing the anisotropic volume averages \( \langle P_n V \rangle [B_1, B_2] \) for \( n \geq 2 \) is technically more complicated than computing \( \langle P_1 V \rangle [B_1, B_2] \), although conceptually this task is not much different from that just accomplished in the preceding section. As shown in Appendix A2, this computation led quite naturally to the introduction of a number of shape functionals that extend the classical Minkowski functionals \( M \) and \( S \). They are defined for all \( n \geq 2 \) as follows:

\[
M_n[B] := \int_{\partial B} P_n(m \cdot n)Hda(n), \tag{24a}
\]

\[
M_n'[B] := \int_{\partial B} (n \cdot x)P_n(m \cdot n)Kda(n), \tag{24b}
\]

\[
M_n''[B] := \int_{\partial B} [1 - (m \cdot n)^2]^{1/2}(\sigma_1 - \sigma_2)P_n^{(2,2)}(m \cdot n)da(n), \tag{24c}
\]

\[
S_n[B] := \int_{\partial B} P_n(m \cdot n)da(n), \tag{24d}
\]

\[
S_n'[B] := \int_{\partial B} (n \cdot x)P_n(m \cdot n)Hda(n), \tag{24e}
\]

\[
S_n''[B] := \int_{\partial B} (n \cdot x)[1 - (m \cdot n)^2]^{1/2}(\sigma_1 - \sigma_2)P_n^{(2,2)}(m \cdot n)da(n). \tag{24f}
\]

We shall often refer to them as the extended Minkowski functionals. They give \( \langle P_n V \rangle [B_1, B_2] \) the following concise, explicit representation:

\[
\langle P_n V \rangle [B_1, B_2] = \frac{1}{12\pi} \left( M_n'[B_1]S_n[B_2] + M_n'[B_2]S_n[B_1] \right) + \frac{1}{6\pi} \left( M_n[B_1]S_n'[B_2] + M_n[B_2]S_n'[B_1] \right) + \frac{1}{(4\pi)^2} \left( M_n''[B_1]S_n''[B_2] + M_n''[B_2]S_n''[B_1] \right) \tag{25}
\]

Strictly speaking, in Appendix A2 we arrived at (24) through the representation via radial mapping of the convex bodies in the special class \( \mathcal{H} \). However, the extended Minkowski functionals can be extended by continuity to the whole of \( \mathcal{H} \). Moreover, as clearly shown by (24), their definition actually applies to any cylindrically symmetric body, be it convex or not. The extended \( M \) and \( S \) functionals are invariant under rotations. Their behavior under translations is further discussed in Appendix A5 and the possibility that, despite all appearances, they may not be independent from one another is explored in Appendix A6.

Since the extended Minkowski functionals for a body \( B \) are invariant under central inversion of \( B \) (see Appendix A1), it follows from (25) that \( \langle P_n V \rangle [B_1, B_2^*] = \langle P_n V \rangle [B_1, B_2] \), and so equation (14) becomes

\[
B_n = (2n + 1)(-1)^n \langle P_n V \rangle [B_1, B_2], \tag{26}
\]

which by (25) expresses the Legendre coefficients of \( V_e \) in (4) in terms of shape functionals evaluated on the individual bodies \( B_1 \) and \( B_2 \). Formula (26) will be applied in the following section to a special class of bodies.

---

8 More shortly, also as the extended \( M \) and \( S \) functionals.
V. CIRCULAR CONES

We denote by $C^\alpha$ a circular cone with semi-amplitude $\alpha \in [0, \pi/2]$, radius $R$, and height $h$, both related through (A32) to the slant height $L$ (see Fig. 2). It is a simple matter to show that the classical Minkowski functionals for $C^\alpha$

![FIG. 2. (Color online) A circular cone with vertex in the origin $o$, semi-amplitude $\alpha$, radius $R$, height $h$, and slant height $L$.](image)

... take the explicit forms (see also (A61) and (A62) of [15]),

$$M[C^\alpha] = \pi L \left[ \cos \alpha + \left( \frac{\pi}{2} + \alpha \right) \sin \alpha \right], \quad (27a)$$

$$S[C^\alpha] = \pi L^2 \sin \alpha (1 + \sin \alpha), \quad (27b)$$

$$V[C^\alpha] = \frac{1}{3} \pi L^3 \cos \alpha \sin^2 \alpha. \quad (27c)$$

As follows easily from (A34), the Gaussian curvature $K$ vanishes identically on all smooth components of $\partial C^\alpha$. Moreover, the contribution of the vertex $o$ to all the integrals in (24) vanishes, as can be seen by replacing $o$ with a fitting spherical cap of radius $\varepsilon$ (whose area surface scales like $\varepsilon^2$) and then taking the limit as $\varepsilon \to 0^+$, in complete analogy to the method used in Appendix A 4 a to compute the extended Minkowski functionals on a circular ridge $\mathcal{R}$. The formulae (A38) obtained there for a $\mathcal{R}$ can be directly applied here to the rim of the cone’s base by simply setting $\theta_1 = \frac{\pi}{2} - \alpha$ and $\theta_2 = \pi$. Use of (A32) finally leads us to

$$M_n[C^\alpha] = \pi L \left( P_n(\sin \alpha) \cos \alpha + \sin \alpha \int_{\frac{\pi}{2}-\alpha}^{\pi} P_n(\cos \vartheta)d\vartheta \right), \quad (28a)$$

$$M'_n[C^\alpha] = -2\pi L \int_{\frac{\pi}{2}-\alpha}^{\pi} \cos(\vartheta + \alpha) P_n(\cos \vartheta) \sin \vartheta d\vartheta, \quad (28b)$$

$$M''_n[C^\alpha] = -\pi L \left( P^{(2,2)}_{n-2}(\sin \alpha) \cos^2 \alpha \sin \alpha \int_{\frac{\pi}{2}-\alpha}^{\pi} P^{(2,2)}_{n-2}(\cos \vartheta) \sin^2 \vartheta d\vartheta \right), \quad (28c)$$

$$S_n[C^\alpha] = \pi L^2 \sin \alpha \left[ P_n(\sin \alpha) + (-1)^n \sin \alpha \right], \quad (28d)$$

$$S'_n[C^\alpha] = -\pi L^2 \sin \alpha \int_{\frac{\pi}{2}-\alpha}^{\pi} \cos(\vartheta + \alpha) P_n(\cos \vartheta)d\vartheta, \quad (28e)$$

$$S''_n[C^\alpha] = -\pi L^2 \sin \alpha \int_{\frac{\pi}{2}-\alpha}^{\pi} \cos(\vartheta + \alpha) P^{(2,2)}_{n-2}(\cos \vartheta) \sin^2 \vartheta d\vartheta, \quad (28f)$$

for all $n \geq 2$. Inserting (28) in (26), we obtain explicit, analytic formulae for the Legendre coefficients $B_n$ of the excluded volume of two congruent circular cones, $C^\alpha_1$ and $C^\alpha_2$, which for completeness are recorded in (A50) for the first seven indices $n \geq 1$. They are plotted in Fig. 3 as functions of $\alpha$. Inserting (27) in (15), we also obtain the isotropic average $B_0$ in (16), which is plotted in Fig. 4 with two possible normalizations, relative to the volume $V_c$ of each cone delivered by (27c) in Fig. 4(a) and relative to $L^3$ in Fig. 4(b). The even-indexed coefficients $B_n$’s are mostly negative, indicating by (6) a tendency for the corresponding terms in the sum (4) to minimize $V_c$ for either $\vartheta = 0$ or $\vartheta = \pi$, irrespectively. On the contrary, the odd-indexed coefficients are mostly positive (apart from $B_3$ which is never negative), indicating a tendency for the corresponding terms in (4) to minimize $V_c$ for $\vartheta = \pi$, that is, when the cones $C^\alpha_1$ and $C^\alpha_2$ are in the antiparallel configuration, with $m_2 = -m_1$. This suggests that the excluded volume of
this paper. For a given reconstruction algorithm outlined in Appendix B. Our strategy was completely different from that adopted so far in two congruent circular cones is minimized in the antiparallel configuration, as shown by direct computation in [15] in accord with the general minimum property established more recently in [26].

The crosses superimposed to the graphs in Fig. 3 represent the values of $B_n$ extracted numerically from the volume of the excluded body $R_e\{C_1^\alpha, C_2^\alpha\}$, the region in space that cone $C_2^\alpha$ cannot access by the presence of cone $C_1^\alpha$. Determining $R_e\{C_1^\alpha, C_2^\alpha\}$ is indeed necessary for a direct determination of $V_e\{C_1^\alpha, C_2^\alpha\}$, as the general proper geometric definition of the excluded volume of bodies $R_1$ and $R_2$ is precisely the volume of the excluded body $R_e\{R_1, R_2\}$, $V_e\{R_1, R_2\} := V[R_e\{R_1, R_2\}]$ (see also [15]). Here $R_e\{C_1^\alpha, C_2^\alpha\}$ was obtained from the shape-reconstruction algorithm outlined in Appendix B. Our strategy was completely different from that adopted so far in this paper. For a given $\alpha$, we reconstructed $R_e\{C_1^\alpha, C_2^\alpha\}$ for a number of values of the angle $\vartheta$ made by the cones’ axes $m_1$ and $m_2$; we computed numerically the excluded volume $V_e$ as a function of $\vartheta$ by applying (A12c) to a

![Graph](image1)

(a)

![Graph](image2)

(b)
triangulation of $\partial \mathcal{B}_e \{ \mathcal{C}_1^\alpha, \mathcal{C}_2^\alpha \}$ and we extracted from this function the coefficients $B_n$ through (5). To what extent the two methods agree, thus granting support to each other, is left to the reader to judge from Fig. 3. Quantitative details about both the shape-reconstruction algorithm employed here (including its adaptation to the specific case of cones, which with their sharp edge and pointed vertex required special attention) and the way the coefficients $B_n$ were computed can be found in Appendix B below.

Figure 5 shows three graphs representing the excluded volume $V_e$ of $\mathcal{C}_1^\alpha$ and $\mathcal{C}_2^\alpha$ scaled to their common volume $V_c$ (given by (27c)) as a function of the angle $\vartheta$ between their axes. The semi-amplitude $\alpha$ of both cones is taken here to be $\alpha_0 = 0.14 \pi$, for which, as shown in Fig. 4, the isotropic average $\langle V_e \rangle$ scaled to $V_c$ takes on its minimum value. The graphs in Fig. 5 correspond to the function in (12) truncated at $n = 3$ and $n = 9$; they are both contrasted against the octupolar approximation, which in [15] was shown to be rather accurate. While, by construction, the latter takes on the exact values of $V_e$ at both $\vartheta = 0$ (parallel cones) and $\vartheta = \pi$ (antiparallel cones), which are $14V_c$ and $8V_c$, respectively, both truncated expansions do not. Actually, as expected, the convergence of the series in (4) at these points is rather slow: for example, a computation with 61 terms was required to obtain

$$\frac{V_e}{V_c} \approx 14.01 \quad \text{and} \quad \frac{V_e}{V_c} \approx 8.153,$$

at $\vartheta = 0$ and $\vartheta = \pi$, respectively. Thus, if for cones the explicit octupolar approximation of the excluded volume could still be a good choice, for other cylindrically symmetric convex bodies, the general method proposed in this paper might be even a better choice.

VI. CONCLUSIONS

The major objective of this paper was to express explicitly the excluded volume $V_e \{ \mathcal{B}_1, \mathcal{B}_2 \}$ of two arbitrary cylindrically symmetric, convex bodies $\mathcal{B}_1$ and $\mathcal{B}_2$ (with symmetry axes $\mathbf{m}_1$ and $\mathbf{m}_2$), in terms of shape functionals to be evaluated separately for $\mathcal{B}_1$ and $\mathcal{B}_2$. We accomplished this task by relating the coefficients $B_n$ that represent $V_e \{ \mathcal{B}_1, \mathcal{B}_2 \}$ in the basis of Legendre polynomials $P_n(\mathbf{m}_1 \cdot \mathbf{m}_2)$ to certain anisotropic volume averages which, in

\[\text{FIG. 5. Excluded volume } V_e \text{ of two congruent circular cones, } \mathcal{C}_1^\alpha \text{ and } \mathcal{C}_2^\alpha \text{ with slant height } L \text{ and semi-amplitude } \alpha_0 = 0.14 \pi \text{ corresponding to the minimum value of the scaled average } \langle V_e \rangle / V_c, \text{ where } V_c \text{ is the volume of each cone. Two graphs, plotted against the angle } 0 \leq \vartheta \leq \pi \text{ made by the cones’ axes, are delivered by (4) truncated at } n = 3 \text{ (solid line) and } n = 9 \text{ (dashed line). The third graph (dotted line) represents the octupolar approximation proposed in [15], which interpolates the excluded volumes of parallel } (\vartheta = 0) \text{ and antiparallel } (\vartheta = \pi) \text{ configurations.}\]

\[\text{(29)}\]

\[9 \text{ Since the expansion in (4) is an approximation in the } L^2\text{-norm, and not pointwise.}\]
complete analogy with the classical Minkowski formula for the isotropic average of the excluded volume, were expressed in terms of shape functionals that extend Minkowski’s. As demonstrated by the example of cones, which we worked out in full details, the extended Minkowski functionals can be evaluated exactly. A large number of them might be required to obtain $V_e\{B_1, B_2\}$ at a high degree of accuracy, but the proposed method provides them exactly in any desired number.

As also witnessed by the room taken by cones in this paper, one motivation of our study was to explore the role of shape polarity in the excluded volume of tapered bodies. It has already been shown that when such congruent bodies $B_1$ and $B_2$ are convex and cylindrically symmetric, $V_e\{B_1, B_2\}$ attains its minimum in the antiparallel configuration. Therefore, one could think of assigning a shape dipole $d$ to these bodies by extracting from $V_e\{B_1, B_2\}$ the dipolar component, $B_1 m_1 \cdot m_2$, and rewriting it formally as $d_1 \cdot d_2$. Instead, we proved that $B_1 \equiv 0$, thus making elusive the definition of the any shape dipole for a tapered, cylindrically symmetric, convex body. Clearly, the antipolar property revealed by the minimum of $V_e\{B_1, B_2\}$ remains valid, but it can in general be read off from the coefficient $B_3$, and so properly speaking it is an octupolar effect.

Cones indeed interested us because they are tapered, but they are not the easiest cylindrically symmetric, convex bodies for which one would compute the excluded volume. Perhaps, ellipsoids of revolution come first in anyone’s wish list, as little is known about their excluded volume. Yes, there are overlap criteria used in computer simulations, as there are also approximations such as that stipulated in the Gaussian overlap model originally introduced in [28].

Several other applications could be foreseen for our representation formula. In tune again with Onsager’s paper [1], we mention just one: the role of shape in steric interactions of filamentous viruses. This was indeed the original motivation of Onsager’s work, which intended to provide a theoretical explanation for the liquid crystalline behavior of tobacco mosaic viruses, which were the first to be isolated and purified [33]. An up-to-date review of the recent applications of Onsager’s theory to viruses of various elongated shapes can be found in [34]. We trust that our representation formula for the excluded volume could help making the role of viruses’ shape more explicit.

ACKNOWLEDGMENTS

One of us (EGV) is indebted to Peter Palffy-Muhoray for having raised the question about which would be the most appropriate definition of shape dipole for a cylindrically symmetric rigid body, which prompted the study presented here.

Appendix A: Mathematical details

In this appendix we record for completeness the mathematical details needed to make our development rigorous, but which would have hampered our presentation if dispersed in the main body of the paper. We start by recalling the essentials of convex body geometry; they are extracted from the wider treatment presented in Appendix A of [15], to which the interested reader is referred for a better appreciation of the formalism adopted in this paper.

1. Essentials of convex body geometry

A convex body $B$ in the three-dimensional space $E$ is represented here through the radial mapping $\nu \mapsto r(\nu)$, which associates to each unit vector $\nu$ in the unit sphere $S^2$ of $E$ the point on the boundary $\partial B$ of $B$ where the outward unit normal is precisely $\nu$. Such a representation requires $S^2$ to be mapped univocally onto $\partial B$, which is the case whenever $B$ belongs to the class $X^+$ of convex bodies with smooth boundaries and strictly positive curvatures. Such an assumption is not a true limitation to our development, as $X^+$ is indeed dense in the whole class $X$ of convex bodies with respect to the Hausdorff metric. Thus, the values attained in $X \setminus X^+$ by a continuous functional defined in $X^+$ can be computed as limits on appropriate approximating sequences of bodies in $X^+$. This property

\[10\] Actually, for selected $m_1$ and $m_2$ on the symmetry axes of the congruent bodies $B_1$ and $B_2$, one could either orient the vectors $d_1$ and $d_2$ along $m_1$ and $m_2$, respectively, or in the opposite directions, provided their orientations are reverted in both bodies.

\[11\] An Onsager theory for hard-ellipsoids based on this approximation can be found in [29], a paper well aware of the possible inaccuracies stemming from the hard-body modification of the simple Gaussian overlap model [30]. See also [31] for a recent review of the Gaussian overlap model for hard-ellipsoids.

\[12\] The excluded area of two ellipses is obtained at once from their distance of closest approach. Unfortunately, the extension to ellipsoids in three space dimensions of the method that was successful in two dimensions can only be performed numerically [32].
is for example exploited in Sec. A4a below to compute the contribution of a sharp ridge to the extended Minkowski functionals introduced in Sec. IV.\textsuperscript{13}

Figure 6 illustrates our representation of $B$ through its radial mapping $r$. It also shows that the unit outward normal $n$ to $\partial B$, which by construction at the point $r(\nu)$ coincides with $\nu$, can also be regarded as a field on $\partial B$. Its surface gradient $\nabla_s n$ is the curvature tensor and can be represented as

$$\nabla_s n = \sigma_1 e_1 \otimes e_1 + \sigma_2 e_2 \otimes e_2,$$

where the positive scalars $\sigma_1$ and $\sigma_2$ are the principal curvatures of $\partial B$, and the orthogonal unit vectors $e_1$ and $e_2$, both tangent to $\partial B$, designates the principal directions of curvature. In this paper, fully devoted to cylindrically symmetric bodies, we have conventionally taken $e_1$ along the local meridian, so that $e_1$, $n$, and the symmetry axis $m$ of $B$ are everywhere in one and the same plane (possibly varying with the point selected on $\partial B$). Figure 7 shows the geometric situation envisaged here.

The mean curvature $H$ and the Gaussian curvature $K$ are defined in terms of the principal curvatures as

$$H := \frac{1}{2}(\sigma_1 + \sigma_2) \quad \text{and} \quad K := \sigma_1 \sigma_2. \tag{A2}$$

The former can also be expressed as

$$H = \text{tr} \nabla_s n = \frac{1}{2} \text{div}_s n, \tag{A3}$$

where $\text{tr}$ is the trace operator and $\text{div}_s$ denotes the surface divergence. Similarly, letting $A^*$ denote the adjugate of a second-rank tensor $A$,\textsuperscript{14} we also have that

$$(\nabla_s n)^* = Kn \otimes n = K\nu \otimes \nu. \tag{A4}$$

The surface gradient $\nabla_s r$ of the radial mapping $r$ over $S^2$ has an expression similar to (A1),

$$\nabla_s r = \rho_1 e_1 \otimes e_1 + \rho_2 e_2 \otimes e_2, \tag{A5}$$

\textsuperscript{13} The very same property makes it possible to arrive at the expressions for the extended $M$ and $S$ functionals of a cone $\mathcal{C}^n$ listed in Sec. V.

\textsuperscript{14} $A^*$ is characterized by requiring that $A^*(u \times v) = Au \times Av$, for all vectors $u$ and $v$, where $\times$ denotes the cross product of vectors (see also Sec. 2.11 of [18]).
where

\[ \rho_1 := \frac{1}{\sigma_1} \quad \text{and} \quad \rho_2 := \frac{1}{\sigma_2} \quad \text{(A6)} \]

are the principal radii of curvature of \( \partial \mathcal{B} \). In complete analogy with (A1), we have that

\[ (\nabla_s r)^* = \frac{1}{K} \nu \otimes \nu, \quad \text{(A7)} \]

whence it follows that the surface dilation ratio induced by the mapping \( r \) that sends \( S^2 \) onto \( \partial \mathcal{B} \) is given by\(^\text{15}\)

\[ \frac{da(n)}{da(\nu)} = |(\nabla_s r)^*| = \frac{1}{K}. \quad \text{(A8)} \]

Putting together (A5), (A6), (A3), and (A2), we can also write

\[ \text{div}_s r = \rho_1 + \rho_2 = \frac{1}{K} \text{div}_s n. \quad \text{(A9)} \]

In the following, we shall also denote by \( x \) the position vector on \( \partial \mathcal{B} \). Formally, the fields \( \nu \) and \( n \) are related through \( x \) by the relations

\[ \nu = n(x) \quad \text{and} \quad x = r(\nu). \quad \text{(A10)} \]

A theorem that we have often used in this paper is the surface-divergence theorem.\(^\text{16}\) It says that

\[ \int_{\mathcal{F}} \text{div}_s u \, da(n) = \int_{\mathcal{F}} (\text{div}_s n) u \cdot n \, da(n) = 2 \int_{\mathcal{F}} H u \cdot n \, da(n), \quad \text{(A11)} \]

for any continuously differentiable field \( u \) defined on a closed smooth surface \( \mathcal{F} \) with unit outer normal \( n \) and mean curvature \( H \).

Three continuous functionals defined on the whole class \( \mathcal{X} \) of convex bodies were introduced by Minkowski. They are the total mean curvature \( M \), the surface area \( S \), and the volume \( V \). For a body \( \mathcal{B} \in \mathcal{X}^+ \), they are defined and represented as follows:\(^\text{17}\)

\[ M[\mathcal{B}] := \int_{\partial \mathcal{B}} H \, da(n) = \int_{S^2} r \cdot \nu \, da(\nu), \quad \text{(A12a)} \]

\[ S[\mathcal{B}] := \int_{\partial \mathcal{B}} \, da(n) = \int_{S^2} \frac{1}{K} \, da(\nu) = \int_{S^2} \nu \cdot (\nabla_s r)^* \, da(\nu), \quad \text{(A12b)} \]

\[ V[\mathcal{B}] := \frac{1}{3} \int_{\partial \mathcal{B}} n \cdot x \, da(n) = \frac{1}{3} \int_{S^2} r \cdot \nu \frac{1}{K} \, da(\nu) = \frac{1}{3} \int_{S^2} (\nu \cdot r) \nu \cdot (\nabla_s r)^* \, da(\nu). \quad \text{(A12c)} \]

As shown in greater details in \([15]\), one of the advantages of representing a body \( \mathcal{B} \) in \( \mathcal{X}^+ \) through its radial mapping \( r \) is that the Minkowski sum \( \mathcal{B}_1 + \mathcal{B}_2 \) of two bodies, \( \mathcal{B}_1 \) and \( \mathcal{B}_2 \), represented by the radial mappings \( r_1 \) and \( r_2 \), respectively, is represented by the radial mapping \( r_{12} = r_1 + r_2 \). Correspondingly, the fundamental functionals in (A12) evaluated on the Minkowski sum of two bodies, \( \mathcal{B}_1 \) and \( \mathcal{B}_2 \), of \( \mathcal{X}^+ \) are delivered by\(^\text{18}\)

\[ M[\mathcal{B}_1 + \mathcal{B}_2] = M[\mathcal{B}_1] + M[\mathcal{B}_2], \quad \text{(A13a)} \]

\[ S[\mathcal{B}_1 + \mathcal{B}_2] = S[\mathcal{B}_1] + S[\mathcal{B}_2] + \int_{S^2} \left[ \sin^2 \phi \left( \rho_1^{(1)} \rho_1^{(2)} + \rho_2^{(1)} \rho_2^{(2)} \right) + \cos^2 \phi \left( \rho_1^{(1)} \rho_2^{(2)} + \rho_2^{(1)} \rho_1^{(2)} \right) \right] \, da(\nu), \quad \text{(A13b)} \]

\(^15\) See also Sec. 5.2 of \([18]\).

\(^16\) See also Sec. 5.2.3 of \([35]\).

\(^17\) See Appendix A of \([15]\), for more details

\(^18\) See (A25), (A43), and (A49) of \([15]\).
\[
V[B_1 + B_2] = V[B_1] + V[B_2] + \frac{1}{3} \int_{\mathbb{S}^2} \left( \mathbf{\nu} \cdot \mathbf{r}_1 \frac{1}{K^{(1)}} + \mathbf{\nu} \cdot \mathbf{r}_2 \frac{1}{K^{(2)}} \right) da(\mathbf{\nu}) \\
+ \frac{1}{3} \int_{\mathbb{S}^2} (\mathbf{\nu} \cdot \mathbf{r}_1 + \mathbf{\nu} \cdot \mathbf{r}_2) \sin^2 \phi \left( \rho_1^{(1)} \rho_1^{(2)} + \rho_2^{(1)} \rho_2^{(2)} \right) + \cos^2 \phi \left( \rho_1^{(1)} \rho_2^{(2)} + \rho_2^{(1)} \rho_1^{(2)} \right) da(\mathbf{\nu}),
\]

where \(\rho_1^{(1)}\) and \(\rho_2^{(1)}\) are the principal radii of curvature of \(\partial B_1\), \(\rho_1^{(2)}\) and \(\rho_2^{(2)}\) are those of \(\partial B_2\), \(\phi \in [0, 2\pi]\) is the angle of the rotation about \(\mathbf{\nu}\) that brings the pair of principal curvature directions \((e_1^{(1)}, e_2^{(1)})\) of \(B_1\) into the pair of principal curvature directions \((e_1^{(2)}, e_2^{(2)})\) of body \(B_2\), and \(K^{(1)} = (\rho_1^{(1)} \rho_2^{(1)})^{-1}, K^{(2)} = (\rho_1^{(2)} \rho_2^{(2)})^{-1}\) are the Gaussian curvatures of \(\partial B_1\) and \(\partial B_2\), respectively.

We finally remark that for a body \(B \in \mathcal{K}^+\) represented by the radial mapping \(\mathbf{r}(\mathbf{\nu})\), the central inverse \(B^*\) (relative to the same origin \(o\)) is represented by the radial mapping \(\mathbf{r}^*(\mathbf{\nu})\) defined by

\[
\mathbf{r}^*(\mathbf{\nu}) := -\mathbf{r}(\mathbf{\nu}).
\]

As a result, if \(\mathbf{r}_1\) and \(\mathbf{r}_2\) are the radial mappings representing the bodies \(B_1\) and \(B_2\) in \(\mathcal{K}^+\), the body \(B_1 + B_2^*\), whose volume is the excluded volume \(V_e\{B_1, B_2\}\) of the pair \((B_1, B_2)\), is represented by the radial mapping

\[
\mathbf{r}_e(\mathbf{\nu}) := \mathbf{r}_1(\mathbf{\nu}) - \mathbf{r}_2(\mathbf{\nu}).
\]

It is not difficult to show with aid of (A15) that the shape functionals defined in (24) for \(B \in \mathcal{K}^+\) are invariant under the transformation \(B \mapsto B^*\).

2. Anisotropic volume averages

The anisotropic volume averages \(\langle P_n(\mathbf{V}) \rangle_{B_1, B_2}\) are defined in (13). The first average \(\langle P_1(\mathbf{V}) \rangle_{B_1, B_2}\) has been computed in Sec. III; here we compute all others. The method employed will be the same as in Sec. III, but to make it effective we need to replace (19) with the more general addition formula (see Sec. 18.18.9 of [19]),

\[
P_n(m_1 \cdot m_2) = P_n(\sin \vartheta_1 \sin \vartheta_2 \cos \phi + \cos \vartheta_1 \cos \vartheta_2) = P_n(\cos \vartheta_1) P_n(\cos \vartheta_2) \\
+ 2 \sum_{k=1}^{n} \frac{(n-k)! (n+k)!}{2^{2k} (n!)^2} (\sin \vartheta_1)^k (\sin \vartheta_2)^k P^{(k,k)}_{n-k} \cos \vartheta_1 P^{(k,k)}_{n-k} \cos \vartheta_2 \cos k \phi,
\]

where \(P_n^{(\alpha,\beta)}\) is the Jacobi polynomial of degree \(n\) and indices \((\alpha, \beta)\). Jacobi polynomials are defined in the interval \([-1, 1]\) and are orthogonal relative to the weight function \(w(x) = (1-x)^{\alpha}(1+x)^{\beta}\). They enjoy the symmetry property

\[
P_n^{(\alpha,\beta)}(-x) = (-1)^n P_n^{(\beta,\alpha)}(x)
\]

and can be represented as finite sums (see Sec. 18.5.8 of [19]),

\[
P_n^{(\alpha,\beta)}(x) = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n+\alpha}{k} \binom{n+\beta}{n-k} (x-1)^{n-k} (x+1)^k.
\]

The first three Jacobi polynomials that interest us are

\[
P_0^{(2,2)}(x) = 1, \quad P_1^{(2,2)}(x) = 3x, \quad P_2^{(2,2)}(x) = 7x^2 - 1.
\]

With the aid of (18) and (A17), we establish the identity,

\[
\frac{1}{2\pi} \int_{0}^{2\pi} P_n(m_1 \cdot \mathbf{\nu}) P_n(m_2 \cdot \mathbf{\nu}) \left[ \sin^2 \phi \left( \rho_1^{(1)} \rho_1^{(2)} + \rho_2^{(1)} \rho_2^{(2)} \right) + \cos^2 \phi \left( \rho_1^{(1)} \rho_2^{(2)} + \rho_2^{(1)} \rho_1^{(2)} \right) \right] d\phi \\
= P_n(m_1 \cdot \mathbf{\nu}) P_n(m_2 \cdot \mathbf{\nu}) \left( \rho_1^{(1)} + \rho_2^{(1)} \right) \left( \rho_1^{(2)} + \rho_2^{(2)} \right) \\
- \frac{(n-2)! (n+2)!}{(4n!)^2} \left[ (m_1 \cdot \mathbf{\nu})^2 \right] \left[ (m_2 \cdot \mathbf{\nu})^2 \right] P_{n-2}^{(2,2)}(m_1 \cdot \mathbf{\nu}) P_{n-2}^{(2,2)}(m_2 \cdot \mathbf{\nu}) \left( \rho_1^{(1)} - \rho_2^{(1)} \right) \left( \rho_1^{(2)} - \rho_2^{(2)} \right),
\]

where, as stipulated above, the principal directions of curvatures \(e_1^{(1)}\) and \(e_1^{(2)}\) for bodies \(B_1\) and \(B_2\), respectively, to which the principal radii of curvature \(\rho_1^{(1)}\) and \(\rho_1^{(2)}\) are correspondingly associated, lie orderly on the planes \((m_1, n)\)
and \((m_2, n)\). Use of (17), (A17), and (A20) in (A14) leads us to

\[
\langle P_n V \rangle [\mathcal{B}_1, \mathcal{B}_2] = \frac{1}{3} \left( \mathbb{P}_n \frac{(m_2 \cdot \nu)}{K^{(2)}} \right)_\nu \int_{S^2} (\nu \cdot r_1) P_n (m_1 \cdot \nu) da(\nu) + (\nu \cdot r_2) P_n (m_2 \cdot \nu) \int_{S^2} \frac{P_n (m_1 \cdot \nu)}{K^{(1)}} \\nu 
+ \frac{1}{6} \left( \mathbb{P}_n (m_2 \cdot \nu) \left( \rho_1^{(1)} + \rho_2^{(2)} \right) \right)_\nu \int_{S^2} (\nu \cdot r_1) P_n (m_1 \cdot \nu) \left( \rho_1^{(1)} + \rho_2^{(1)} \right) da(\nu) 
+ \frac{1}{6} \left( (\nu \cdot r_2) P_n (m_2 \cdot \nu) \left( \rho_1^{(1)} + \rho_2^{(2)} \right) \right)_\nu \int_{S^2} P_n (m_1 \cdot \nu) \left( \rho_1^{(1)} + \rho_2^{(1)} \right) da(\nu) 
- \frac{1}{6} \frac{(n - 2)! (n + 2)!}{(4n)!^2} \langle 1 - (m_2 \cdot \nu)^2 \rangle P_n^{(2, 2)} (m_2 \cdot \nu) \left( \rho_1^{(1)} - \rho_2^{(1)} \right) da(\nu) 
\times \int_{S^2} [1 - (m_1 \cdot \nu)^2] (\nu \cdot r_1) P_n^{(2, 2)} (m_1 \cdot \nu) \left( \rho_1^{(1)} - \rho_2^{(2)} \right) da(\nu) 
- \frac{1}{6} \frac{(n - 2)! (n + 2)!}{(4n)!^2} \langle 1 - (m_2 \cdot \nu)^2 \rangle (\nu \cdot r_2) P_n^{(2, 2)} (m_2 \cdot \nu) \left( \rho_1^{(2)} - \rho_2^{(2)} \right) da(\nu) 
\times \int_{S^2} [1 - (m_1 \cdot \nu)^2] (\nu \cdot r_2) P_n^{(2, 2)} (m_1 \cdot \nu) \left( \rho_1^{(2)} - \rho_2^{(2)} \right) da(\nu) .
\]

(A21)

To accomplish our task we need now compute all the integrals featuring in (A21). To make this easier, it is expedient to realize that they result from parameterizing some general shape functionals through the radial mappings \(r_1\) and \(r_2\) of bodies \(\mathcal{B}_1\) and \(\mathcal{B}_2\). For a cylindrically symmetric body \(\mathcal{B} \in \mathcal{K}^+\), by (A8), we see that

\[
\int_{S^2} \frac{P_n (m \cdot \nu)}{K} da(\nu) = \int_{\partial \mathcal{B}} P_n (m \cdot n) da(n).
\]

(A22a)

Similarly, also by use of (A5), (A6), and (A2), we easily arrive at

\[
\int_{S^2} (\nu \cdot r) P_n (m \cdot \nu) da(\nu) = \int_{\partial \mathcal{B}} (\nu \cdot x) P_n (m \cdot n) K da(n),
\]

(A22b)

\[
\int_{S^2} P_n (m \cdot \nu) (\rho_1 + \rho_2) da(\nu) = 2 \int_{\partial \mathcal{B}} P_n (m \cdot n) H da(n),
\]

(A22c)

\[
\int_{S^2} (\nu \cdot r) P_n (m \cdot \nu) (\rho_1 + \rho_2) da(\nu) = 2 \int_{\partial \mathcal{B}} (n \cdot x) P_n (m \cdot n) H da(n),
\]

(A22d)

\[
\int_{S^2} [1 - (m \cdot \nu)^2] (\nu \cdot r) P_n^{(2, 2)} (m \cdot \nu) (\rho_1 - \rho_2) da(\nu) = -2 \int_{\partial \mathcal{B}} [1 - (m \cdot n)^2] (n \cdot x) P_n^{(2, 2)} (m \cdot n) \frac{1}{2} (\sigma_1 - \sigma_2) da(n),
\]

(A22e)

\[
\int_{S^2} [1 - (m \cdot \nu)^2] P_n^{(2, 2)} (m \cdot \nu) (\rho_1 - \rho_2) da(\nu) = -2 \int_{\partial \mathcal{B}} [1 - (m \cdot n)^2] P_n^{(2, 2)} (m \cdot n) \frac{1}{2} (\sigma_1 - \sigma_2) da(n).
\]

(A22f)

In formulae (A22) we readily recognize the shape functionals defined in (24). With the aid of these definitions, we give (A21) the form (25) used in the main text.

3. Generating curve

Here we represent the boundary \(\partial \mathcal{B}\) of a cylindrically symmetric convex body \(\mathcal{B}\) as generated by the \(2\pi\)-rotation of a plane curve \(y(s)\) parameterized in the generic scalar \(s\). Such a curve crosses the symmetry axis along \(m\) in two poles, the uppermost of which is taken as the origin \(o\) (see Fig. 8). Identifying \(m\) with the unit vector \(e_z\) of a Cartesian frame \((e_x, e_y, e_z)\), we can then represent \(\partial \mathcal{B}\) as the surface

\[
x(s, \varphi) = r(s)e_r - a(s)e_z,
\]

(A23)

where

\[
e_r = \cos \varphi e_x + \sin \varphi e_y
\]

(A24a)

is the radial unit vector and

\[
e_\varphi = -\sin \varphi e_x + \cos \varphi e_y
\]

(A24b)
FIG. 8. (Color online) The plane curve \( y \), which generates \( \partial B \) by a \( 2\pi \)-rotation about \( m \), is parameterized in the generic scalar \( s \) as \( y(s) = x(s,0) \), where \( x(s,\varphi) \) is given by (A23).

is the associate orthogonal unit vector in the plane \( (e_x, e_y) \).

By letting \( s \) and \( \varphi \) depend on a parameter \( t \), we obtain a trajectory \( t \mapsto \xi(t) := x(s(t), \varphi(t)) \) on \( \partial B \). It follows from (A23) that

\[
\dot{\xi} = \dot{s} \sqrt{r'^2 + a'^2} t + \varphi r e_\varphi, \tag{A25}
\]

where a prime ’ denotes differentiation with respect to \( s \), a superimposed dot denotes differentiation with respect to \( t \), and

\[
t = \frac{r' e_r - a' e_z}{\sqrt{r'^2 + a'^2}} \tag{A26}
\]

is the unit tangent vector to \( y(s) \). From (A26) and (A25), we easily arrive at both the unit outward normal to \( \partial B \),

\[
n = \frac{a' e_r + r' e_z}{\sqrt{r'^2 + a'^2}} \tag{A27}
\]

and the surface area element

\[
da(n) = r \sqrt{r'^2 + a'^2} ds d\varphi. \tag{A28}
\]

By further differentiating \( n \) along the trajectory \( \xi(t) \), we obtain that

\[
\dot{n} = \frac{s(a'' r' - a' r'')}{\sqrt{r'^2 + a'^2}} t + \frac{\dot{\varphi} a'}{\sqrt{r'^2 + a'^2}} e_\varphi. \tag{A29}
\]

Since \( \dot{n} = (\nabla_s n) \dot{\xi} \) and, by (A25),

\[
\dot{s} = \frac{\dot{\xi} \cdot t}{\sqrt{r'^2 + a'^2}} \quad \text{and} \quad \dot{\varphi} = \frac{\dot{\xi} \cdot e_\varphi}{r}, \tag{A30}
\]

for \( \dot{\xi} \) is arbitrary, we conclude that

\[
\nabla_s n = \frac{a'' r' - a' r''}{(r'^2 + a'^2)^{3/2}} t \otimes t + \frac{a'}{r \sqrt{r'^2 + a'^2}} e_\varphi \otimes e_\varphi, \tag{A31}
\]

whence we read off at once the principal curvatures of \( \partial B \).

Figure 9 depicts the generating curve for a circular cone \( C^\alpha \) with vertex in the origin \( o \), semi-amplitude \( \alpha \), radius \( R \) and height \( h \), which are related to the slant height \( L \) through the equations

\[
R = L \sin \alpha, \quad h = L \cos \alpha. \tag{A32}
\]

The functions \( r(s) \) and \( a(s) \) featuring in (A23) are correspondingly given by

\[
r(s) = s \sin \alpha \quad \text{and} \quad a(s) = s \cos \alpha, \tag{A33}
\]

where now \( s \) has been chosen as the arc-length along the slant height of the cone; it follows from (A31) that

\[
\sigma_1 = 0 \quad \text{and} \quad \sigma_2 = \frac{\cot \alpha}{s}. \tag{A34}
\]
FIG. 9. (Color online) The generating curve of a circular cone \( \varphi^\alpha \) with semi-amplitude \( \alpha \), radius \( R \) and height \( h \), the two latter related to the slant height \( L \) as in (A32). The parameter \( s \) here represents the arc-length along the slant side of the cone.

4. Extended \( M \) and \( S \) functionals of a circular ridge

Here we apply the formalism presented in Sec. A 3 to compute the extended \( M \) and \( S \) functionals defined in Sec. IV for a circular ridge \( \mathcal{R} \) of radius \( R \), where neither \( H \) nor \( K \) are defined. To this end, we replace \( \mathcal{R} \) with a toroidal approximation \( \mathcal{R}_\varepsilon \) with equatorial radius \( R \) and meridian radius \( \varepsilon \), whose outer unit normal \( n \) spans the sector in which the angle \( \theta \) that it makes with the symmetry axis \( m \) ranges in the interval \( [\theta_1, \theta_2] \). To afford a greater generality (and in view of our application to cones in Sec. V above), we choose the origin \( o \) on the symmetry axis at the generic distance \( h \) from the ridge’s plane (see Fig. 10). Our strategy will be to compute the extended \( M \) and \( S \) functionals on \( \mathcal{R}_\varepsilon \) and then take the limit as \( \varepsilon \to 0^+ \). The functions \( r(s) \) and \( a(s) \) introduced in Sec. A 3 which here describe \( \mathcal{R}_\varepsilon \) are

\[
r(s) = R + \varepsilon \sin \theta(s), \quad a(s) = h - \varepsilon \cos \theta(s),
\]

(A35)

where \( \theta \) and \( s \) are related through \( s - s_1 = \varepsilon (\theta(s) - \theta_1) \), with \( s_1 \) an arbitrary constant. It easily follows from (A31) and (A35) that

\[
\sigma_1 = \frac{1}{\varepsilon}, \quad \sigma_2 = \frac{\sin \theta}{R + \varepsilon \sin \theta}.
\]

(A36)

Moreover, (A28) yields

\[
da(n) = (R + \varepsilon \sin \theta) \varepsilon d\theta d\varphi.
\]

(A37)

Using (A36) and (A37) in the definitions of the extended \( M \) and \( S \) functionals in (24), and then taking the limit...
as \( \varepsilon \to 0^+ \), we arrive at the following expressions:

\[
M_n[R] = \pi R \int_{\theta_1}^{\theta_2} P_n(\cos \theta) d\theta, \quad (A38a)
\]

\[
M'_n[R] = 2\pi \int_{\theta_1}^{\theta_2} (R \sin \theta - h \cos \theta) \sin \theta P_n(\cos \theta) d\theta, \quad (A38b)
\]

\[
M''_n[R] = \pi R \int_{\theta_1}^{\theta_2} \sin^2 \theta P_{n-2}^{(2,2)}(\cos \theta) d\theta, \quad (A38c)
\]

\[
S_n[R] = 0, \quad (A38d)
\]

\[
S'_n[R] = \pi R \int_{\theta_1}^{\theta_2} (R \sin \theta - h \cos \theta) P_n(\cos \theta) d\theta, \quad (A38e)
\]

\[
S''_n[R] = \pi R \int_{\theta_1}^{\theta_2} (R \sin \theta - h \cos \theta) \sin^2 \theta P_{n-2}^{(2,2)}(\cos \theta) d\theta. \quad (A38f)
\]

a. Extended \( M \) and \( S \) functionals for a disk

Formulae (A38) are instrumental to obtaining the explicit expressions for the extended \( M \) and \( S \) functionals of a disk \( D \) of radius \( R \). As before, we start by replacing \( D \) with an approximating rounded body, the spherodisk \( D_\varepsilon \) defined as the Minkowski sum of \( D \) and a ball \( B^{3}_\varepsilon \) of radius \( \varepsilon \) and center coincident with the center of \( D \). Figure 11 illustrates both \( D_\varepsilon \) and the generating curve of its boundary. The extended \( M \) and \( S \) functionals for \( D_\varepsilon \) will be obtained by taking the limit as \( \varepsilon \to 0^+ \) in those computed for \( D_\varepsilon \). Since \( \partial D_\varepsilon \) consists of two flat parallel disks, for which both principal curvatures vanish, and the toroidal approximation \( R_\varepsilon \) of the circular rim \( R \) of \( D \), for which the angles \( \theta_1 \) and \( \theta_2 \) in Fig. 10 are \( \theta_1 = 0 \) and \( \theta_2 = \pi \), respectively. Apart from the limit as \( \varepsilon \to 0^+ \) of \( S_n[D_\varepsilon] \), which is immediate to compute, for all other functionals this limit follows directly from (A38) by setting \( h = 0 \) and choosing \( \theta_1 \) and \( \theta_2 \) as above. We thus arrive at

\[
M_n[D] = \pi R \int_{\theta_1}^{\pi} P_n(\cos \theta) d\theta, \quad (A39a)
\]

\[
M'_n[D] = 2\pi R \int_{0}^{\pi} P_n(\cos \theta) \sin^2 \theta d\theta, \quad (A39b)
\]

\[
M''_n[D] = \pi R \int_{0}^{\pi} P_{n-2}^{(2,2)}(\cos \theta) \sin^2 \theta d\theta, \quad (A39c)
\]

\[
S_n[D] = \pi R^2 \left( P_n(1) + P_n(-1) \right), \quad (A39d)
\]

\[
S'_n[D] = \pi R^2 \int_{0}^{\pi} P_n(\cos \theta) \sin \theta d\theta, \quad (A39e)
\]

\[
S''_n[D] = \pi R^2 \int_{0}^{\pi} P_{n-2}^{(2,2)}(\cos \theta) \sin^3 \theta d\theta. \quad (A39f)
\]

In particular, it follows from (A39) that all extended \( M \) and \( S \) functionals with an odd index \( n \) vanish for a disk.
5. Invariance under translations

The anisotropic volume averages for which we found in (25) an explicit representation in terms of the extended Minkowski functionals are clearly invariant under the full Euclidean group comprising both translations and rotations. On the other hand, as clearly shown by equations (24), while all extended $M$ and $S$ functionals are invariant under translations, those that also appear to be invariant under translations are only $M_n$, $M_n''$, and $S_n$, $M_n'[\mathcal{B}]$, $S_n'[\mathcal{B}]$, and $S_n''[\mathcal{B}]$ are expressed as integrals over the boundary $\partial \mathcal{B}$ of the body $\mathcal{B}$ of fields that depend explicitly on the origin $o$ through the position vector $x$. Here we shall show that, despite all appearances, $M_n'$ is indeed invariant under translations, whereas both $S_n'$ and $S_n''$ are not. For the latter two, we shall also give explicit formulae that describe how they are affected by a translation. Of course, the combination of these functionals in (25) must be translation-invariant. We shall exploit this fact in Sec. A 6 below to show that functionals $M_n''$ and $M_n'$ are not independent, a conclusion which would be hard to reach by direct comparison of their definitions.

Translating a body $\mathcal{B}$ by the vector $a$ is formally equivalent to taking the Minkowski sum $\mathcal{B} + a$ of $\mathcal{B}$ and the point in space identified by $a$. Moreover, since all extended $M$ and $S$ functionals are invariant under rotations, computed on $\mathcal{B} + a$ for any given $\mathcal{B}$, they are isotropic functions of $a$. It readily follows from (24b) that

$$M_n'[\mathcal{B} + a] = M_n'[\mathcal{B}] + a \cdot \int_{\partial \mathcal{B}} P_n(m \cdot n) K \, da(n).$$

(A40)

The integral on the right side of (A40) is an isotropic vector-valued function of $m$; as such, by the Cauchy theorem on isotropic vector-valued functions, it must be proportional to $m$. Thus, (A40) becomes

$$M_n'[\mathcal{B} + a] = M_n'[\mathcal{B}] + a \cdot m \int_{\partial \mathcal{B}} (m \cdot n) P_n(m \cdot n) K \, da(n).$$

(A41)

For $\mathcal{B} \in \mathcal{K}^+$, by use of (A8), we see that

$$\int_{\partial \mathcal{B}} (m \cdot n) P_n(m \cdot n) K \, da(n) = \int_{\mathbb{R}} P_1(m \cdot \nu) P_n(m \cdot \nu) \, da(\nu) = 2\pi \int_{-1}^1 P_1(x) P_n(x) \, dx = 0 \quad \forall \ n \geq 2,$$

(A42)

where the last equality follows from the orthogonality of Legendre polynomials. Since we have already proved in Sec. III that $M_1[\mathcal{B}]$ vanishes identically for all $\mathcal{B} \in \mathcal{K}^+$, by (A42) we conclude that all functionals $M_n$ are invariant under translations.

This is not the case for both $S_n'$ and $S_n''$. Reasoning precisely as above and making use of the recurrence relations

$$xP_n(x) = \frac{n+1}{2n+1} P_{n+1}(x) + \frac{n}{2n+1} P_{n-1}(x),$$

(A43a)

$$xP_{n-2}(x) = \frac{(n-1)(n+3)}{(n+1)(2n+1)} P_{n-1}(x) + \frac{n}{2n+1} P_{n-3}(x),$$

(A43b)

the latter valid for $n \geq 2$ and with the postulation that $P_{-1}^{(2,2)} \equiv 0$, we arrive at

$$S_n'[\mathcal{B} + a] = S_n'[\mathcal{B}] + a \cdot m \left( \frac{n+1}{2n+1} M_{n+1}[\mathcal{B}] + \frac{n}{2n+1} M_{n-1}[\mathcal{B}] \right),$$

(A44a)

$$S_n''[\mathcal{B} + a] = S_n''[\mathcal{B}] + a \cdot m \left( \frac{(n-1)(n+3)}{(n+1)(2n+1)} M_{n+1}''[\mathcal{B}] + \frac{n}{2n+1} M_{n-1}''[\mathcal{B}] \right),$$

(A44b)

the latter valid for $n \geq 2$ and with the postulation that $M_n''[\mathcal{B}] \equiv 0$.

6. Reduction formulae

Here we take advantage of the general formulae (A44) just established and of the specific expressions for the extended $M$ and $S$ functionals obtained in (A39) to show that each functional $M_n''$ reduces to $M_n$ and to substantiate our conjecture that so should equally do each $M_n'$.

---

19 See, for example, Sec. 18.9.1 of [19].
a. $M''_n$ reduced to $M_n$

By requiring that the anisotropic volume averages, as expressed by (25), be invariant under translations for all bodies $B_1$ and $B_2$, a laborious but easy computation relying on (A44) and the translation-invariance of $M'_n$ shows that

$$M''_n[B] = a''_nM_n[B], \quad \text{(A45)}$$

where the coefficients $a''_n$ must obey the recurrence equation

$$\frac{(n+3)(n+2)}{16(n+1)n}a''_{n+1}a''_n = 1, \quad \text{(A46)}$$

whose explicit solution is

$$a''_n = \frac{4n}{n+2}. \quad \text{(A47)}$$

b. $M'_n$ reduced to $M_n$?

Inspired by (A47), we computed the ratio $a'_n$ of $M'_n[B]$ to $M_n[B]$ for a disk $D$; with the aid of (A39a) and (A39b), we realized that for a large number of values of $n$ it agrees with

$$a'_n = -\frac{2}{(n-1)(n+1)} \quad \forall \ n \geq 2. \quad \text{(A48)}$$

We were thus led to conjecture that

$$M'_n[B] = -\frac{2}{(n-1)(n+1)}M_n[B] \quad \forall \ n \geq 2 \quad \text{(A49)}$$

for all bodies $B$. Although we could not establish (A49) on a firmer basis, we checked by use of (28a) and (28b) that it is valid when $B$ is taken to be the cone $C'^{\alpha}$, for all values of the semi-amplitude $\alpha$. We are aware that (A47) and (A48) have a completely different standing, as the former has been proved rigorously, whereas the latter can at most be conjectured. Our development in the main body of the paper relies neither on (A47) nor on (A48). We heeded them here to witness the inquiries we have made on the general structure of the extended Minkowski functionals introduced in this work.

7. Legendre coefficients for the excluded volume of cones

Letting $B_1$ and $B_2$ be two congruent circular cones, $C'^{\alpha}$ and $C'^{\beta}$, with semi-amplitude $\alpha$, with the aid of (12), (25), and (28) we arrived at the following explicit formulae for the first eight Legendre coefficients $B_n$ plotted in Figs. 3
and 4(b) as functions of $\alpha$:

$$B_0 = \frac{15}{12} \pi L^3 \sin \alpha (6 \alpha \sin^2 \alpha + 3 \pi \sin^2 \alpha + 14 \sin \alpha \cos \alpha + 6 \alpha \sin \alpha + 3 \pi \sin \alpha + 6 \cos \alpha),$$  \hfill (A50a)

$$B_1 = 0,$$  \hfill (A50b)

$$B_2 = \frac{5}{12} \pi L^3 \sin \alpha (-18 \cos^5 \alpha + 18 \cos^3 \alpha - 4 \cos \alpha + 4 \alpha \cos^2 \alpha - 4 \alpha + 2 \alpha \cos^2 \alpha - 2 \pi$$
$$+ 12 \sin \alpha \cos^3 \alpha + 6a \sin \alpha \cos^2 \alpha + 3 \pi \sin \alpha \cos^2 \alpha - 4 \sin \alpha \cos \alpha - 4 \alpha \sin \alpha - 2 \pi \sin \alpha),$$  \hfill (A50c)

$$B_3 = \frac{35}{12} \pi L^3 \sin^3 \alpha \cos^5 \alpha,$$  \hfill (A50d)

$$B_4 = -\frac{3}{2048} \pi L^3 \sin \alpha (-10150 \cos 7 \alpha + 6530 \cos 3 \alpha - 1280 \cos 3 \alpha + 48 \cos \alpha + 4900 \sin 3 \alpha - 24 \pi \cos^2 \alpha$$
$$+ 24 \pi - 48 \alpha \cos^2 \alpha + 48 \alpha + 1120 \sin 5 \alpha \sin \alpha + 105 \pi \cos 4 \alpha \sin \alpha \sin \alpha + 210 \pi \cos 4 \alpha \sin \alpha$$
$$- 1040 \sin \alpha \cos 3 \alpha - 120 \alpha \sin \alpha \cos^2 \alpha - 240 \alpha \sin \alpha \cos^2 \alpha$$
$$+ 48 \sin \alpha \cos \alpha + 24 \pi \sin \alpha + 48 \alpha \sin \alpha),$$  \hfill (A50e)

$$B_5 = \frac{13}{65536} \pi L^3 \sin^3 \alpha \cos^5 \alpha (243 \cos 4 \alpha - 396 \cos^2 \alpha + 160),$$  \hfill (A50f)

$$B_6 = \frac{11}{65536} \pi L^3 \sin \alpha (-1074570 \cos^9 \alpha + 596498 \cos^7 \alpha - 149044 \cos^5 \alpha + 12656 \cos^3 \alpha - 160 \cos \alpha$$
$$+ 899052 \cos 11 \alpha + 80 \pi \cos^2 \alpha - 80 \pi + 160 \alpha \cos^2 \alpha - 160 \alpha - 284592 \cos 13 \alpha + 19712 \cos^7 \alpha \sin \alpha$$
$$+ 2310 \sin \alpha \cos \alpha + 1155 \pi \sin \alpha \cos \alpha - 30016 \cos^5 \alpha \sin \alpha - 1890 \pi \cos^4 \alpha \sin \alpha$$
$$- 3780 \pi \cos^4 \alpha \sin \alpha + 10976 \sin \alpha \cos^3 \alpha + 840 \pi \sin \alpha \cos^2 \alpha + 1680 \sin \alpha \sin \alpha$$
$$- 160 \sin \alpha \cos \alpha - 80 \pi \sin \alpha - 160 \alpha \sin \alpha),$$  \hfill (A50g)

$$B_7 = \frac{3}{2177} \pi L^3 \sin^3 \alpha \cos^5 \alpha (102245 \cos 8 \alpha - 273702 \cos^6 \alpha + 274472 \cos^4 \alpha - 121968 \cos^2 \alpha + 20160),$$  \hfill (A50h)

where $L$ is the cone’s slant height. They are recorded here both for completeness and as an illustration of the method proposed in this paper.

### Appendix B: Shape-reconstruction method

In this appendix we describe the method adopted for reconstructing the boundary of the excluded body $\partial B_e \{ C_1^a, C_2^a \}$ for two congruent circular cones $C_1^a$ and $C_2^a$ of semi-amplitude $\alpha$ and slant height $L$, hereafter simply denoted $\partial B_e$ for short. More precisely, the method reconstructs a triangular surface mesh that, depending on a fundamental parameter to be described, approximates $\partial B_e$ at any degree of precision. From the surface mesh, the approximate value of the excluded volume $V[\partial B_e]$ can be computed immediately.

The method adopted for this task is a pipeline of two algorithmic components:

1. an online vector quantization algorithm that includes a generator of random point samples from $\partial B_e$ and which produces a configuration of reference vectors $W$;

2. a surface reconstruction algorithm that produces from $W$ the triangulated surface mesh that represents an approximation to $\partial B_e$;

The method described is similar to that in [15]. In particular, the random generator of point samples from $\partial B_e$ is essentially the same. In that context, however, all target surfaces $\partial B_e$ were generated from spheri-cones and could be assumed to be smooth, so that the reconstruction process could be embedded into step 1 above via the SOAM algorithm [36]. By contrast, in the case of cones considered here, the presence of ridges and cusps in $\partial B_e$ forces adopting a different strategy. In the rest of this appendix, the main aspects of this new strategy are discussed in detail.

#### 1. Sampling the surface boundary

Random point samples from $\partial B_e$ can be generated with a procedure based on equation (A16), reproduced here for convenience:

$$r_e(\nu) = r_1(\nu) - r_2(-\nu).$$

Here $r_e$ reaches a point on $\partial B_e$ and $r_1$ and $r_2$, in this specific case, designate points on $\partial C_1^a$ and $\partial C_2^a$, respectively. Random points on $\partial B_e$ can be obtained either by generating a random vector reaching a point on $\partial C_1^a$ and then...
finding a vector to a point on $\partial B_e$ that has opposite normal $-\mathbf{v}$ or by reverting this very procedure: the sum of the vectors thus obtained will belong to $\partial B_e$.

The main difficulty in implementing such a random generator is to guarantee positive sampling probability almost everywhere on $\partial B_e$, that is, apart from subsets of zero area measure. On all smooth components of a circular cone, in fact, the Gaussian curvature $K$ vanishes and this means that in general a normal vector $\mathbf{v}$ does not identify uniquely one point on the cone’s surface. Furthermore, the Minkowski sum of two straight lines on the boundary of each cone can result in a surface patch with positive area measure on $\partial B_e$, despite the fact that each line has zero area measure and thus no chances of being sampled, unless specific provisions are introduced. Appendix B in [15] describes how these problems can be circumvented in actual computations.

Although the requirement of positive sampling probability almost everywhere can be enforced in practice, no known method guarantees uniform sampling probability over $\partial B_e$. As shown in Fig. 12(a), the overall sampling obtained with the chosen random point generation method is indeed non-uniform.

2. Vector quantization: adaptive neural gas

Many well-known algorithms for surface reconstruction work considerably better when the input point cloud is as close as possible to a uniform sample of the target surface and are often hampered when this is not the case. Apart from greater time complexity, these difficulties can lead in practice to the need for accurate verification of results and possibly to manual post-processing, to correct imperfections.

The intended purpose of a vector quantization algorithm in this context is to obtain both an improvement in the uniformity of sampling and a quantitative reduction in the number of points to be used for surface reconstruction. The algorithm of choice is an adaptive variant of the neural gas (NG) algorithm [39] and works as follows:

1. initialize $W$ with a pre-defined number $k$ of reference vectors $w_i$ positioned at random on $\partial B_e$;
2. generate a random point $p$ from $\partial B_e$;
3. find the nearest reference vector in $W$, i.e. $w_i := \arg\min_{w_j \in W} \|p - w_j\|$;
4. if $\|p - w_i\| \leq r$, where $r$ is a fixed threshold, adapt all reference vectors in $W$ by
   \[ \Delta w_i = \varepsilon \cdot h_\lambda(k_i(p))(p - w_i) \]
   where $k_i(p) := \#\{w_j : \|p - w_j\| < \|p - w_i\|\}$ (# denotes cardinality), $\varepsilon > 0$ is a real parameter and
   \[ h_0(n) := \delta_0n \quad \text{and} \quad h_\lambda(n) := e^{-\lambda n}, \text{ for } \lambda > 0; \]
5. otherwise, if $p$ is farther away from $w_i$, add a new reference vector $p$ to $W$;

20 Known methods for uniform sampling presuppose knowledge of the surface’s analytic description plus further specific conditions [37].
21 More precisely, the relevant requisite in this respect is that the point sampling should be at least locally uniform [38].
6. unless a maximum number of iterations $T$ has been reached, return to step 2.

As evident from step 5, this algorithm is adaptive in the number of reference vectors in $W$; in particular, this means that the level of refinement of the sampling of $\partial B_e$ provided by $W$ can be controlled through the value of the fundamental threshold $r$.

In [39] it is proven that, when the value of the constant $\varepsilon$ tends to 0 as the iterations progress, the NG algorithm performs a stochastic gradient descent towards a (local) minimum of an overall cost function and that its configuration tends to obey the power law

$$
\rho(w) \propto P(w)^\gamma \quad \text{with} \quad \gamma := \frac{d}{d+2},
$$

where $d$ is the dimension of the input space being sampled, that is $d = 2$ in this case. Here $\rho(w)$ is the density of reference vectors in $W$ at $w$ and $P(w)$ is the sampling probability. Since the exponent $\gamma$ is smaller than 1, the overall configuration of $W$ tends to be closer to uniformity than the sampling probability $P$. This effect is clearly visible in Fig. 12(b).

### 3. Surface reconstruction

With proper parameter settings (see below), the reconstruction of a triangular mesh from the final configuration $W$ produced by the adaptive NG algorithm poses no particular problem and could be performed in full automation. In this work we used the ball-pivoting algorithm [40] which joins in a triangular face any three vectors in $W$ whose ends are touched by a ball of a given radius $r$ that does not contain any other vector’s end from the same set. One example of the results of this procedure is shown in Figs. 12(c) and (d). Further examples are shown in Fig. 13, which contains a gallery of shapes produced with the method described above.

![Fig. 13](image-url)

**FIG. 13.** Gallery of reconstructed boundaries $\partial B_e$ for pairs of congruent circular cones of semi-amplitude $\alpha$. Rows correspond to values of $\alpha$ equal to $\frac{\pi}{32}$, $\frac{\pi}{6}$ and $\frac{15}{32}\pi$, respectively, while columns correspond to values of the angle $\vartheta$ between the symmetry axes $m_1$ and $m_2$ equal to 0, $\frac{\pi}{2}$ and $\pi$, respectively. All figures are in the same scale and frame of reference.
4. Implementation and benchmark

The adaptive NG vector quantization algorithm, together with the generator of random points from $\partial \mathcal{B}_e$, has been implemented in Java. In order to speed the execution up, the algorithm has been converted to a multi-threaded version suitable for multi-core computers, along the lines described in [41]. For surface reconstruction, we used the implementation of the ball-pivoting algorithm included in the Meshlab open-source tool [42].

The overall method for shape reconstruction was validated using Minkowski’s formula for isotropic volume average (15) together with the cone-specific functionals (27). For benchmarking, pairs of congruent circular cones $C^1$ and $C^2$ having slant height $L$ and semi-amplitude $\alpha$ varying from $\frac{\pi}{2}$ to $\frac{15\pi}{8}$ with step $\frac{\pi}{8}$ were considered. For each such pair, the value of $V[\mathcal{B}_e]$ was computed for angles $\theta$ between the two symmetry axes $m_1$ and $m_2$ varying from $0$ to $\pi$ with step $\frac{\pi}{32}$; the isotropic average of the resulting sequence of volumes was then computed and compared with the exact value of $\langle V[\mathcal{B}_e] \rangle$. The fundamental threshold $r$, which governs the density of reference vectors in $W$ with respect to $\partial \mathcal{B}_e$, was determined empirically with the objective of having a difference less than 0.02% between the exact value of each isotropic average and the corresponding value computed numerically. A value $r = \frac{\pi}{160}L$ was found to be adequate (see also the comparative plots in Figs. 4(a) and (b)). Also the value of $T = 120\text{M}$ maximum equivalent iterations of the NG algorithm was determined empirically. In the actual experiments, the execution was split into 4 concurrent threads, each processing in multi-signal mode (see [41]) 250 random points per iteration. Being dependent on the area of $\partial \mathcal{B}_e$, the number of reference vectors in the final configurations of $W$ varied greatly, from 3,592 to 41,689.

All numerical experiments were run on a workstation based on an Intel® Xeon® CPU E3-1240 v3, 3.4 GHz CPU with 8 GB of RAM. As for computing times, the most demanding part of the method is running the $T = 120\text{M}$ equivalent iterations of the adaptive NG algorithm. For each pair of cones and for each pose, with the precision required, this computation took on average about 4.254 seconds (i.e. about 71 minutes) to complete.

[1] L. Onsager, “The effects of shape on the interaction of colloidal particles,” Ann. N.Y. Acad. Sci. 51, 627–659 (1949), reprinted in [43], pp. 625–657.
[2] D. Frenkel, “Perspective on “The effect of shape on the interaction of colloidal particles”,” Theor. Chem. Acc. 103, 212–213 (2000).
[3] D. Frenkel, “Entropy-driven phase transitions,” Physica A 263, 26–38 (1999), Proceedings of the 20th IUPAP International Conference on Statistical Physics.
[4] X. Zheng and P. Palffy-Muhoray, “Distance of closest approach of two arbitrary hard ellipses in two dimensions,” Phys. Rev. E 75, 061709 (2007).
[5] J. Vieillard-Baron, “Phase transitions of the classical hard-ellipse system,” J. Chem. Phys. 56, 4729–4744 (1972).
[6] W. M. Gelbart and A. Gelbart, “Effective one-body potentials for orientationally anisotropic fluids,” Mol. Phys. 33, 1387–1398 (1977).
[7] L. Mederos, E. Velasco, and Y. Martínez-Ratón, “Hard-body models of bulk liquid crystals,” J. Phys.: Condens. Matter 26, 463101 (2014).
[8] J.-P. Hansen and I. R. McDonald, Theory of Simple Liquids, 4th ed. (Academic Press, Oxford, 2013) with Applications to Soft Matter.
[9] D. Frenkel, “Onsager’s spherocylinders revisited,” J. Phys. Chem. 91, 4912–4916 (1987).
[10] D. Frenkel, “Onsager’s spherocylinders revisited [Erratum],” J. Phys. Chem. 92, 5314–5314 (1988).
[11] H. Brunn, “Über Ovale und Eiflächen,” München (1887).
[12] H. Minkowski, “Volumen und Oberflächen,” Math. Ann. 57, 447–495 (1903).
[13] T. Bonnesen and W. Fenchel, Theory of Convex Bodies (BCS Associates, Moscow, Idaho, USA, 1987) translated from the German Theorie der konvexen Körper (Springer, Berlin, 1934) and edited by L. Boron, C. Christenson, and B. Smith, with the collaboration of W. Fenchel.
[14] R. Schneider, Convex Bodies: The Brunn-Minkowski Theory, Encyclopedia of Mathematics and its Applications, Vol. 44 (Cambridge University Press, Cambridge, 1993).
[15] M. Piastra and E. G. Virga, “Octupolar approximation for the excluded volume of axially symmetric convex bodies,” Phys. Rev. E 88, 032507 (2013).
[16] G. S. Singh and B. Kumar, “Molecular fluids and liquid crystals in convex-body coordinate systems,” Ann. Phys. 294, 24–47 (2001).
[17] B. M. Mulder, “The excluded volume of hard spheroidotopes,” Mol. Phys. 103, 1411–1424 (2005).
[18] M. E. Gurtin, E. Fried, and L. Anand, The Mechanics and Thermodynamics of Continua (Cambridge University Press, Cambridge, 2010).
[19] DLMF, “NIST Digital Library of Mathematical Functions,” http://dlmf.nist.gov/, Release 1.0.6 of 2013-05-06, online companion to [44].
[20] I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic Press, New York, 1980) corrected and enlarged edition prepared by A. Jeffrey.

[21] T. Kihara, “Virial coefficients and models of molecules in gases,” Rev. Mod. Phys. 25, 831–843 (1953).

[22] T. Kihara, “On Ishihara-Hayashida’s theory of the second virial coefficient for rigid convex molecules,” J. Phys. Soc. Japan 8, 686–687 (1953).

[23] A. Ishihara, “Determination of molecular shape by osmotic measurement,” J. Chem. Phys. 18, 1446–1449 (1950).

[24] A. Ishihara and T. Hayashida, “Theory of high polymer solutions. I. Second virial coefficient for rigid ovaloids model,” J. Phys. Soc. Japan 6, 40–45 (1951).

[25] A. Ishihara and T. Hayashida, “Theory of high polymer solutions. II. Special forms of second osmotic coefficient,” J. Phys. Soc. Japan 6, 46–50 (1951).

[26] P. Palffy-Muhoray, E. G. Virga, and X. Zheng, “The minimum excluded volume of convex shapes,” J. Phys. A: Math. Theor. 47, 415205 (2014).

[27] J. W. Perram and M. S. Wertheim, “Statistical mechanics of hard ellipsoids. I. overlap algorithm and the contact function,” J. Comp. Phys. 58, 409–416 (1985).

[28] B. J. Berne and P. Pechukas, “Gaussian model potentials for molecular interactions,” The Journal of Chemical Physics 56, 4213–4216 (1972).

[29] S.-D. Lee, “The Onsager-type theory for nematic ordering of finite-length hard ellipsoids,” J. Chem. Phys. 89 (1988).

[30] V. R. Bhethanabotla and William Steele, “A comparison of hard-body models for axially-symmetric molecules,” Mol. Phys. 60, 249–251 (1987).

[31] R. C. Singh, “Structure of hard ellipsoids: The Gaussian overlap model,” J. Mol. Liquids 122, 1–10 (2005).

[32] X. Zheng, W. Iglesias, and P. Palffy-Muhoray, “Distance of closest approach of two arbitrary hard ellipsoids,” electronic-Liquid Crystals Communications (2008), http://www.e-lc.org/docs/2008_10_12_23_11_56.

[33] J. D. Bernal F. C. Bawden, N. W. Pirie and I. Fankuchen, “Liquid crystalline substances from virus-infected plants,” Nature 138, 1051–1052 (1936).

[34] Z. Dogic and S. Fraden, “Ordered phases of filamentous viruses,” Curr. Opin. Colloid Interface Sci. 11, 47–55 (2006).

[35] A. M. Sonnet and E. G. Virga, *Dissipative Ordered Fluids. Theories for Liquid Crystals* (Springer, New York, 2012).

[36] M. Piastra, “Self-organizing adaptive map: Autonomous learning of curves and surfaces from point samples,” Neural Networks 41, 96–112 (2013).

[37] M. Arndt, “A method for generating uniform point distributions on a sample surface,” Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment 588, 509 – 513 (2008).

[38] T. K. Dey, *Curve and Surface Reconstruction* (Cambridge University Press, 2006).

[39] T. M. Martinetz, S. G. Berkovich, and K. J. Schulten, “Neural-gas network for vector quantization and its application to time-series prediction,” IEEE Trans. Neural Networks 4, 558–569 (1993).

[40] F. Bernardini, J. Mittleman, H. Rushmeier, C. Silva, and G. Taubin, “The ball-pivoting algorithm for surface reconstruction,” Visualization and Computer Graphics, IEEE Transactions on 5, 349–359 (1999).

[41] G. Parigi, A. Stramieri, D. Pau, and M. Piastra, “A multi-signal variant for the gpu-based parallelization of growing self-organizing networks,” in *Informatics in Control, Automation and Robotics* (Springer, 2014) pp. 83–100.

[42] P. Cignoni, M. Corsini, and G. Ranzuglia, “Meshlab: an open-source 3d mesh processing system,” Ercim news 73, 45–46 (2008).

[43] T. J. Sluckin, D. A. Dunmur, and H. Stegemeyer, *Crystals that Flow* (Taylor & Francis, London, New York, 2004).

[44] F. W. J. Olver, D. W. Lozier, R. F. Boisvert, and C. W. Clark, eds., *NIST Handbook of Mathematical Functions* (Cambridge University Press, New York, NY, 2010) print companion to [19].