Distance of closest approach of two arbitrary hard ellipsoids

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The distance of closest approach of particles with hard cores is a key parameter in statistical theories and computer simulations of liquid crystals and colloidal systems. In this Brief Report, we provide an algorithm to calculate the distance of closest approach of two ellipsoids of arbitrary shape and orientation. This algorithm is based on our previous analytic result for the distance of closest approach of two-dimensional ellipses. The method consists of determining the intersection of the ellipsoids with the plane containing the line joining their centers and rotating the plane. The distance of closest approach of the two ellipses formed by the intersection is a periodic function of the plane orientation, whose maximum corresponds to the distance of closest approach of the two ellipsoids.

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I. INTRODUCTION

The distance of closest approach of particles with hard cores is a key parameter in statistical theories and computer simulations of liquid crystals and colloidal systems. Although ellipsoids are the simplest nonspherical shapes, no analytic solution exists for the distance of their closest approach. For this reason, in liquid crystal theories, spherocylindrical hard cores are often used, for which the excluded volume and the shape of the excluded region can be exactly determined [1,2]. The latter is important for the determination of the effective single-particle potential in mean-field theories [2]. In computer simulations of ellipsoids, overlap criteria are typically used [3,4]. We have recently succeeded in obtaining a closed-form analytic expression for the distance of closest approach of two hard ellipses of arbitrary size and eccentricity [5]. Here we present an algorithm for finding the closest approach of two ellipsoids based on this analytic result. This algorithm may be useful for calculating excluded volumes and related quantities, such as elastic constants, for liquid crystals and colloids, and it may also provide an overlap criterion for ellipsoids in computer simulations.

II. DESCRIPTION AND SOLUTION OF THE PROBLEM

Consider two ellipsoids, each with a given shape and orientation, whose centers are on a line with a given direction. We wish to determine the distance between the centers when the ellipsoids are in point contact externally. This distance of closest approach is a function of the shapes of the ellipsoids and their orientation. There is no analytic solution for this problem, since solving for the distance requires the solution of a sixth-order polynomial equation [5]. Here we present an algorithm to determine this distance based on our analytic results for the distance of closest approach of ellipses in two dimensions (2D), which can be implemented numerically. Our algorithm consists of three steps.

(1) Constructing a plane containing the line joining the centers of the two ellipsoids and finding the equations of the ellipses formed by the intersection of this plane and the ellipsoids.

(2) Determining the distance of closest approach of the ellipses; that is, the distance between the centers of the ellipses when they are in point contact externally.

(3) Rotating the plane until the distance of closest approach of the ellipses is a maximum. The distance of closest approach of the ellipsoids is this maximum distance.

We detail steps 1 and 3 in the sections below. Step 2 is described in Refs. [5,6].

A. Step 1: Ellipses formed by the intersection of the ellipsoids and the plane

The shapes of the ellipsoids are specified by the lengths a, b, and c of their principal axes; the orientations are given by the unit vectors $\hat{\mathbf{l}}$, $\hat{\mathbf{m}}$, and $\hat{\mathbf{n}}$ along the principal axes (Fig. 1). The equations of the ellipsoids have the form

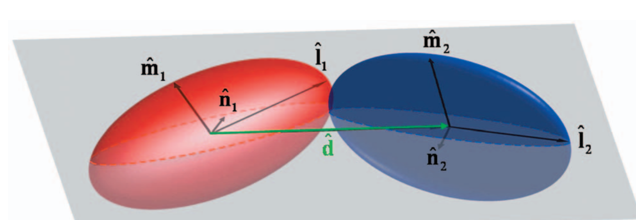

FIG. 1. (Color) Two externally tangent ellipsoids intersecting with a plane containing the line joining the centers. The semiaxes of the ellipsoid on the left are 10, 4, and 2, while those of the one on the right are 8, 6, and 2. The vector joining the centers has direction ⟨1,0,0⟩. The distance of their closest approach is 14.7163.

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$$\mathbf{r}\cdot\left(\frac{\hat{\mathbf{l}}\hat{\mathbf{l}}}{a^2}+\frac{\hat{\mathbf{m}}\hat{\mathbf{m}}}{b^2}+\frac{\hat{\mathbf{n}}\hat{\mathbf{n}}}{c^2}\right)\cdot\mathbf{r}=1. \quad (1)$$

We next assume that their centers are on a line whose direction is given by $\hat{\mathbf{d}}$.

We construct a plane which contains the line connecting the centers of the ellipsoids. The normal to the plane is $\hat{\mathbf{p}}$, and we define $\hat{\mathbf{s}}=\hat{\mathbf{p}}\times\hat{\mathbf{d}}$.

Since we want to rotate the plane, we define the initial direction of the normal $\hat{\mathbf{p}}_0$ as

$$\hat{\mathbf{p}}_0=\frac{\hat{\mathbf{d}}\times\hat{\mathbf{l}}_1}{|\hat{\mathbf{d}}\times\hat{\mathbf{l}}_1|}. \quad (2)$$

If $\hat{\mathbf{p}}_0=0$, then

$$\hat{\mathbf{p}}_0=\frac{\hat{\mathbf{d}}\times\hat{\mathbf{m}}_1}{|\hat{\mathbf{d}}\times\hat{\mathbf{m}}_1|}. \quad (3)$$

We denote rotation by the angle θ, then

$$\hat{\mathbf{p}}=(\cos\,\theta)\hat{\mathbf{p}}_0+(\sin\,\theta)(\hat{\mathbf{p}}_0\times\hat{\mathbf{d}}),\qquad \theta\in[0,\pi). \quad (4)$$

The unit vectors along the principal axes of the ellipsoids can be expressed in term of these coordinates,

$$\hat{\mathbf{l}}=l_x\hat{\mathbf{d}}+l_y\hat{\mathbf{s}}+l_z\hat{\mathbf{p}}, \quad (5)$$

$$\hat{\mathbf{m}}=m_x\hat{\mathbf{d}}+m_y\hat{\mathbf{s}}+m_z\hat{\mathbf{p}}, \quad (6)$$

$$\hat{\mathbf{n}}=n_x\hat{\mathbf{d}}+n_y\hat{\mathbf{s}}+n_z\hat{\mathbf{p}}. \quad (7)$$

Substitution into the equations of the ellipsoids, and noting that in the plane $\hat{\mathbf{r}}\cdot\hat{\mathbf{p}}=0$, gives, for the intersection of each ellipsoid with the plane,

$$\mathbf{r}\cdot\left[\left(\frac{l_x^2}{a^2}+\frac{m_x^2}{b^2}+\frac{n_x^2}{c^2}\right)\hat{\mathbf{d}}\hat{\mathbf{d}}+\left(\frac{l_yl_x}{a^2}+\frac{m_ym_x}{b^2}+\frac{n_yn_x}{c^2}\right)\hat{\mathbf{s}}\hat{\mathbf{d}} +\left(\frac{l_xl_y}{a^2}+\frac{m_xm_y}{b^2}+\frac{n_xn_y}{c^2}\right)\hat{\mathbf{d}}\hat{\mathbf{s}}+\left(\frac{l_y^2}{a^2}+\frac{m_y^2}{b^2}+\frac{n_y^2}{c^2}\right)\hat{\mathbf{s}}\hat{\mathbf{s}}\right]\cdot\mathbf{r}=1,$$

which can be written as

$$\mathbf{r}\mathbb{A}\mathbf{r}=1, \quad (8)$$

where

$$\mathbb{A}=\alpha\hat{\mathbf{d}}\hat{\mathbf{d}}+\beta\hat{\mathbf{s}}\hat{\mathbf{d}}+\beta\hat{\mathbf{d}}\hat{\mathbf{s}}+\gamma\hat{\mathbf{s}}\hat{\mathbf{s}}, \quad (9)$$

and we note that $\mathbb{A}$ is in 2D, in the space formed by the orthogonal vectors $\hat{\mathbf{d}}$ and $\hat{\mathbf{s}}$.

We next write

$$\mathbb{A}=u\mathbf{I}-v\hat{\mathbf{k}}\hat{\mathbf{k}}. \quad (10)$$

If u, v, and $\hat{\mathbf{k}}$ are determined, the equation of the ellipse in the plane is obtained in standard form [5,6]. We write

$$\hat{\mathbf{k}}=\cos\,\phi\hat{\mathbf{d}}+\sin\,\phi\hat{\mathbf{s}},$$

and then

$$\mathbb{A}=(\alpha\hat{\mathbf{d}}\hat{\mathbf{d}}+\beta\hat{\mathbf{s}}\hat{\mathbf{d}}+\beta\hat{\mathbf{d}}\hat{\mathbf{s}}+\gamma\hat{\mathbf{s}}\hat{\mathbf{s}}) =u\mathbf{I}-v(\cos\,\phi\hat{\mathbf{d}}+\sin\,\phi\hat{\mathbf{s}})(\cos\,\phi\hat{\mathbf{d}}+\sin\,\phi\hat{\mathbf{s}}).$$

Solving for ϕ, v and u gives

$$v=\sqrt{4\beta^2+(\alpha-\gamma)^2}, \quad (11)$$

$$\phi=\frac{1}{2}\tan^{-1}\left(\frac{-2\beta}{\gamma-\alpha}\right), \quad (12)$$

and

$$u=\gamma+v\,\sin^2\,\phi. \quad (13)$$

This enables writing the equations for the ellipses in standard form, and the analytic results of Refs. [5,6] can be used to determine the distance of closest approach $d(\theta)$ for the two ellipses as function of the orientation θ of the plane. The maximum distance of closest approach of the ellipses is the distance of closest approach d_c of the two ellipsoids.

B. Step 3: Maximizing the distance of closest approach of the ellipses as function of orientation of the plane

1. Uniqueness of the maximum

As the plane is rotated about the line joining the centers of the ellipsoids, the distance of closest approach of the ellipses has only one maximum and one minimum as function of the angle of rotation in the interval $[0,\pi)$. Consider the intersection of the two ellipsoids with the plane with arbitrary orientation. The distance of closest approach of the ellipses is d' ($<d_c$). If the two ellipsoids are now placed so that their centers are separated by distance d', they will interpenetrate, and their intersection will be one or two simple closed curves. Since the two ellipses on the plane are now tangent to each other at the point of contact, this point must be on one of the intersection curve as well as on the plane. If there are two intersection curves, this point will be on the curve which is closer to the line of centers. Furthermore, this point is the only point that the plane shares with the intersection curve. That is because if the plane were to share two points with the intersection curve, then either there should be another two ellipses on the plane tangent to each other, which is geometrically impossible, or the two ellipses share two common points, which contradicts the fact that they are tangent. Thus the plane has only one point in common with the intersection curve. Since the plane contains only one point on the intersection curve, there are at most two orientations θ of the plane containing only one point on the intersection curve. Therefore there are at most two values of θ giving the same distance d', which guarantees that there is a unique maximum and a unique minimum within the interval $[0,\pi)$.

2. Fast algorithm to locate the maximum

Standard numerical methods exist to find the extrema of functions. For example, the line search algorithm is an efficient method of unconstrained optimization [7]. More efficient special schemes exist which exploit special properties of functions. The golden section search is a fast scheme to

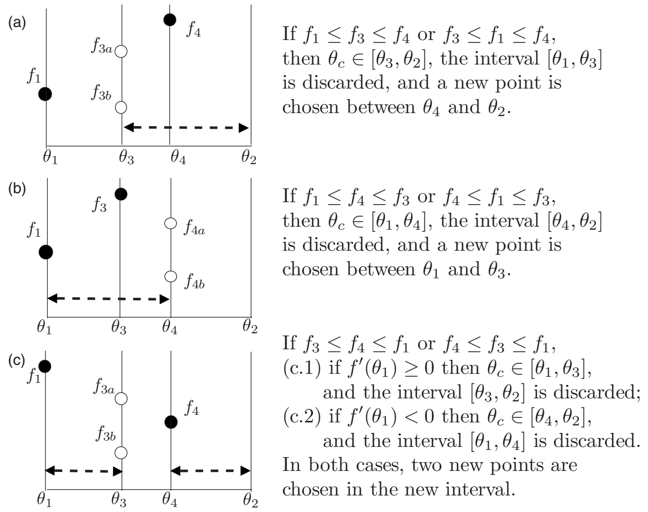

FIG. 2. Diagram illustrating scenarios for identifying the subinterval containing the maximum.

determine the extremum of a unimodal function [8]. Since $d(\theta)$ possesses a maximum as well as a minimum, the golden section search is not applicable. We have developed a fast algorithm, a modified version of the golden section search, to find the maximum of a periodic function with a single maximum and a single minimum per period.

We note that the maximum value of θ must occur between $\theta_1=0$ and $\theta_2=\pi$. As in the golden section search, we choose two points θ_3 and θ_4 inside the interval $[\theta_1, \theta_2)$, and they must satisfy

$$\theta_4 - \theta_1 = \theta_2 - \theta_3 = \frac{1}{\varphi}(\theta_2 - \theta_1), \quad \varphi = \frac{1+\sqrt{5}}{2}. \tag{14}$$

We next examine the relative positions of the first three leftmost values of the function. The three possible scenarios are illustrated in Fig. 2. In two of them, Figs. 2(a) and 2(b), the interval size can be reduced by discarding one subinterval at one end. In the next step, the remaining three points are relabeled, and one more point is chosen from the larger subinterval according to Eq. (14). In the third case, Fig. 2(c), the derivative at the first point must be evaluated in order to decide in which of the two subintervals the maximum is located. If the derivative is positive, the maximum is in the subinterval immediately to the right of the first point. If it is negative, the maximum is in the second disjoint subinterval. If the derivative is zero, the maximum is at the first point. Once the subinterval containing the maximum is identified, the appropriate subintervals are discarded, and two new points are chosen according to Eq. (14) in the remaining subinterval. The process is then repeated until the size of interval reaches the specified tolerance. This algorithm is fast, with the same speed of convergence as the golden section search, i.e., the size of the search interval converges linearly to zero.

C. Computational details

To make the results presented in this Brief Report more accessible, we have provided our source code in FORTRAN and C implementing this algorithm in the Appendix of Ref. [9]. In both programs, we used double precision throughout.

We note that in our implementations there may be a loss of accuracy for ellipsoids with large aspect ratios (e.g., ≥200) when using double precision. In the ellipse program, when the aspect ratio gets large, the ratios of the coefficients in the quartic equation get extremely large, and large number cancellations and/or rounding errors can lead to inaccurate results. If the aspect ratios of the ellipsoids are large (≥200), quadruple precision should be used. Benchmarks of computation time are given in the Appendix of Ref. [9].

We point out that the existing overlap criteria proposed by Vieillard-Baron [3] and by Perram and Wertheim [4] can also be used to determine the distance of closest approach. This can be accomplished via a 1D search (as in our case), essentially by varying the center-to-center distance and avoiding overlap. However, Ref. [3] works only for identical ellipsoids of revolution, whereas our scheme works in general. Reference [4] works for general ellipsoids; however, an optimization algorithm is required to determine overlap, making this scheme effectively a 2D search. Finally, our algorithm provides information that others do not, namely, the contact point.

III. CONCLUSION

We have developed an algorithm to calculate the distance of closest approach of two arbitrary hard ellipsoids. The algorithm is based on analytic results in the 2D case; it consists of determining the distance of closest approach of two ellipses formed by the intersection of a plane with the ellipsoids as the plane is rotated. The distance of closest approach of the ellipsoids is the maximum distance of closest approach of the ellipses. We have shown that there is only a single maximum and have developed a fast algorithm to find it. We expect these results to be useful in theoretical and numerical studies of condensed-matter systems consisting of ellipsoidal particles.

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