Distance of closest approach of two arbitrary hard ellipses in 2D

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Abstract

The distance of closest approach of hard particles is a key parameter of their interaction and plays an important role in the resulting phase behavior. For non-spherical particles, the distance of closest approach depends on orientation, and its calculation is surprisingly difficult. Although overlap criteria have been developed for use in computer simulations [1, 2], no analytic solutions have been obtained for the distance of closest approach of ellipsoids in 3-D, or, until now, for ellipses in 2-D. We have derived an analytic expression for the distance of closest approach of the centers of two arbitrary hard ellipses as function of their orientation relative to the line joining their centers. We describe our method for solving this problem, illustrate our result, and discuss its usefulness in modeling and simulating systems of anisometric particles such as liquid crystals.

I.   INTRODUCTION

Short range repulsive forces between atoms and molecules in soft condensed matter are often modeled by an effective hard core, which governs the proximity of neighbors. Since the attractive interaction with a few nearest neighbors usually dominates the potential energy, the distance of closest approach is a key parameter in statistical descriptions of condensed phases. Simple atoms and molecules with spherical symmetry can be viewed as having spherical hard cores; the distance of closest approach of the centers of identical hard spheres in 3-D or of hard circles in 2-D is the diameter. For non-spherical molecules, such as the constituents of liquid crystals, the distance depends on orientation, and its calculation is surprisingly difficult [3]. The simplest smooth non-spherical shapes are the ellipse and the ellipsoid. Although overlap criteria have been developed for use in computer simulations [1, 2], no analytic solutions for the distance of closest approach have been obtained for ellipsoids in 3-D, or, up to now, for ellipses in 2-D. The problem of determining the distance of closest approach for two ellipses is particularly intriguing because of its seductive apparent simplicity [3]. We have recently succeeded in deriving an analytic expression for the distance of closest approach of the centers of two arbitrary hard ellipses as function of their orientation relative to the line joining their centers. We describe our method for solving this problem, give the solution, illustrate our results, and discuss its usefulness in modeling and simulating systems of anisometric particles such as liquid crystals.

II.   STATEMENT OF THE PROBLEM

We consider two ellipses E_1 and E_2 in 2D with semi-axes lengths a_i and b_i where $a_i > b_i$, eccentricity $e_i = \sqrt{1 - \dfrac{b_i^2}{a_i^2}}$, and major axes oriented along the unit vectors $\hat{\mathbf{k}}_i$ ($i = 1, 2$). Initially the ellipses are distant so that they have no point in common. One ellipse is then translated towards the other along the line joining their centers until they are in point contact externally (see Fig. 1). The problem is to find the distance d between centers when the ellipses are so tangent; that is, to find the distance of closest approach.

The equation of the ellipses are:

$$E_1: \quad \mathbf{r}_1 \mathbb{A}_1 \mathbf{r}_1 = 1, \quad \mathbb{A}_1 = \frac{1}{b_1^2}\left(\mathbf{I} + \left(\frac{b_1^2}{a_1^2} - 1\right)\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1\right) = \frac{1}{b_1^2}(\mathbf{I} - e_1^2\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1) \qquad (1)$$
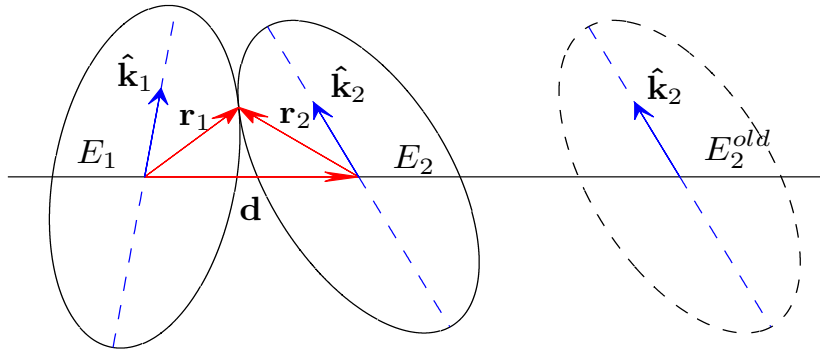
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FIG. 1: Two externally tangent ellipses E_1 and E_2. The directions of the major axes are given by $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$, the centers are joined by the vector $\mathbf{d}$.

and

$$E_2: \quad \mathbf{r}_2 \mathbb{A}_2 \mathbf{r}_2 = 1, \quad \mathbb{A}_2 = \frac{1}{b_2^2}\left(\mathbf{I} + \left(\frac{b_2^2}{a_2^2} - 1\right)\hat{\mathbf{k}}_2\hat{\mathbf{k}}_2\right) = \frac{1}{b_2^2}(\mathbf{I} - e_2^2\hat{\mathbf{k}}_2\hat{\mathbf{k}}_2), \tag{2}$$

where $\mathbf{I}$ is the identity matrix and $\hat{\mathbf{k}}_i\hat{\mathbf{k}}_i$ is the dyad product. The vector joining the centers is given by $\mathbf{d} = d\hat{\mathbf{d}}$; $\hat{\mathbf{d}}$ is a given unit vector. Our goal is to find the distance d as function of ellipse parameters a_1, b_1, a_2, b_2 and orientations $\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}$, $\hat{\mathbf{k}}_2 \cdot \hat{\mathbf{d}}$ and $\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2$.

It is tempting to seek a solution by solving the quadratic equations

$$\mathbf{r}_1 \mathbb{A}_1 \mathbf{r}_1 = 1 \tag{3}$$

and

$$(\mathbf{r}_1 - \mathbf{d})\mathbb{A}_2(\mathbf{r}_1 - \mathbf{d}) = 1 \tag{4}$$

simultaneously for the points of intersection, and then requiring that the distance d between centers be such that there is intersection exactly at one point. This approach fails for the following reason: although the components of $\mathbf{r}_1$ at the points of intersection can be obtained by solving a quartic equation (say for the x-component of $\mathbf{r}_1$), the condition requiring that

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the quartic have exactly one double real root is not straightforward to implement (there are four roots, and it is not clear which two roots need to coalesce to yield the required tangency condition) and it further gives an equation in d whose order is higher than quartic, and which cannot therefore be solved analytically.

III.   THE SOLUTION

Our approach proceeds via three steps:

(1) Transformation of the two tangent ellipses E_1 and E_2, whose centers are joined by the vector $\mathbf{d}$, into a circle C_1' and an ellipse E_2', whose centers are joined by the vector $\mathbf{d}'$. The circle C_1' and the ellipse E_2' remain tangent after the transformation.

(2) Determination of the distance d' of closest approach of C_1' and E_2' analytically.

(3) Determination of the distance d of closest approach of E_1 and E_2 by inverse transformation of the vector $\mathbf{d}'$.
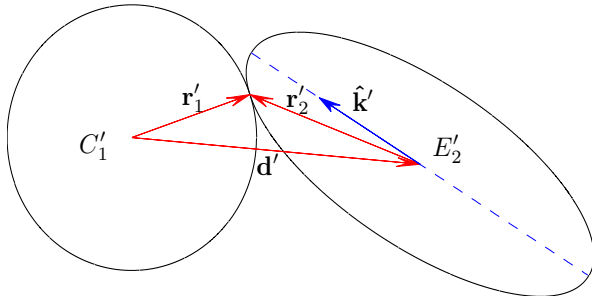
A.   Transformations

FIG. 2: The transformed circle C_1' and ellipse E_2' after applying transformation $\mathbb{T}$ to the ellipses in Fig. 1. The major axis of transformed ellipse E_2' is along $\hat{\mathbf{k}}'$, and the centers are joined by the vector $\mathbf{d}'$.

An ellipse can be transformed into a unit circle by anisotropic scaling. We introduce for this purpose the matrix $\mathbb{T}$, which transforms the ellipse E_1 into a unit circle C_1' and the ellipse E_2 into another ellipse E_2'. The transformation is a scaling by the factor $1/a_1$ along the $\hat{\mathbf{k}}_1$ direction and by the factor $1/b_1$ in the direction perpendicular to $\hat{\mathbf{k}}_1$. The transformation matrix $\mathbb{T}$, which transforms position $\mathbf{r}$ to a position $\mathbf{r}'$ in a space with dimensionless coordinates, is

$$\mathbb{T} = \frac{1}{b_1}\left(\mathbf{I} + \left(\frac{b_1}{a_1} - 1\right)\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1\right) \tag{5}$$

and the inverse, $\mathbb{T}^{-1}$, is

$$\mathbb{T}^{-1} = b_1\left(\mathbf{I} + \eta\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1\right), \tag{6}$$

where

$$\eta = \left(\frac{a_1}{b_1} - 1\right). \tag{7}$$

One can easily verify that $\mathbb{T}^{-1}\mathbb{A}_1\mathbb{T}^{-1} = \mathbf{I}$.

If $\mathbf{r}_i' = \mathbb{T}\mathbf{r}_i$, or, equivalently, $\mathbf{r}_i = \mathbb{T}^{-1}\mathbf{r}_i'$ ($i = 1, 2$), substitution into Eq. (1) gives a unit circle C_1' and a new ellipse E_2' (see Fig. 2). That is,

$$C_1': \quad \mathbf{r}_1\mathbb{A}_1\mathbf{r}_1 = \mathbf{r}_1'\mathbb{T}^{-1}\mathbb{A}_1\mathbb{T}^{-1}\mathbf{r}_1' = \mathbf{r}_1'\mathbf{r}_1' = 1 \tag{8}$$

and

$$E_2': \quad \mathbf{r}_2\mathbb{A}_2\mathbf{r}_2 = \mathbf{r}_2'\mathbb{T}^{-1}\mathbb{A}_2\mathbb{T}^{-1}\mathbf{r}_2' = \mathbf{r}_2'\mathbb{A}'\mathbf{r}_2' = 1. \tag{9}$$

$\mathbb{A}'$ can be written as

$$\mathbb{A}' = \frac{b_1^2}{b_2^2}(\mathbf{I} + \eta\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1)(\mathbf{I} - e_2^2\hat{\mathbf{k}}_2\hat{\mathbf{k}}_2)(\mathbf{I} + \eta\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1). \tag{10}$$

The eigenvectors of $\mathbb{A}'$ provide information about the directions of the principal axes and the eigenvalues about the lengths of the semi-axes of the transformed ellipse E_2'. Since $\mathbb{A}'$ is real symmetric, its eigenvalues λ_+ and λ_- are real, and the corresponding eigenvectors $\hat{\mathbf{k}}_+'$ and $\hat{\mathbf{k}}_-'$ are orthogonal. Explicit expressions for these are given in the Appendix. The lengths of the semi-axes, if $\lambda_+ > \lambda_-$, are given by

$$b_2' = \frac{1}{\sqrt{\lambda_+}},$$
$$a_2' = \frac{1}{\sqrt{\lambda_-}}, \tag{11}$$

and we note that $a_2' > b_2'$.

Under the transformation $\mathbb{T}$, the vector $\mathbf{d}$ is transformed to

$$\mathbf{d}' = \mathbb{T}\mathbf{d} = d\mathbb{T}\hat{\mathbf{d}} = d'\hat{\mathbf{d}}', \tag{12}$$

where $\hat{\mathbf{d}}' = \dfrac{\mathbb{T}\hat{\mathbf{d}}}{|\mathbb{T}\hat{\mathbf{d}}|}$ is a unit vector. Explicitly,

$$\mathbb{T}\hat{\mathbf{d}} = \frac{1}{b_1}\left(\hat{\mathbf{d}} + \left(\frac{b_1}{a_1} - 1\right)(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})\hat{\mathbf{k}}_1\right) \tag{13}$$

and

$$|\mathbb{T}\hat{\mathbf{d}}| = \frac{1}{b_1}\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}. \tag{14}$$

B. Distance d' of closest approach of a circle and an ellipse

We next derive the a useful relation between the position vector $\mathbf{r}$ of a point on the ellipse and the unit outward normal $\hat{\mathbf{n}}$ at that point. For an ellipse, given by $\mathbf{r}\mathbb{A}\mathbf{r} = 1$, the unit normal $\hat{\mathbf{n}}$ is

$$\hat{\mathbf{n}} = \frac{\nabla(\mathbf{r}\mathbb{A}\mathbf{r})}{|\nabla(\mathbf{r}\mathbb{A}\mathbf{r})|} = \frac{\mathbb{A}\mathbf{r}}{\sqrt{\mathbf{r}\mathbb{A}^2\mathbf{r}}}. \tag{15}$$

Multiplying Eq. (15) by $\mathbb{B} = \mathbb{A}^{-1}$ gives

$$\mathbb{B}\hat{\mathbf{n}} = \frac{\mathbf{r}}{\sqrt{\mathbf{r}\mathbb{A}^2\mathbf{r}}} \tag{16}$$

and multiplying $\mathbb{B}\hat{\mathbf{n}}$ by $\hat{\mathbf{n}}$ gives

$$\hat{\mathbf{n}}\mathbb{B}\hat{\mathbf{n}} = \frac{1}{\mathbf{r}\mathbb{A}^2\mathbf{r}}. \tag{17}$$

Substituting into (16), we obtain $\mathbf{r}$ in terms of the unit normal $\hat{\mathbf{n}}$

$$\mathbf{r} = \frac{\mathbb{B}\hat{\mathbf{n}}}{\sqrt{\hat{\mathbf{n}}\mathbb{B}\hat{\mathbf{n}}}}. \tag{18}$$

If a unit circle and an ellipse are externally tangent, then the directions of their normals at the point of contact must be opposite. If the unit outward normal of the unit circle C_1' at the point of contact is $\hat{\mathbf{n}}'$, then

$$\mathbf{r}_1' = \hat{\mathbf{n}}', \quad \mathbf{r}_2' = -\frac{\mathbb{B}'\hat{\mathbf{n}}'}{\sqrt{\hat{\mathbf{n}}'\mathbb{B}'\hat{\mathbf{n}}'}} \tag{19}$$

and we have, for the vector $\mathbf{d}'$ joining the centers,

$$\mathbf{d}' = \mathbf{r}_1' - \mathbf{r}_2' = \hat{\mathbf{n}}' + \frac{\mathbb{B}'\hat{\mathbf{n}}'}{\sqrt{\hat{\mathbf{n}}'\mathbb{B}'\hat{\mathbf{n}}'}}, \tag{20}$$

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where

$$\mathbb{B}' = \mathbb{A}'^{-1} = b_2'^2 \left(\mathbf{I} + \delta \hat{\mathbf{k}}'_- \hat{\mathbf{k}}'_- \right) \tag{21}$$

and

$$\delta = \frac{a_2'^2}{b_2'^2} - 1 > 0. \tag{22}$$

Eq. (20) is a key result. It is a vector equation with only two unknowns: the magnitude of $\mathbf{d}'$ and the direction of $\hat{\mathbf{n}}'$. It can be solved for d' as follows. We multiply both sides of Eq. (20) by $\hat{\mathbf{k}}'_-$ and by $\hat{\mathbf{k}}'_+$, and letting

$$\hat{\mathbf{k}}'_- \cdot \hat{\mathbf{d}}' = \sin\phi, \quad \hat{\mathbf{k}}'_- \cdot \hat{\mathbf{n}}' = \sin\psi, \quad \hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{d}}' = \cos\phi, \quad \hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{n}}' = \cos\psi, \tag{23}$$

we get, from Eq. (20),

$$d' \sin\phi = \sin\psi \left(1 + \frac{b_2'(1+\delta)}{\sqrt{1 + \delta \sin^2\psi}} \right) \tag{24}$$

and

$$d' \cos\phi = \cos\psi \left(1 + \frac{b_2'}{\sqrt{1 + \delta \sin^2\psi}} \right). \tag{25}$$

Here the unknowns are ψ and d'. In the special case of $\delta = 0$, $d' = 1 + b_2' = 1 + a_2'$, and in the case of $\phi = \dfrac{\pi}{2}$, $d' = 1 + b_2'\sqrt{1+\delta} = 1 + a_2'$. In general, $\phi \neq \dfrac{\pi}{2}$, and the solution for d' is more challenging.

We let $q = \sqrt{1 + \delta \sin^2\psi}$, then

$$\sin^2\psi = \frac{q^2 - 1}{\delta} \tag{26}$$

and

$$\cos^2\psi = 1 - \frac{q^2 - 1}{\delta}. \tag{27}$$

Substitution into Eq. (24)(a-b), squaring both sides and dividing these two equations to eliminate d' gives a quartic equation for q,

$$\tan^2\phi (\delta + 1 - q^2)(\frac{q}{b_2'} + 1)^2 = (q^2 - 1)(\frac{q}{b_2'} + 1 + \delta)^2. \tag{28}$$

This can be written in the standard form $Aq^4 + Bq^3 + Cq^2 + Dq + E = 0$, where the coefficients are

$$A = -\frac{1}{b_2'^2}(1 + \tan^2\phi), \tag{29a}$$

$$B = -\frac{2}{b_2'}(1 + \tan^2\phi + \delta), \tag{29b}$$

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$$C = -\tan^2\phi - (1+\delta)^2 + \frac{1}{b_2'^2}(1+(1+\delta)\tan^2\phi), \tag{29c}$$

$$D = \frac{2}{b_2'}(1+\tan^2\phi)(1+\delta), \tag{29d}$$

$$E = (1+\tan^2\phi+\delta)(1+\delta) \tag{29e}$$

and

$$\tan^2\phi = \frac{(\hat{\mathbf{k}}_-' \cdot \hat{\mathbf{d}}')^2}{1 - (\hat{\mathbf{k}}_-' \cdot \hat{\mathbf{d}}')^2}. \tag{30}$$

The roots of Eq. (28) can be obtained explicitly as follows.

To make contact with the standard solution of the quartic equation, using Ferrari's method [4], we define

$$\alpha = -\frac{3B^2}{8A^2} + \frac{C}{A}, \tag{31a}$$

$$\beta = \frac{B^3}{8A^3} - \frac{BC}{2A^2} + \frac{D}{A}, \tag{31b}$$

$$\gamma = \frac{-3B^4}{256A^4} + \frac{CB^2}{16A^3} - \frac{BD}{4A^2} + \frac{E}{A} \tag{31c}$$

and

$$P = -\frac{\alpha^2}{12} - \gamma, \tag{31d}$$

$$Q = -\frac{\alpha^3}{108} + \frac{\alpha\gamma}{3} - \frac{\beta^2}{8} \tag{31e}$$

and

$$U = \left(-\frac{Q}{2} + \sqrt{\frac{Q^2}{4} + \frac{P^3}{27}}\right)^{1/3}, \tag{31f}$$

where we take the principal values of the roots. If $U = 0$, then

$$y = -\frac{5}{6}\alpha - Q^{1/3}, \tag{32}$$

otherwise

$$y = -\frac{5}{6}\alpha + U - \frac{P}{3U}. \tag{33}$$

In terms of these, the one real positive root q is

$$q = -\frac{B}{4A} + \frac{1}{2}\left(\sqrt{\alpha + 2y} + \sqrt{-\left(3\alpha + 2y + \frac{2\beta}{\sqrt{\alpha + 2y}}\right)}\right). \tag{34}$$

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In the special case when $\alpha + 2y = 0$, then $\beta = 0$ (which we have not observed in this problem, but include here for completeness) and the positive real root is given by

$$q = -\frac{B}{4A} + \sqrt{\frac{-\alpha + \sqrt{\alpha^2 - 4\gamma}}{2}}. \tag{35}$$

Knowing q, d' can be found by squaring both sides of Eqs. (24)(a-b) and adding; this gives

$$d' = \sqrt{\frac{q^2 - 1}{\delta}\left(1 + \frac{b_2'(1+\delta)}{q}\right)^2 + \left(1 - \frac{q^2 - 1}{\delta}\right)\left(1 + \frac{b_2'}{q}\right)^2}. \tag{36}$$

The vector joining the centers of the circle and the ellipse is given by

$$\mathbf{d}' = d'\hat{\mathbf{d}}'. \tag{37}$$

C. Distance d of closest approach

The distance of closest approach of the two ellipses is obtained via the transformation from $\mathbf{d}'$ to $\mathbf{d}$,

$$\mathbf{d} = \mathbb{T}^{-1}\mathbf{d}' = d'\mathbb{T}^{-1}\hat{\mathbf{d}}' = d'\mathbb{T}^{-1}\frac{\mathbb{T}\hat{\mathbf{d}}}{|\mathbb{T}\hat{\mathbf{d}}|} = \frac{d'}{|\mathbb{T}\hat{\mathbf{d}}|}\hat{\mathbf{d}} = \frac{d'}{\frac{1}{b_1}\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}}\hat{\mathbf{d}}, \tag{38}$$

and finally we have

$$d = \frac{d'}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}}b_1. \tag{39}$$

This is the solution for the distance of closest approach, which is our main result.

D. Contact point

In addition to the distance of closest approach, it is interesting and useful to locate the point contact. We denote the vector from the center of Ellipse 1 to the point of contact as $\boldsymbol{r}_c$. In the transformed coordinate system, where Ellipse 1 has become a unit circle after the affine transformation, the vector from the center of circle to the point of contact is $\boldsymbol{r}_c' = \hat{\mathbf{n}}'$ where $\hat{\mathbf{n}}'$ is the unit normal at the point of contact, whose components along the orthogonal unit vectors $\hat{\mathbf{k}}_+'$ and $\hat{\mathbf{k}}_-'$ are known Thus, to obtain $\boldsymbol{r}_c$, it is only necessary to perform the transformation of $\hat{\mathbf{n}}'$, that is,

$$\boldsymbol{r}_c = \mathbb{T}^{-1}\hat{\mathbf{n}}' \tag{40}$$

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The components of $\hat{\mathbf{n}}'$ are given by

$$\hat{\mathbf{k}}'_- \cdot \hat{\mathbf{n}}' = \sin \psi, \quad \hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{n}}' = \cos \psi \tag{41}$$

where ψ is given by

$$\sin \psi = sgn(\sin \phi)\sqrt{\frac{q^2 - 1}{\delta}}, \tag{42}$$

$$\cos \psi = sgn(\cos \phi)\sqrt{1 - \frac{q^2 - 1}{\delta}}. \tag{43}$$

where $sgn(x)$ gives the sign of x and the angle ϕ is known.

It follows that

$$\hat{\mathbf{n}}' = \cos \psi \hat{\mathbf{k}}'_+ + \sin \psi \hat{\mathbf{k}}'_- \tag{44}$$

Writing $\hat{\mathbf{k}}'_+$ and $\hat{\mathbf{k}}'_-$ in terms of $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$

$$\hat{\mathbf{k}}'_+ = \cos \gamma \frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \sin \gamma \frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \tag{45}$$

where

$$\cos \gamma = \hat{\mathbf{k}}'_+ \cdot \frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \tag{46}$$

and

$$\sin \gamma = \hat{\mathbf{k}}'_+ \cdot \frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \tag{47}$$

$$\hat{\mathbf{k}}'_- = -\sin \gamma \frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \cos \gamma \frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \tag{48}$$

Substitution gives $\hat{\mathbf{n}}'$ in terms of $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$ gives

$$\hat{\mathbf{n}}' = \cos(\psi + \gamma)\frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \sin(\psi + \gamma)\frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \tag{49}$$

Now

$$\boldsymbol{r}_c = \mathbb{T}^{-1}\hat{\mathbf{n}}' = b_1\left(\mathbf{I} + \eta\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1\right)\hat{\mathbf{n}}' \tag{50}$$

and so

$$\boldsymbol{r}_c = b_1 \cos(\psi + \gamma)\frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + b_1 \sin(\psi + \gamma)\frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} +$$
$$(a_1 - b_1)\cos(\psi + \gamma)\frac{(1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\hat{\mathbf{k}}_1}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + (a_1 - b_1)\sin(\psi + \gamma)\frac{(1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\hat{\mathbf{k}}_1}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \tag{51}$$

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and finally

$$
\begin{aligned}
\boldsymbol{r}_c = &[(a_1 + (a_1 - b_1)\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\frac{\cos(\psi + \gamma)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + (a_1 - (a_1 - b_1)\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\frac{\sin(\psi + \gamma)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}]\hat{\mathbf{k}}_1 + \\
&[b_1 \cos(\psi + \gamma)\frac{1}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} - b_1 \sin(\psi + \gamma)\frac{1}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}]\hat{\mathbf{k}}_2 \qquad (52)
\end{aligned}
$$

IV. DISCUSSION

The above methods give a closed form expression for the distance of closest approach and the position of the point of contact for two ellipses of arbitrary size, eccentricity and orientation. Detailed steps of the calculation are given in the Appendix. To demonstrate the applicability of the method, we give two examples: calculation of the excluded area and the locus of the point of contact while one ellipse is fixed and the other is rotated.
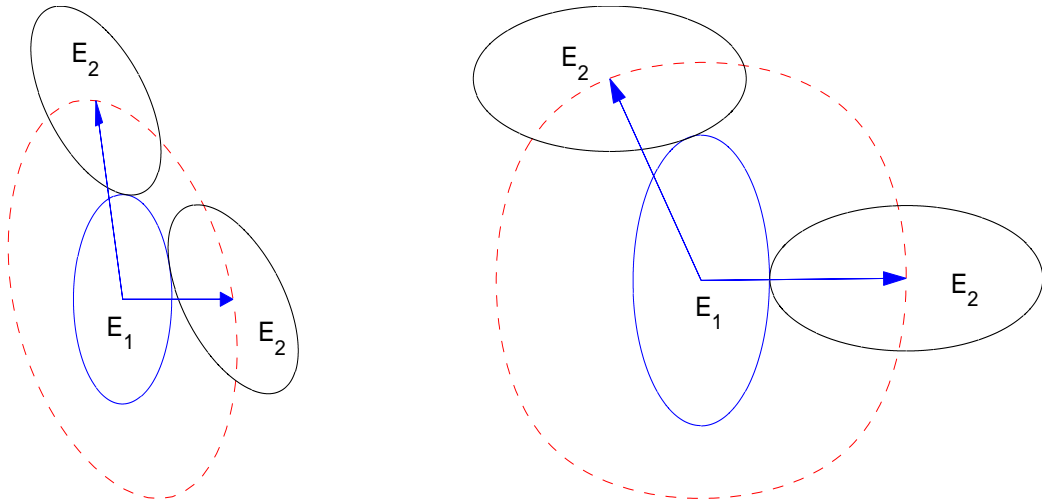
A. Excluded area A_{ex}

FIG. 3: Excluded area for two ellipses. Ellipse E_1 is fixed at origin, and ellipse E_2 rotates around it, keeping its orientation fixed and remaining tangent to E_1. The center of E_2 traces out the dashed curve. The area bounded by the dashed curve is the excluded area A_{ex}.

From the analytical solution provided in Section III, one can easily compute, numerically, the excluded area for two identical ellipses whose orientation is fixed by integrating

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$d^2(\hat{\mathbf{d}}, a_1, b_1, a_2, b_2, \hat{\mathbf{k}}_1, \hat{\mathbf{k}}_2)$ over $\hat{\mathbf{d}}$;

$$A_{ex} = \frac{1}{2} \int d^2(\hat{\mathbf{d}}, a_1, b_1, a_2, b_2, \hat{\mathbf{k}}_1, \hat{\mathbf{k}}_2) |d\hat{\mathbf{d}}|. \tag{53}$$

Fig. 3 shows the locus of the center of ellipse E_2 rotating around E_1 while keeping the orientation of both ellipses fixed. Here $a_1 = a_2 = 2$, $b_1 = b_2 = 1$. When the angle between the major axes is $30°$, the excluded area is 26.4 (Fig. 3.a). If the angle is increased to $45°$, then the excluded area is 27.6. If the angle is $90°$, then the excluded area is 29.7 (Fig. 3.b). The excluded area increases monotonically with the angle between major axes of two ellipses; it is the smallest when the major axes are parallel, and the largest when the major axes are normal to each other.
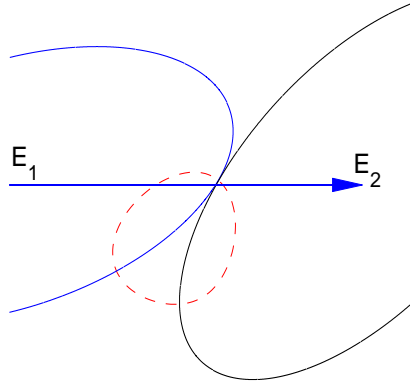
B.   Locus of the point of contact

FIG. 4: Locus of the point of contact. Ellipse E_1 is rotated about its center, while ellipse E_2 keeps its orientation fixed. The center of E_2 moves so that E_2 remains tangent to E_1. The point of contact traces out the dashed curve.

Fig. 4 shows that locus of the point of contact when ellipse E_1 is rotating about its center while ellipse E_2 keeps its orientation. It is interesting and unexpected that the locus has dipolar rather than quadrupolar symmetry.

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C. Potential Applications

Our result, the analytical expression for the distance of closest approach of two hard ellipses, has a number of potential applications. It may be useful in modeling 2-D liquid crystals, both analytically and numerically. The excluded area, discussed above, is a key parameter in statistical models [5] which can be calculated for ellipses from our result. Another potential application is in the theory of nematic liquid crystals. One important contribution to the elastic constants of nematics is due to anisotropic dispersion forces. The average Van der Waals interaction energy of a molecule with its neighbors is an algebraic function of the distance of closest approach. The origin of three distinct elastic constants in nematics is still unresolved. Our result may be useful in modeling elastic constants in 2-D nematics, and possibly giving insights towards understanding their origins in general.

Monte Carlo calculations have played an important role in modeling the phase behavior of isotropic fluids and liquid crystals [6]. Vieillard-Baron developed the first overlap criterion for identical hard ellipses [1]. He derived a contact function $\Psi(a, b, \hat{\mathbf{k}}_1, \hat{\mathbf{k}}_2, \mathbf{d})$ such that $\Psi = 0$ when the ellipses are tangent (either exteriorly or interiorly), and this function is positive and at least one of two auxiliary functions are negative if the ellipses have no real point in common. This overlap criterion has been used in Monte-Carlo simulations of hard ellipse systems [1, 7]. It may be possible to solve $\Psi(a, b, \hat{\mathbf{k}}_1, \hat{\mathbf{k}}_2, \mathbf{d}) = 0$ for d (this involves solving a quartic equation), and thus obtain a result similar to ours; to our knowledge this has not yet been done. However, Vieillard-Baron's contact function Ψ is only valid for identical ellipses, and so this result would not be as general as ours, presented here.

According to the Hohenberg-Mermin-Wagner theorem, long range order corresponding to broken continuous symmetry is not allowed in 2D systems with short-range interactions [8]. The possibility of long-range order in 2D nematics has been discussed theoretically [9] and examined using Monte-Carlo simulations with Lennard-Jones like potentials [10] as well as with hard rods [11]. Although it has been shown that true long range order cannot exist if the interparticle potential is separable into a positional and an orientational part [10], it is not clear what the implications are for systems of hard ellipses. Frenkel has shown that only quasi-long range order exists for hard spherocylinders [11], that is, the correlations in orientational order decay algebraically. Hard ellipsoids, however, can show dramatically different behavior from hard spherocylinders [12] (hard ellipses do not form smectic phases,

whereas spherocylinders do [13]), and for this reason Monte Carlo simulations of hard ellipses, on systems larger than studied by Vieillard-Baron, would be of considerable interest. Our result for the distance provides an overlap criterion which could be usefully applied here.

Another area of interest is phase separation in hard particle systems [14, 15]. For example, simulations of hard disks and hard parallel squares have been studied, and phase separation has been observed. Theoretical studies, on the other hand predict no phase separation in 2D [16]. Our results could provide the criterion for the overlap of ellipses of different sizes, and thus enable Monte-Carlo simulations of binary mixtures of hard ellipses.

Vieillard-Baron also provides an overlap criterion for two identical ellipsoids of revolution in 3D [1]. This involves the evaluation of a contact function Ψ and five auxiliary functions, three of which must be non-negative and at least one among the remaining three must be negative to avoid overlap. Perram and Wertheim provided a more general overlap criterion for hard ellipsoids [2]. Their scheme for evaluating the criterion involves an iterative numerical technique to find the maximum of a scalar function. Our results can provide the basis of a simple algorithm to determine the distance of closest approach of two ellipsoids in 3D. This involves passing a plane through the line joining the centers of the two ellipsoids, determining the distance of closest approach of the ellipses in the plane, then rotating the plane and finding the largest such distance. The details of this algorithm will be published elsewhere.

V.   CONCLUSION

We have derived an analytic expression for the distance of closest approach of two hard ellipses with arbitrary orientation in 2D. The strategy is to transform the ellipses into a circle and a new ellipse by a scaling transformation. The relation between the position of a point on the ellipse and the normal at that point allows the tangency condition between the circle and ellipse to be written as a simple vector equation with two unknowns, which may be solved analytically for the distance between the centers. The solution requires the solution of a quartic equation, whose single positive real root can be uniquely determined. The final result for the distance is obtained by the inverse scaling transformation. Explicit instructions for calculating the distance are given in the Appendix. Our result may be useful in analytic and numerical models of orientationally ordered systems.

VI. APPENDIX

A. Detailed calculation of the distance of closest approach

We start by specifying all the quantities required for the calculation of d.

a_1 and b_1 are the lengths $(a_1 > b_1)$ of the major and minor axes of ellipse E_1.

a_2 and b_2 are the lengths $(a_2 > b_2)$ of the major and minor axes of ellipse E_2.

$e_1 = \sqrt{1 - \dfrac{b_1^2}{a_1^2}}$ is the eccentricity of ellipse E_1.

$e_2 = \sqrt{1 - \dfrac{b_2^2}{a_2^2}}$ is the eccentricity of ellipse E_2.

$\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}$ is the cosine of the angle between the major axis $\hat{\mathbf{k}}_1$ of ellipse E_1 and the direction $\hat{\mathbf{d}}$ of the line joining the centers.

$\hat{\mathbf{k}}_2 \cdot \hat{\mathbf{d}}$ is the cosine of the angle between the major axis $\hat{\mathbf{k}}_2$ of ellipse E_2 and the direction $\hat{\mathbf{d}}$ of the line joining the centers.

$\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2$ is the cosine of the angle between the major axis $\hat{\mathbf{k}}_1$ of ellipse E_1 and the major axis $\hat{\mathbf{k}}_2$ of ellipse E_2.

The above quantities are specified in the statement of the problem.

The following quantities are derived from these.

$$\eta = \frac{a_1}{b_1} - 1. \tag{54}$$

In the coordinate system with the basis $(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)/\sqrt{2 + 2\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}$ and $(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)/\sqrt{2 - 2\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}$, the components of $\mathbb{A}'$ are

$$\mathbb{A}'_{11} = \frac{b_1^2}{b_2^2}\left(1 + \frac{1}{2}(1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)(\eta(2 + \eta) - e_2^2(1 + \eta(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2))^2)\right), \tag{55}$$

$$\mathbb{A}'_{22} = \frac{b_1^2}{b_2^2}\left(1 + \frac{1}{2}(1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)(\eta(2 + \eta) - e_2^2(1 - \eta(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2))^2)\right) \tag{56}$$

and

$$\mathbb{A}'_{12} = \mathbb{A}'_{21} = \frac{b_1^2}{b_2^2}\frac{1}{2}\sqrt{1 - (\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)^2}(\eta(2 + \eta) + e_2^2(1 - \eta^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)^2)). \tag{57}$$

The eigenvalues of $\mathbb{A}'$, in terms of these, are

$$\lambda_+ = \frac{1}{2}(\mathbb{A}'_{11} + \mathbb{A}'_{22}) + \sqrt{\frac{1}{4}(\mathbb{A}'_{11} - \mathbb{A}'_{22})^2 + \mathbb{A}'^2_{12}} \tag{58}$$

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and

$$\lambda_- = \frac{1}{2}(\mathbb{A}'_{11} + \mathbb{A}'_{22}) - \sqrt{\frac{1}{4}(\mathbb{A}'_{11} - \mathbb{A}'_{22})^2 + \mathbb{A}'^2_{12}}. \tag{59}$$

It follows that

$$b'_2 = \frac{1}{\sqrt{\lambda_+}} \tag{60}$$

and

$$a'_2 = \frac{1}{\sqrt{\lambda_-}}. \tag{61}$$

The eigenvectors are given by

$$\hat{\mathbf{k}}'_+ = \frac{1}{\sqrt{2}\sqrt{\mathbb{A}'^2_{12} + (\lambda_+ - \mathbb{A}'_{11})^2}} \left(\frac{\mathbb{A}'_{12}(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \frac{(\lambda_+ - \mathbb{A}'_{11})(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \right) \tag{62}$$

and

$$\hat{\mathbf{k}}'_- = \frac{1}{\sqrt{2}\sqrt{\mathbb{A}'^2_{12} + (\lambda_+ - \mathbb{A}'_{11})^2}} \left(-\frac{(\lambda_+ - \mathbb{A}'_{11})(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \frac{\mathbb{A}'_{12}(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} \right). \tag{63}$$

Then

$$\hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{d}}' = \cos\phi = \frac{1}{\sqrt{2}\sqrt{\mathbb{A}'^2_{12} + (\lambda_+ - \mathbb{A}'_{11})^2}\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}} \times$$

$$\left(\frac{\mathbb{A}'_{12}}{\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}(\frac{b_1}{a_1}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}) + (\hat{\mathbf{k}}_2 \cdot \hat{\mathbf{d}}) + \left(\frac{b_1}{a_1} - 1\right)(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)) + \right.$$

$$\left. \frac{(\lambda_+ - \mathbb{A}'_{11})}{\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}(\frac{b_1}{a_1}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}) - (\hat{\mathbf{k}}_2 \cdot \hat{\mathbf{d}}) - \left(\frac{b_1}{a_1} - 1\right)(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)) \right). \tag{64}$$

If $\hat{\mathbf{k}}_1 = -\hat{\mathbf{k}}_2$, then $-\hat{\mathbf{k}}_2$ may be replaced by $+\hat{\mathbf{k}}_2$ without the loss of generality. If $\hat{\mathbf{k}}_1 = \hat{\mathbf{k}}_2$, care must be taken evaluating the above expression. Letting $\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2 = \cos\theta$, in the limit as $\theta \to 0$ we find that if $\mathbb{A}'_{11} > \mathbb{A}'_{22}$, then $(\lambda_+ - \mathbb{A}'_{11}) \sim \mathbb{A}'^2_{12}$, and

$$\hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{d}}' = \cos\phi = \frac{1}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}} \frac{b_1}{a_1}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}), \tag{65}$$

while if $\mathbb{A}'_{11} < \mathbb{A}'_{22}$, then

$$\hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{d}}' = \cos\phi = \frac{\sqrt{1 - (\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}}. \tag{66}$$

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Next,

$$\delta = \frac{a_2'^2}{b_2'^2} - 1. \tag{67}$$

If $\phi = \pi/2$ or if $\delta = 0$, then $d' = 1 + a_2'$, and Eq. (73) can be evaluated directly. Otherwise,

$$\tan^2 \phi = \frac{1}{(\hat{\mathbf{k}}_+' \cdot \hat{\mathbf{d}}')^2} - 1, \tag{68}$$

$$A = -\frac{1}{b_2'^2}(1 + \tan^2 \phi), \tag{69a}$$

$$B = -\frac{2}{b_2'}(1 + \tan^2 \phi + \delta), \tag{69b}$$

$$C = -\tan^2 \phi - (1 + \delta)^2 + \frac{1}{b_2'^2}(1 + (1 + \delta) \tan^2 \phi), \tag{69c}$$

$$D = \frac{2}{b_2'}(1 + \tan^2 \phi)(1 + \delta), \tag{69d}$$

$$E = (1 + \tan^2 \phi + \delta)(1 + \delta), \tag{69e}$$

$$\alpha = -\frac{3B^2}{8A^2} + \frac{C}{A} \tag{70a}$$

and

$$\beta = \frac{B^3}{8A^3} - \frac{BC}{2A^2} + \frac{D}{A}. \tag{70b}$$

If $\beta \neq 0$, then

$$\gamma = \frac{-3B^4}{256A^4} + \frac{CB^2}{16A^3} - \frac{BD}{4A^2} + \frac{E}{A}, \tag{70c}$$

$$P = -\frac{\alpha^2}{12} - \gamma, \tag{70d}$$

$$Q = -\frac{\alpha^3}{108} + \frac{\alpha\gamma}{3} - \frac{\beta^2}{8}, \tag{70e}$$

$$U = \left(-\frac{Q}{2} + \sqrt{\frac{Q^2}{4} + \frac{P^3}{27}}\right)^{1/3} \tag{70f}$$

and the principal values of the roots are taken throughout;

$$y = \begin{cases} -\dfrac{5}{6}\alpha + U - \dfrac{P}{3U} & \text{if } U \neq 0, \\ -\dfrac{5}{6}\alpha - Q^{1/3} & \text{if } U = 0, \end{cases} \tag{70g}$$

and

$$q = -\frac{B}{4A} + \frac{1}{2}\left(\sqrt{\alpha + 2y} + \sqrt{-\left(3\alpha + 2y + \frac{2\beta}{\sqrt{\alpha + 2y}}\right)}\right). \tag{70h}$$

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If $\beta = 0$, then

$$q = -\frac{B}{4A} + \sqrt{\frac{-\alpha + \sqrt{\alpha^2 - 4\gamma}}{2}}, \tag{71}$$

$$d' = \sqrt{\frac{q^2 - 1}{\delta}\left(1 + \frac{b_2'(1+\delta)}{q}\right)^2 + \left(1 - \frac{q^2 - 1}{\delta}\right)\left(1 + \frac{b_2'}{q}\right)^2}, \tag{72}$$

and finally

$$d = \frac{d'}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}} b_1. \tag{73}$$

B. Detailed calculation of the position of the point of contact

To obtain the vector $\boldsymbol{r}_c$ from the center of Ellipse 1 to the point of contact, we first need to compute $\hat{\mathbf{n}}'$ and then perform the inverse affine transformation. Explicitly, $\boldsymbol{r}_c = \mathbb{T}^{-1}\hat{\mathbf{n}}'$. The components of $\hat{\mathbf{n}}'$ can be defined though the inner product with $\hat{\mathbf{k}}_+'$ and $\hat{\mathbf{k}}_-'$::

$$\hat{\mathbf{k}}_+' \cdot \hat{\mathbf{n}}' = \cos\psi = sgn(\cos\phi)\sqrt{1 - \frac{q^2 - 1}{\delta}}, \tag{74}$$

$$\hat{\mathbf{k}}_-' \cdot \hat{\mathbf{n}}' = \sin\psi = sgn(\sin\phi)\sqrt{\frac{q^2 - 1}{\delta}}. \tag{75}$$

where $sgn(x)$ gives the sign of x. The expression for $\cos\phi$ is given in Eq. **??**. $\sin\phi$ can be calculated similarly, and

$$\hat{\mathbf{k}}_-' \cdot \hat{\mathbf{d}}' = \sin\phi = \frac{1}{\sqrt{2}\sqrt{{\mathbb{A}_{12}'}^2 + (\lambda_+ - \mathbb{A}_{11}')^2}\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}} \times$$
$$\left(-\frac{(\lambda_+ - \mathbb{A}_{11}')}{\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}\left(\frac{b_1}{a_1}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}) + (\hat{\mathbf{k}}_2 \cdot \hat{\mathbf{d}}) + \left(\frac{b_1}{a_1} - 1\right)(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\right) +$$
$$\frac{\mathbb{A}_{12}'}{\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}\left(\frac{b_1}{a_1}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}) - (\hat{\mathbf{k}}_2 \cdot \hat{\mathbf{d}}) - \left(\frac{b_1}{a_1} - 1\right)(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\right). \tag{76}$$

It follows that

$$\hat{\mathbf{n}}' = \cos\psi\,\hat{\mathbf{k}}_+' + \sin\psi\,\hat{\mathbf{k}}_-'. \tag{77}$$

Writing $\hat{\mathbf{k}}_+'$ and $\hat{\mathbf{k}}_-'$ in terms of $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$

$$\hat{\mathbf{k}}_+' = \cos\gamma\frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \sin\gamma\frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}, \tag{78}$$

$$\hat{\mathbf{k}}'_- = -\sin\gamma \frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \cos\gamma \frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}, \tag{79}$$

where

$$\cos\gamma = \hat{\mathbf{k}}'_+ \cdot \frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}, \tag{80}$$

and

$$\sin\gamma = \hat{\mathbf{k}}'_+ \cdot \frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}. \tag{81}$$

The angle γ can be calculated explicitly, since $\hat{\mathbf{k}}'_+$ and $\hat{\mathbf{k}}'_-$ are known. Substitution gives $\hat{\mathbf{n}}'$ in terms of $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$ and gives

$$\hat{\mathbf{n}}' = \cos(\psi + \gamma) \frac{(\hat{\mathbf{k}}_1 + \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + \sin(\psi + \gamma) \frac{(\hat{\mathbf{k}}_1 - \hat{\mathbf{k}}_2)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}. \tag{82}$$

Finally, after the transformaton $\mathbb{T}^{-1}$, the contact point $\boldsymbol{r}_c$ is given by a linear combination of $\hat{\mathbf{k}}_1$ and $\hat{\mathbf{k}}_2$:

$$
\begin{aligned}
\boldsymbol{r}_c &= \mathbb{T}^{-1}\hat{\mathbf{n}}' = b_1\left(\mathbf{I} + \eta\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1\right)\hat{\mathbf{n}}' \\
&= [(a_1 + (a_1 - b_1)\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\frac{\cos(\psi + \gamma)}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} + (a_1 - (a_1 - b_1)\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2)\frac{\sin(\psi + \gamma)}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}]\hat{\mathbf{k}}_1 + \\
&\quad [b_1\cos(\psi + \gamma)\frac{1}{\sqrt{2}\sqrt{1 + \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}} - b_1\sin(\psi + \gamma)\frac{1}{\sqrt{2}\sqrt{1 - \hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}}_2}}]\hat{\mathbf{k}}_2. \tag{83}
\end{aligned}
$$

There are some special cases, when either q is not given or ϕ is not well defined We treat these separately below.

1. If $\delta = 0$ or $\phi = \pi/2$, then $\cos\psi$ and $\sin\psi$ are not required, since that $\hat{\mathbf{n}}' = \hat{\mathbf{d}}'$ and

$$\boldsymbol{r}_c = \mathbb{T}^{-1}\hat{\mathbf{d}}' = \frac{\mathbb{T}^{-1}\mathbb{T}\hat{\mathbf{d}}}{\left|\mathbb{T}\hat{\mathbf{d}}\right|} = \frac{\hat{\mathbf{d}}}{\frac{1}{b_1}\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}}. \tag{84}$$

2. If $\hat{\mathbf{k}}_1 = \hat{\mathbf{k}}_2$, care must to be taken in evaluating the angle ϕ. Since $\hat{\mathbf{k}}_1 = \hat{\mathbf{k}}_2$, these vectors do not span the space, and a new vector $\hat{\mathbf{k}}_1^\perp$, perpendicular to $\hat{\mathbf{k}}_1$, needs to be introduced. .

(a) If $A_{11} > A_{22}$, then $\hat{\mathbf{k}}'_+ = \hat{\mathbf{k}}_1$, and $\hat{\mathbf{k}}'_- = \hat{\mathbf{k}}_1^\perp$, and $\cos\phi$ and $\sin\phi$ are given by

$$\hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{d}}' = \cos\phi = \frac{1}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}} \frac{b_1}{a_1}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}), \tag{85}$$

$$\hat{\mathbf{k}}'_- \cdot \hat{\mathbf{d}}' = \sin\phi = \frac{1}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}}(\hat{\mathbf{k}}_1^\perp \cdot \hat{\mathbf{d}}), \tag{86}$$

Here $\hat{\mathbf{n}}' = \cos\psi\hat{\mathbf{k}}_1 + \sin\psi\hat{\mathbf{k}}_1^\perp$, and the $\boldsymbol{r}_c$ is given by

$$\boldsymbol{r}_c = \mathbb{T}^{-1}\hat{\mathbf{d}}' = b_1\left(\mathbf{I} + \eta\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1\right)(\cos\psi\hat{\mathbf{k}}_1 + \sin\psi\hat{\mathbf{k}}_1^\perp)$$
$$= a_1\cos\psi\hat{\mathbf{k}}_1 + b_1\sin\psi\hat{\mathbf{k}}_1^\perp. \tag{87}$$

(b) If $A_{11} < A_{22}$, $\hat{\mathbf{k}}'_+ = \hat{\mathbf{k}}_1^\perp$, and $\hat{\mathbf{k}}'_- = \hat{\mathbf{k}}_1$, then

$$\hat{\mathbf{k}}'_+ \cdot \hat{\mathbf{d}}' = \cos\phi = \frac{1}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}}(\hat{\mathbf{k}}_1^\perp \cdot \hat{\mathbf{d}}), \tag{88}$$

$$\hat{\mathbf{k}}'_- \cdot \hat{\mathbf{d}}' = \sin\phi = \frac{1}{\sqrt{1 - e_1^2(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}})^2}} \frac{b_1}{a_1}(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{d}}), \tag{89}$$

and $\hat{\mathbf{n}}' = \cos\psi\hat{\mathbf{k}}_1^\perp + \sin\psi\hat{\mathbf{k}}_1$ We then have

$$\boldsymbol{r}_c = \mathbb{T}^{-1}\hat{\mathbf{d}}' = b_1\left(\mathbf{I} + \eta\hat{\mathbf{k}}_1\hat{\mathbf{k}}_1\right)(\cos\psi\hat{\mathbf{k}}_1^\perp + \sin\psi\hat{\mathbf{k}}_1)$$
$$= b_1\cos\psi\hat{\mathbf{k}}_1^\perp + a_1\sin\psi\hat{\mathbf{k}}_1. \tag{90}$$

VII.   ACKNOWLEDGMENTS

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[2] J. W. Perram and M. S. Wertheim, "Statistical mechanics of hard ellipsoids. I. overlap algorithm and the contact function", J. Comput. Phys., **58**, 409 (1985).

[3] At first glance, this problem seems simple enough for a high school geometry homework assignment. Further consideration shows, however, that it is not simple at all. One of us (P.P-M.) has thought about it since his graduate student days, and has attempted to interest others in it with varying degrees of success. A prize for its solution was informally announced at the Liquid Crystal Gordon Conference in 1983 (attended by W.M. Gelbart and R.B. Meyer), this, however, did not generate a solution. J. Vieillard-Baron, an early worker on this problem, was reportedly greatly disturbed by the difficulties he encountered. It is a great pleasure therefore to have finally found a solution.

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