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A FAST ALGORITHM TO EVALUATE THE SHORTEST DISTANCE BETWEEN RODS

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Abstract—We present a fast algorithm to evaluate the shortest distance between rods of either the same or different length. The presented algorithm speeds up considerably the evaluation of the shortest distance with respect to other previously reported algorithms. As an application, this algorithm has allowed a fast development of the statistical mechanics of molecular fluids interacting through potentials depending on the shortest distance as, e.g. the Kihara model. The reported algorithm has proved to be very useful to study the liquid state either by simulation (Monte Carlo or Molecular Dynamics) or by perturbation theory and to obtain thermodynamic properties of Kihara-like fluids.

INTRODUCTION

Kihara proposed in 1951 an intermolecular potential model in which the interaction energy between a pair of molecules only depends on the shortest distance ρ between the molecular cores. The molecular cores are chosen to reproduce the molecular shape. The Kihara potential model has been mainly applied to evaluate the second virial coefficient B_2 because analytical expressions are known (Kihara, 1982; Maitland *et al.*, 1981). Its application to the study of molecular fluids in liquid state, however, has not been carried out until recently. The reason is that it is difficult to find a computationally efficient algorithm to evaluate ρ. Furthermore, the computation of ρ is a usual problem in a lot of problems of quantum chemistry and statistical mechanics. In the application familiar to us, the natural choice of the core for a linear molecule (i.e. N_2, CO_2) is a linear rod. Hence the importance of finding fast algorithms to evaluate ρ between linear rods of the same or different length, able to model pure liquids or mixtures, respectively. The algorithm should be fast so that it is possible to carry out simulation studies (Allen & Tildesley, 1987; Ciccotti *et al.*, 1987) of liquid state by Monte Carlo (Vega & Lago, 1988; Kantor & Boublik, 1988) or Molecular Dynamics (Vega & Lago, 1990) techniques or by perturbation theory (Hansen & McDonald, 1986; Vega & Lago, 1991a, b). In these kinds of studies the evaluation of ρ is typically performed many millions of times and, therefore, it is absolutely necessary to find fast algorithms to obtain ρ. The method can be extended to non-linear rigid molecules as for instance ozone, propane, ciclo-propane, iso-butane that can be treated as a set of rods of uniform length (Vega *et al.*, 1992). When the length to breadth ratio of the molecule is very high the evaluation of ρ allows to perform studies of phase transition to liquid crystal by computer simulation (Stroobants *et al.*, 1987; Frenkel, 1988).

Previously, two algorithms to evaluate ρ between linear rods have been reported. The first applied to the evaluation of ρ between rods of the same length (Sevilla & Lago, 1985) and the second extended the method to consider the rods of different length (Lago & Vega, 1988). In this work we present an algorithm to evaluate the shortest distance ρ between linear rods of either the same or different length. This algorithm is approximately four times faster than the other two previously proposed (Sevilla & Lago, 1985; Lago & Vega, 1988). We believe that the proposed algorithm will contribute to the statistical mechanics of molecular systems which interact through potentials depending on the shortest distance between the cores.

The scheme of the paper is very simple. In the following section we shall present the details of the algorithm and in the Appendix we shall supply a FORTRAN subroutine to evaluate the shortest distance between linear rods of different length.

ALGORITHM

We shall start by describing the algorithm to find the shortest distance ρ between rods of the same length and later we shall show how it can be extended to rods of different length.

Let us define $\mathbf{r}$ as the vector connecting two arbitrary points of the lines denoted as 1 and 2 respectively (see Fig. 1). The rod numbered as 1 is contained in the straight line labelled as 1 and the

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rod 2 in the straight line 2. We can write the vector $\mathbf{r}$ as:

$$\mathbf{r} = \mathbf{r}_{12} + \mu\, \mathbf{u}_2 - \lambda\, \mathbf{u}_1 \tag{1}$$

where $\mathbf{u}_1$ $\mathbf{u}_2$ are unit vectors contained in the lines 1 and 2, respectively, $\mathbf{r}_{12}$ is the vector connecting the centre of the rod 1 with the centre of the rod 2 and μ and λ are two arbitrary parameters which range in the interval $(-\infty, +\infty)$. Let us define l as the length of the rod. Then when λ and μ simultaneously range in the interval $[-l/2, l/2]$ the vector $\mathbf{r}$ connects a point of rod 1 with a point of rod 2. Thus, the evaluation of ρ reduces to the evaluation of the absolute minimum of the modulus of $\mathbf{r}$ in the range $\mu = [-l/2, l/2]$ $\lambda = [-l/2, l/2]$. Let us now construct a new map by representing in the abcissa axis the values of the parameter λ and in the ordinate axis the values of μ, and let us denote this plane as the (λ, μ) plane. From the definition, every point in the (λ, μ) plane represents a vector connecting a point of line 1 with a point of line 2 in the real space (See Fig. 1). Then the area enclosed by the intervals $\mu = [-l/2, l/2]$ $\lambda = [-l/2, l/2]$ is a square in the (λ, μ) plane whose sides are also included [see Fig. 1(b)].

The minima of the function $|\mathbf{r}|$ and $\mathbf{r}^2$ occur at the same point of the (λ, μ) plane or conversely between the same pair of points of the real space. For mathematical convenience we shall look for the minimum of $\mathbf{r}^2$. From equation (1) $\mathbf{r}^2$ is given by:

$$\mathbf{r}^2 = \mathbf{r}_{12}^2 + \mu^2 + \lambda^2 + 2\mu\, \mathbf{r}_{12} \cdot \mathbf{u}_2 - 2\lambda\, \mathbf{r}_{12} \cdot \mathbf{u}_1 - 2\lambda\mu\, \mathbf{u}_1 \cdot \mathbf{u}_2. \tag{2}$$

Let us first evaluate the shortest distance between the lines 1 and 2. That can be done by setting to zero the derivative of equation (2) with respect to λ and μ. If we define λ' and μ' as the values minimizing $\mathbf{r}^2$ in the equation (2) then its values are given by:

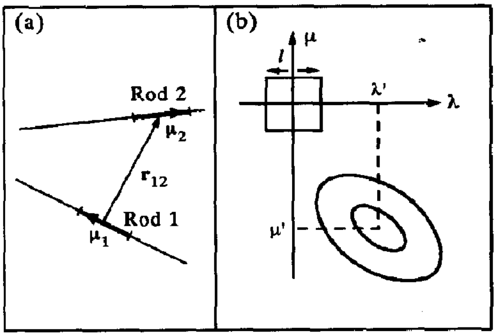

Fig. 1. (a) Definition of $\mathbf{r}_{12}$, $\mathbf{u}_1$, $\mathbf{u}_2$ for a pair of rods labelled as rod 1 and rod 2 respectively. We show the pair of rods in real space. (b) View of the (λ, μ) plane. Every point of the square centred at the origin correspond to a pair of points in real space, one contained in rod 1 and the other in rod 2. The shortest distance between the lines 1 and 2 where the rods are embedded occurs at (λ', μ'). The ellipses show contours where the function $\mathbf{r}^2$ [see equation (2)] takes the same value.

$$\lambda' = \frac{((\mathbf{r}_{12} \cdot \mathbf{u}_1) - (\mathbf{u}_1 \cdot \mathbf{u}_2)(\mathbf{r}_{12} \cdot \mathbf{u}_2))}{(1 - (\mathbf{u}_1 \cdot \mathbf{u}_2)^2)} \tag{3}$$

$$\mu' = \frac{(-(\mathbf{r}_{12} \cdot \mathbf{u}_2) + (\mathbf{u}_1 \cdot \mathbf{u}_2)(\mathbf{r}_{12} \cdot \mathbf{u}_1))}{(1 - (\mathbf{u}_1 \cdot \mathbf{u}_2)^2)}. \tag{4}$$

By substituting these values of λ' and μ' in equation (1) the square of the shortest distance between the lines 1 and 2 is obtained. If the point (λ', μ') is inside the square mapping the two rods on the (λ, μ) plane, then the shortest distance between the rods ρ is equal to the shortest distance between the lines and the problem of the evaluation of ρ is then solved. When the point (λ', μ') is not inside the square then the following discussion explains how to determine ρ.

The interior part of the square of Fig. 1(b) corresponds to interior points of rod 1 and rod 2. The sides of the square correspond to an interior point of a rod and an extreme of the other rod. Finally, the corners of the square correspond to an extreme of one of the rods and an extreme of the other. Let us now study the mapping on the (λ, μ) plane of all the pair of points of lines 1 and 2 which are at the same distance. For that purpose let us set the value of $\mathbf{r}^2$ to a positive constant which we shall call d^2. Equation (2) is then written as:

$$\lambda^2 - 2\lambda\mu\, \mathbf{u}_1 \cdot \mathbf{u}_2 + \mu^2 - 2\lambda\, \mathbf{r}_{12} \cdot \mathbf{u}_1 + 2\mu\, \mathbf{r}_{12} \cdot \mathbf{u}_2 + (\mathbf{r}_{12}^2 - d^2) = 0. \tag{5}$$

The general equation of a conic in the plane (x_1, x_2) is given by (Apostol, 1980):

$$\alpha x_1^2 + \beta x_1 x_2 + \gamma x_2^2 + \delta x_1 + \epsilon x_2 + \phi = 0 \tag{6}$$

and has the same form as the equation (5) with the constants α, β, γ, δ, ϵ, ϕ being given by:

$$\alpha = 1 \quad \beta = -2\,\mathbf{u}_1 \cdot \mathbf{u}_2 \quad \gamma = 1$$

$$\delta = -2\,\mathbf{r}_{12} \cdot \mathbf{u}_1 \quad \epsilon = 2\,\mathbf{r}_{12} \cdot \mathbf{u}_2 \quad \phi = (\mathbf{r}_{12}^2 - d^2). \tag{7}$$

It is easy to show that equation (5) is the equation of an ellipse in the plane (λ, μ). The centre of the ellipse, namely, the point where the two principals semi-axes cross, has (λ', μ') as coordinates where λ' and μ' are given by equations (3) and (4) respectively. It can also easily be shown that the direction of the two main semi-axes of the ellipse bisects the angle determined by the λ and μ axes independently of the value of β, and, therefore, independently of the relative orientation of lines 1 and 2. The eccentricity of the ellipse, however, depends on the relative orientation between the lines 1 and 2. Therefore, all the pair of points of lines 1 and 2 in real space at a given distance d^2 map onto an ellipse centred on (λ', μ'),whose main principal axes form and angle of 45°to the axes λ and μ in the (λ, μ) space. This is illustrated in Fig. 1(b). Finally, it is also easy to show that the length of the ellipse axes increases when d^2 increases.

Let us now divide the (λ, μ) plane into four different regions and let us assign a side of the square to

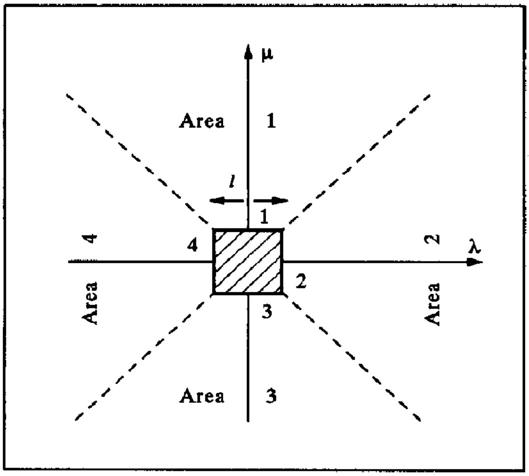

Fig. 2. The four areas or regions in which the (λ, μ) plane is divided for rods of equal length. The areas are labelled from 1 to 4 according to the number of the square side.

a given region as it is shown in Fig. 2. Let us assume, for example, that for a pair of rods in a given relative orientation the point (λ', μ') falls inside the region labelled as 3. Furthermore, let us consider the set of ellipses centred on (λ', μ') (each mapping equidistant pair of points in real space) and whose principal semi-axes form an angle of 45° with the axes λ and μ. Obviously, one ellipse of this set is tangent to the square in the side labelled as 3 because their semi-axes are parallel to the bisecting lines of quadrants. This is so regardless of the eccentricity of the ellipses. The contact point of the side 3 of the square correspond to the coordinates of a point P of rod 1 and a point P′ of rod 2 in real space. Therefore, the shortest distance between the rods ρ that we are looking for, occurs between the points P and P′. In the same way if for another given relative orientation of rods 1 and 2, the point (λ', μ') falls in the region labelled as 1 then an analogous argument drives us to the conclusion that the shortest distance between the rods occurs on a point of the side 1 of the square of the (λ, μ) space and so on. In general, if (λ', μ') falls inside the regions labelled as i, then the shortest distance between the rods occurs on a point of the side i of the square. In previous algorithms the four sides of the square were explored to find ρ regardless of the value of (λ', μ'). Now, once we know in which region falls (λ', μ'), we shall only look for ρ in the corresponding side of the square. Thus, the present algorithm is about four times faster because only one side of the square is investigated.

Let us explain now how to determine ρ on the side of the square of interest. For that purpose, we take again the above example where (λ', μ') falls in region 3. From the preceding argument, ρ is given by a pair of points of real space represented by a point π' on the side 3 of the square in the (λ, μ) plane. We want to determine the coordinates of that point π' of side 3. Let us recall that the side 3 of the square represents a given extreme of the rod 2 and any point of rod 1. The side of the square labelled as 3 is along the line $\mu = -l/2$ of the plane (λ, μ). This line corresponds in the real space to a given extreme of the rod 2 (the obtained as $\mathbf{r}_2 - l/2\ \mathbf{u}_2$) and any point of the line 1. Let us first calculate the minimum of the function given by equation (2) in the range represented by the line $\mu = -l/2$. This can be done from elementary analytical geometry since it is just the problem of finding the shortest distance of a point to a straight line. Let us assume that the shortest distance of the extreme 2 of rod 1 to the line 1, occurs in the point $(\lambda'', -l/2)$ of the (λ, μ) plane. Then according to the value of λ'' there are three different cases:

$$\lambda'' < -l/2 \tag{8}$$

$$-l/2 < \lambda'' < l/2 \tag{9}$$

$$\lambda'' < l/2. \tag{10}$$

Let us now remark that the function $\mathbf{r}^2$ defined by equation (2) has only a minimum (the shortest distance of the extreme 2 of rod 2 to the line 1) along $\mu = -l/2$. The coordinates of that minimum are $(\lambda'', -l/2)$. The function given by equation (2) increases monotonously when we move away from the point $(\lambda'', -l/2)$ on the line $\mu = -l/2$. Consequently if the condition given by equation (9) is satisfied then the shortest distance between the extreme 2 of rod 2 to line 1 is also the shortest distance between the rods 1 and 2, ρ. By the same reason, if the condition given by equation (8) is satisfied the shortest distance between the rods occurs in the point $(-l/2, -l/2)$ of the (λ, μ) plane. This point of the (λ, μ) plane represents the extreme 2 of molecule 2 ($\mu = -l/2$) and the extreme 2 of molecule 1 ($\lambda = -l/2$). Finally, if the condition given by equation (10) is satisfied then the shortest distance between the rods ρ occurs in the point $(l/2, -l/2)$ of the (λ, μ) plane.

In other words, the conclusion of the last paragraph is that if equation (8) is satisfied then the shortest distance between the rods ρ occurs between the pair of extremes of rods 1 and 2 represented by the point $(-l/2, -l/2)$ of the (λ, μ) plane. If equation (9) is satisfied then ρ occurs between the extreme 2 of rod 2 and an interior point of rod 1 represented by the point $(\lambda'', -l/2)$ of the plane (λ, μ). Finally, if equation (10) is satisfied then ρ occurs between the pair of extremes represented by the point $(l/2, -l/2)$ of the (λ, μ) plane.

For the sake of clarity we have illustrated the algorithm assuming that the point (λ', μ') falls in the area 3. The same arguments can be applied when the point (λ', μ') falls in any of the other areas (i.e. 1, 2 or 4) but now we have to change the side of the square to consider.

The preceding arguments enable us to create a fast algorithm to calculate the shortest distance between rods of the same length. The scheme of the algorithm is shown in Table 1.

Table 1. Scheme of the algorithm for the calculation of the shortest distance between linear rods of the same length

1. Evaluation of (λ', μ') according to equations (3) and (4)
2. Is (λ', μ') in the square $\lambda = [-l/2, l/2]$, $\mu = [-l/2, l/2]$?
   Yes: go to step 8 with $(\lambda, \mu) = (\lambda', \mu')$.
   No: determine the region (1, 2, 3, or 4) where (λ', μ') falls.
3. Select the side of the square (see Fig. 2) corresponding to the region found in step 2. The chosen side corresponds to a given extreme of one rod and all the points of the other rod.
4. Calculate the shortest distance of the considered extreme to the line where the other rod is contained.
5. Evaluate the coordinates in the (λ, μ) plane corresponding to the step 4 and label them as (λ'', μ''). (Either $|\lambda''| = l/2$ or $|\mu''| = l/2$ but not simultaneously.)
6. Label η the coordinate whose absolute value is different from $l/2$.
7. Is $-l/2 < \eta < l/2$
   Yes: go to step 8 with $(\lambda, \mu) = (\lambda'', \mu'')$.
   No: $\eta < -l/2$:
   if $\eta = \mu''$ go to the step 8 with $(\lambda, \mu) = (\lambda'', -l/2)$
   if $\eta = \lambda''$ go to the step 8 with $(\lambda, \mu) = (-l/2, \mu'')$
   $\eta > l/2$
   if $\eta = \mu''$ go to the step 8 with $(\lambda, \mu) = (\lambda'', l/2)$
   if $\eta = \lambda''$ go to the step 8 with $(\lambda, \mu) = (l/2, \mu'')$.
8. Evaluate ρ^2 given by equation (2) of the main text by substituting the values of λ and μ found in the above steps 1–7.

The generalization of the algorithm to rods of different length is straightforward. The domain which contains all the pair of points of the two rods is now represented by a rectangle instead of a square in the (λ, μ) plane. The length of the sides of this rectangle is just the length of the rods. The algorithm shown in Table 1 holds also for rods of different length with minor changes. The definition of the areas should be modified as is illustrated in Fig. 3. This is so because the direction of the main semi-axes of the ellipse of the equi-distant pair of points does not depend on the lengths of the rods. The second change is that $l/2$ should be substituted by $l_1/2$ when associated to the coordinate λ (rod 1) and $l/2$ should be modified by $l_2/2$ when associated to the coordinate μ (rod 2).

We give as an Appendix a FORTRAN subroutine to evaluate the shortest distance between a pair of rods of different length. It can also be applied to rods of the same length by setting the length of the two rods to the same value.

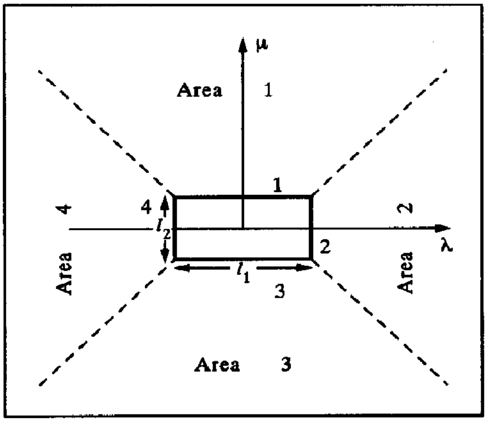

Fig. 3. The four areas or regions in which the (λ, μ) plane is divided for the case of rods of different length. Note that now the pair of rods corresponds to a rectangle instead of a square. The lengths of the sides of the square are l_1 and l_2.

Program availability—The computer program is available from the authors upon request.

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APPENDIX

A FORTRAN subroutine called SDM to evaluate the shortest distance between rods of different length is given below. The input and output variables are:

R12 = Cartesian coordinates of the vector connecting the centre of rod 1 with the centre of rod 2.
U1 = Cartesian coordinates of a unit vector along the rod 1.
U2 = Cartesian coordinates of a unit vector along the rod 2.
XL1D2 = Half of the length of rod 1 (XL1D2 = $l_1/2$).
XL2D2 = Half of the length of rod 2 (XL2D2 = $l_2/2$).
RO2 = Output of the subroutine being the square of the shortest distance between the rods. RO2 = ρ^2.

```
C  SUBROUTINE TO EVALUATE THE SHORTEST DISTANCE BETWEEN TWO RODS
C  OF DIFFERENT LENGTH
C  R12= VECTOR CONNECTING THE GEOMETRICAL CENTERS OF THE TWO RODS
C  U1 = UNITARY VECTOR DEFINIG THE ORIENTATION OF ROD1
C  U2 = UNITARY VECTOR DEFINIG THE ORIENTATION OF ROD2
C  XL1D2= HALF OF THE LENGTH OF ROD1
C  XL2D2= HALF OF THE LENGTH OF ROD2
C  RO2 = SQUARE OF THE SHORTEST DISTANCE BETWEEN THE TWO RODS
      SUBROUTINE SDM(R12,U1,U2,XL1D2,XL2D2,RO2)
      DIMENSION R12(3),U1(3),U2(3)
      R122=R12(1)**2+R12(2)**2+R12(3)**2
      R12EU1=R12(1)*U1(1)+R12(2)*U1(2)+R12(3)*U1(3)
      R12EU2=R12(1)*U2(1)+R12(2)*U2(2)+R12(3)*U2(3)
      U1EU2=U1(1)*U2(1)+U1(2)*U2(2)+U1(3)*U2(3)
      CC=1.-U1EU2**2
C CHECKING WHETHER THE RODS ARE OR NOT PARALLEL
      IF (CC.LT.1.E-6) THEN
         IF (R12EU1.NE.0.) THEN
            XLANDA=SIGN(XL1D2,R12EU1)
            GO TO 10
         ELSE
            XLANDA=0.
            XMU=0.
            GO TO 20
         ENDIF
      ENDIF
C  STEP 1 (SEE TABLE I )
      XLANDA=(R12EU1-U1EU2*R12EU2)/CC
      XMU=(-R12EU2+U1EU2*R12EU1)/CC
C  STEP 2  (SEE TABLE I )
      IF ((ABS(XLANDA).LE.XL1D2).AND.(ABS(XMU).LE.XL2D2)) GO TO 20
      AUXI1=ABS(XLANDA)-XL1D2
      AUXI2=ABS(XMU)-XL2D2
C STEPS 3 TO 7   (SEE TABLE I)
         IF ( AUXI1.GT.AUXI2) THEN
            XLANDA=SIGN(XL1D2,XLANDA)
 10         XMU=XLANDA*U1EU2-R12EU2
            IF ( ABS(XMU).GT.XL2D2) XMU=SIGN(XL2D2,XMU)
         ELSE
            XMU=SIGN(XL2D2,XMU)
            XLANDA=XMU*U1EU2+R12EU1
            IF ( ABS(XLANDA).GT.XL1D2) XLANDA=SIGN(XL1D2,XLANDA)
         ENDIF
C STEP 8   (SEE TABLE I)
  20  RO2=R122+XLANDA**2+XMU**2-2.*XLANDA*XMU*U1EU2
     1     +2.*XMU*R12EU2-2.*XLANDA*R12EU1
      RETURN
      END
```