

On the anisotropy of diffusion in nematic liquid crystals: test of a modified affine transformation model via molecular dynamics

By S. HESS

Institut für Theoretische Physik, Technische Universität Berlin, Sekr. PN 7-1,
Hardenbergstr. 36, D-1000 Berlin 12, Germany

D. FRENKEL

FOM Institute for Atomic and Molecular Physics, PO Box 41883,
1009-DB Amsterdam, The Netherlands

and M. P. ALLEN

H. H. Wills Physics Laboratory, Royal Fort, Tyndall Avenue,
Bristol BS8 1TL, UK

(Received 26 March 1991; accepted 5 June 1991)

An affine transformation model is applied to the diffusion coefficients of perfectly aligned and partially aligned ellipsoidal particles. It is tested against molecular dynamics simulations of hard ellipsoids, free to translate and rotate, in the nematic liquid crystal phase. The theory explains the variation with order parameter of the anisotropy of the diffusion tensor, and approximately relates the average diffusion coefficient to that of an equivalent hard sphere fluid.

1. Introduction

In this paper the anisotropy of self diffusion in nematic liquid crystals is treated by an affine transformation model, which has previously been applied to the explanation of the anisotropy of viscosity [1, 2]. The model was tested successfully in nonequilibrium molecular dynamics computer simulations [2-4] for fluids of perfectly oriented prolate and oblate ellipsoidal particles (Maier-Saupe order parameter $S = 1$) where the viscosity coefficients relevant for shear flow were computed. A modification of the theory is required in order to deal with real nematic liquid crystals, which are only partially ordered ($S < 1$). Here we apply the simple affine transformation model to the diffusion problem, and extend it to account for the effects of partial ordering in the nematic phase. The theory is tested against results obtained from molecular dynamics simulations [5, 6] for fluids of prolate and oblate hard ellipsoidal particles.

2. Affine transformation model

Consider a fluid of perfectly oriented nonspherical particles, where the N -particle potential $\Phi^{(N)}$ is a sum of binary interactions of the particles located at positions r^i and r^j :

$$\Phi^{(N)} = \frac{1}{2} \sum_i \sum_{j \neq i} \Phi_A(r^{ij}), \quad (1)$$

with $r^{ij} = r^i - r^j$. For ellipsoidal particles, the nonspherical binary potential $\Phi_A = \Phi_A(\mathbf{r})$ can be obtained from a spherical interaction potential $\Phi_{\text{sph}}(r^{(A)})$ by an affine transformation

$$\Phi_A(\mathbf{r}) = \Phi_{\text{sph}}(r^{(A)}), \quad (2)$$

with \mathbf{r} and $r^{(A)}$ linked by

$$r^{(A)} \cdot r^{(A)} = \mathbf{r} \cdot \mathbf{A} \cdot \mathbf{r} \quad (3)$$

or

$$r^{(A)} = \mathbf{A}^{1/2} \cdot \mathbf{r}. \quad (4)$$

The transformation matrix \mathbf{A} , with positive eigenvalues A_1, A_2, A_3 , describes the mapping of a sphere

$$r^{(A)} \cdot r^{(A)} = \text{constant}$$

onto an ellipsoid. In order to compare fluids of equal density we use a volume conserving mapping where $A_1 A_2 A_3 = 1$. Then the spherical equipotential surface of $\Phi_{\text{sph}}(r^{(A)})$ encloses the same volume as the corresponding ellipsoidal equipotential surface of $\Phi_A(\mathbf{r})$.

Since all molecules are assumed to be perfectly oriented, the same transformation (4) can be used for all coordinates. The spatial derivative $\partial/\partial\mathbf{r} \equiv \nabla$ is linked with $\nabla^{(A)}$ in the affine space by

$$\nabla^{(A)} = \mathbf{A}^{-1/2} \cdot \nabla. \quad (5)$$

In this way, properties of the fluid of oriented nonspherical particles can be related to properties of a reference fluid (of equal density) of spherical particles. For the viscosity, this method was used in references [2–4, 7]. Here, it is applied to the (self-) diffusion problem where the constitutive law for a diffusion flux \mathbf{j} of labelled particles with density ρ (in the hydrodynamic regime) is given by

$$\mathbf{j} = -\mathbf{D} \cdot \nabla\rho, \quad (6)$$

with the diffusion tensor \mathbf{D} . Use of (5) and $\mathbf{j}^{(A)} = \mathbf{A}^{1/2} \cdot \mathbf{j}$ in accord with (4) leads to

$$\mathbf{j}^{(A)} = -\mathbf{D}^{(A)} \cdot \nabla^{(A)}\rho \quad (7)$$

in the affine space. The diffusion coefficients $\mathbf{D}^{(A)}$ and \mathbf{D} are linked by

$$\mathbf{D} = \mathbf{A}^{-1/2} \cdot \mathbf{D}^{(A)} \cdot \mathbf{A}^{-1/2}. \quad (8)$$

For the affine reference fluid composed of spherical particles, one has

$$\mathbf{D}^{(A)} = D_0 \delta,$$

where δ is the unit tensor and D_0 is the (isotropic) diffusion coefficient of the spherical particles. Then the anisotropic diffusion tensor of the oriented ellipsoidal particles is determined by the transformation matrix \mathbf{A} according to

$$\mathbf{D} = \mathbf{A}^{-1} D_0. \quad (9)$$

Next, the special case of uniaxial ellipsoidal particles with semi-axes a and $b = c$ is considered; $Q = a/b$ is the axis ratio. The unit vector parallel to the symmetry axis is denoted by \mathbf{u} . Then one has [2–4]

$$\mathbf{A} = Q^{2/3} [\delta + (Q^{-2} - 1)\mathbf{u}\mathbf{u}]$$

$$A^{-1} = Q^{-2/3} [\delta + (Q^2 - 1)uu]. \tag{10}$$

The prefactors $Q^{2/3}$ and $Q^{-2/3}$ stem from the condition that the affine transformation conserves the volume. From (9) with (10) one infers that the coefficients D_{\parallel} and D_{\perp} for diffusion parallel and perpendicular to the preferential direction u are given by

$$\begin{aligned} D_{\parallel} &= Q^{4/3} D_0 \\ D_{\perp} &= Q^{-2/3} D_0. \end{aligned} \tag{11}$$

Clearly $D_{\parallel} > D_{\perp}$ ($D_{\parallel} < D_{\perp}$) for prolate (oblate) particles where $Q > 1$ ($Q < 1$).

The anisotropy of the diffusion is characterized by the ratio

$$R = \frac{D_{\parallel} - D_{\perp}}{D_{\parallel} + 2D_{\perp}} \tag{12}$$

which, by definition, lies in the range $-\frac{1}{2} \leq R \leq 1$. Relation (11) implies

$$R = \frac{Q^2 - 1}{Q^2 + 2}. \tag{13}$$

For very long needles ($Q \gg 1$) $R \rightarrow 1$; for very thin platelets ($0 < Q \ll 1$) $R \rightarrow -\frac{1}{2}$.

The average, or arithmetic mean, diffusion coefficient \bar{D} is given by

$$\bar{D} = \frac{1}{3} D_{\parallel} + \frac{2}{3} D_{\perp} = \frac{1}{3} Q^{-2/3} (Q^2 + 2) D_0. \tag{14}$$

Notice that the ratio \bar{D}/D_0 has a minimum at $Q = 1$. Conversely, the geometric mean diffusion coefficient \tilde{D} is predicted to be independent of Q ; from (11) we have

$$\tilde{D} = D_{\parallel}^{1/3} D_{\perp}^{2/3} = D_0. \tag{15}$$

3. Modified affine transformation model

In any real liquid crystal, the orientation of the particles is not perfect. The degree of orientation in a nematic phase is characterized by the Maier-Saupe order parameter

$$S = \langle P_2(\mathbf{n} \cdot \mathbf{u}) \rangle = \frac{3}{2} \langle (\mathbf{n} \cdot \mathbf{u})^2 - \frac{1}{3} \rangle,$$

where P_2 is the second Legendre polynomial. The unit vector \mathbf{n} is the director which specifies an average direction for the molecules; \mathbf{u} represents an individual molecular symmetry axis. The bracket $\langle \dots \rangle$ refers to an average to be evaluated with an orientational (one-particle) distribution function. To generalize relation (9) for the diffusion tensor to a partially ordered fluid, it is assumed that the vicinity of a diffusing molecule has practically the same orientation, such that (9) still applies, but with A^{-1} replaced by $\alpha \langle A^{-1} \rangle$, where the factor α ensures the constant volume in the affine mapping: $\alpha = |\langle A^{-1} \rangle|^{-1/3}$. Instead of the affine transformation model (9), valid for perfect alignment ($S = 1$) we have now the modified version

$$D = \alpha \langle A^{-1} \rangle D_0 \tag{16}$$

for partial alignment ($S < 1$).

For uniaxial particles with a uniaxial average orientation parallel to the director \mathbf{n} one has

$$\langle A^{-1} \rangle = Q^{-2/3} [(1 + \frac{1}{3}(Q^2 - 1)(1 - S))\delta + S(Q^2 - 1)\mathbf{nn}]. \tag{17}$$

Relation (17) follows from (10) due to

$$\langle uu \rangle = \frac{1}{3} \delta(1 - S) + Snn, \tag{18}$$

which is equivalent to

$$\langle \overleftrightarrow{uu} \rangle = S \overleftrightarrow{nn}. \quad (19)$$

Here the symbol $\overleftrightarrow{\cdot}$ refers to the symmetrical traceless part of a tensor, e.g., $\overleftrightarrow{uu} = uu - \frac{1}{3}\delta$. To verify (19), multiply both sides by nn , contract and use

$$\begin{aligned} n \cdot \langle \overleftrightarrow{uu} \rangle \cdot n &= \langle (n \cdot u)^2 - \frac{1}{3} \rangle \\ n \cdot \overleftrightarrow{nn} \cdot n &= \frac{2}{3} \end{aligned}$$

and the definition of S . From (16) and (17) one now infers

$$\begin{aligned} D_{\parallel}/D_0 &= \alpha(Q^{4/3} - \frac{2}{3}Q^{-2/3}(Q^2 - 1)(1 - S)) \\ D_{\perp}/D_0 &= \alpha(Q^{-2/3} + \frac{1}{3}Q^{-2/3}(Q^2 - 1)(1 - S)), \end{aligned} \quad (20)$$

with

$$\begin{aligned} \alpha &= (1 + \frac{2}{3}(Q^{-2} - 1)(1 - S))^{-1/3} (1 + \frac{1}{3}(Q^2 - 1)(1 - S))^{-2/3} \\ &= 3Q^{2/3}(2 + Q^2)^{-1} \left\{ 1 + 2 \left(\frac{Q^2 - 1}{Q^2 + 2} \right) S \right\}^{-1/3} \left\{ 1 - \left(\frac{Q^2 - 1}{Q^2 + 2} \right) S \right\}^{-2/3}. \end{aligned} \quad (21)$$

The ratio

$$\frac{D_{\parallel}}{D_{\perp}} = Q^2 \frac{1 + \frac{2}{3}(Q^{-2} - 1)(1 - S)}{1 + \frac{1}{3}(Q^2 - 1)(1 - S)} \quad (22)$$

approaches the values Q^2 and 1 for $S = 1$ and $S = 0$, respectively. It is remarkable that the anisotropy of diffusion characterized by the ratio R defined by (12) becomes a linear function of S :

$$R = \frac{D_{\parallel} - D_{\perp}}{D_{\parallel} + 2D_{\perp}} = S \left(\frac{Q^2 - 1}{Q^2 + 2} \right). \quad (23)$$

The average diffusion coefficient \bar{D} is now given by

$$\begin{aligned} \bar{D} &= \frac{1}{3}D_{\parallel} + \frac{2}{3}D_{\perp} = \frac{1}{3}Q^{-2/3}(2 + Q^2)\alpha D_0 \\ &= \left\{ 1 + 2 \left(\frac{Q^2 - 1}{Q^2 + 2} \right) S \right\}^{-1/3} \left\{ 1 - \left(\frac{Q^2 - 1}{Q^2 + 2} \right) S \right\}^{-2/3} D_0, \end{aligned} \quad (24)$$

which differs from (14) by the factor α , cf., (21). Owing to (21), one has $\alpha = 1$ for $S = 1$ and $\alpha = 3Q^{2/3}(2 + Q^2)^{-1}$ for $S = 0$. Thus (24) implies $\bar{D} = D_0$ for $S = 0$. As in the simple theory, the geometric mean diffusion coefficient \bar{D} is predicted to be independent of Q and S , being given by (15).

It should be kept in mind that relations (20–24) are exact consequences of the affine transformation equations for $S = 1$, reducing to the equations of the previous section in this limit, but are based on the educated guess (16) for $S < 1$. It is desirable to test these relations with data obtained from a molecular dynamics computer simulation of partially aligned uniaxial ellipsoidal particles.

4. Molecular dynamics simulations

Molecular dynamics simulations have been carried out for hard, uniaxial, ellipsoids of axis ratio $Q = \frac{1}{10}, \frac{1}{5}, \frac{1}{3}, 3, 5, 10$. Here we present a brief summary of the methods used; full technical details have been given elsewhere [5].

Collision by collision dynamics is implemented, with free flight (constant linear and angular momentum for each particle) between collisions. Each forthcoming collision is detected by a method similar to that of Rebertus and Sando [8]. The collision dynamics are completely determined by the conditions that the ellipsoids are hard, smooth bodies, and that energy, linear momentum, and angular momentum are conserved. The molecules are taken to have unit mass m , distributed uniformly throughout the ellipsoid, and the molecular moment of inertia is calculated accordingly. However, the moment of inertia about the symmetry axis is set to zero, and the ellipsoids are treated dynamically as linear rotors with the angular velocity perpendicular to the axis at all times. The temperature T is chosen such that $k_B T = 1$, k_B being Boltzmann's constant: this establishes a convenient time scale for the simulation. The length scale is chosen so that $8ab^2 = 1$, where a and b are the semi-axes; for comparison, hard spheres of the same volume have a diameter $\sigma = 1$.

In these simulations we employed truncated octahedral periodic boundary conditions. For $Q = \frac{1}{3}$, 3 we used system sizes of $N = 125$; for $Q = \frac{1}{5}$, 5 we used $N = 216$; while for $Q = \frac{1}{10}$, 10 we used $N = 500$. We did not systematically investigate the dependence of our results on system size for given Q . Typical production run lengths were $0.5\text{--}1.6 \times 10^6$ collisions, depending on density: thus the results were averaged over times $t_{\text{run}} \sim 2000\text{--}15000t_c$, where t_c is the mean time between collisions per molecule. These run times are usually considered ample for the determination of single-particle properties, although we must bear in mind the slow fluctuations inherent in the nematic phase.

For the least anisometric shapes $Q = \frac{1}{3}$, 3, the isotropic–nematic and nematic–solid transitions have been located by free-energy calculations [9]. The nematic range is quite narrow, extending from about 70% to about 78% of the close-packed density ρ_{cp} . The thermodynamic freezing density of the simple hard sphere $Q = 1$ fluid is $0.67\rho_{\text{cp}}$, but the metastable fluid has been studied up to $0.76\rho_{\text{cp}}$, so some comparison between the two systems is possible.

The isotropic–nematic phase transitions for $Q = \frac{1}{10}$, 10, $\frac{1}{5}$, 5 have not yet been determined by free-energy calculations, but are approximately located by observing the order parameter S . The nematic range is much wider for these values of Q ; ρ_{NI} is about 25% of ρ_{cp} for $Q = \frac{1}{10}$, 10, and about 40–45% for $Q = \frac{1}{5}$, 5. All of the state points studied for these more anisometric systems lie well below the likely freezing density, and we have found no evidence of two-phase coexistence. They are also below the equivalent hard sphere freezing density.

The director \mathbf{n} and the nematic order parameter S were determined in a standard way [10]. Diffusion coefficients D_{\parallel} and D_{\perp} were determined by examining the long-time limit of the mean-squared displacements, and by integrating the velocity autocorrelation function, as described in reference [6].

5. Results

The coefficients D_{\parallel} , D_{\perp} , and S were reported in [6] for $Q = \frac{1}{10}$, 10, $\frac{1}{5}$, 5. For convenience we reproduce those results in table 1, for state points in the nematic region, and supplement them with values for $Q = \frac{1}{3}$, 3 at a single density in each case. The precision is estimated from the results of several independent runs at each state point.

In table 1 we give also the dimensionless ratio $R(12)$, the values of \bar{D}/D_0 and \tilde{D}/D_0 , and the shape scaled order parameter $S(Q^2 - 1)/(Q^2 + 2)$. Hard sphere diffusion

Table 1. Diffusion coefficients and order parameters as functions of elongation and density for the hard ellipsoid fluid. Figures in parentheses indicate the estimated statistical error in the last digit quoted. Hard sphere values D_0 are taken from the formula of reference [11].

Q	ρ/ρ_{cp}	S	$D_{ }$	D_{\perp}	D_0	R	\bar{D}/D_0	\bar{D}/D_0	$s\left(\frac{Q^2-1}{Q^2+2}\right)$
10	0.30	0.60(3)	0.92(3)	0.15(1)	0.32	0.62(2)	0.88(9)	1.29(4)	0.58(3)
10	0.35	0.80(1)	1.56(1)	0.11(1)	0.24	0.82(1)	1.1(1)	2.43(3)	0.78(1)
10	0.50	0.93(1)	1.53(1)	0.052(5)	0.10	0.90(1)	1.5(2)	5.22(5)	0.91(1)
10	0.60	0.95(1)	1.38(1)	0.029(5)	0.047	0.94(1)	2.2(5)	10.1(1)	0.92(1)
10	ideal	1.0				0.97	1.0	7.33	0.97
$\frac{1}{10}$	0.30	0.74(1)	0.077(5)	0.59(1)	0.32	-0.41(1)	0.94(7)	1.32(2)	-0.36(1)
$\frac{1}{10}$	0.35	0.83(1)	0.048(4)	0.58(1)	0.24	-0.44(1)	1.03(9)	1.65(3)	-0.41(1)
$\frac{1}{10}$	0.50	0.94(1)	0.014(4)	0.36(1)	0.10	-0.47(1)	1.2(3)	2.35(7)	-0.46(1)
$\frac{1}{10}$	0.60	0.96(1)	0.007(4)	0.24(1)	0.047	-0.48(1)	1.5(9)	3.4(1)	-0.47(1)
$\frac{1}{10}$	ideal	1.0				-0.49	1.0	3.11	-0.49
5	0.50	0.28(5)	0.20(3)	0.11(2)	0.10	0.22(9)	1.3(4)	1.3(2)	0.25(5)
5	0.55	0.73(1)	0.38(1)	0.056(3)	0.073	0.66(2)	1.4(1)	2.24(5)	0.65(1)
5	0.60	0.82(1)	0.34(1)	0.040(3)	0.047	0.71(2)	1.7(2)	2.93(8)	0.73(1)
5	0.65	0.87(1)	0.26(1)	0.027(3)	0.027	0.74(3)	2.1(3)	3.9(1)	0.77(1)
5	ideal	1.0				0.89	1.0	3.08	0.89
$\frac{1}{5}$	0.45	0.33(1)	0.105(7)	0.18(1)	0.14	-0.16(2)	1.1(1)	1.09(5)	-0.16(1)
$\frac{1}{5}$	0.50	0.70(1)	0.042(5)	0.20(1)	0.10	-0.36(2)	1.1(2)	1.41(7)	-0.33(1)
$\frac{1}{5}$	0.55	0.78(1)	0.030(3)	0.18(1)	0.073	-0.38(1)	1.3(2)	1.74(9)	-0.36(1)
$\frac{1}{5}$	0.60	0.85(1)	0.019(3)	0.15(1)	0.047	-0.41(1)	1.6(3)	2.3(1)	-0.40(1)
$\frac{1}{5}$	0.65	0.88(1)	0.014(2)	0.11(1)	0.027	-0.41(1)	2.0(4)	2.9(2)	-0.42(1)
$\frac{1}{5}$	ideal	1.0				-0.47	1.0	1.99	-0.47
3	0.75	0.70(2)	0.052(4)	0.011(3)	0.0022	0.55(9)	9(3)	11(1)	0.51(2)
3	ideal	1.0				0.73	1.0	1.76	0.73
$\frac{1}{3}$	0.75	0.75(2)	0.006(2)	0.026(3)	0.0022	-0.34(5)	7(3)	9(1)	-0.31(1)
$\frac{1}{3}$	ideal	1.0				-0.42	1.0	1.46	-0.42

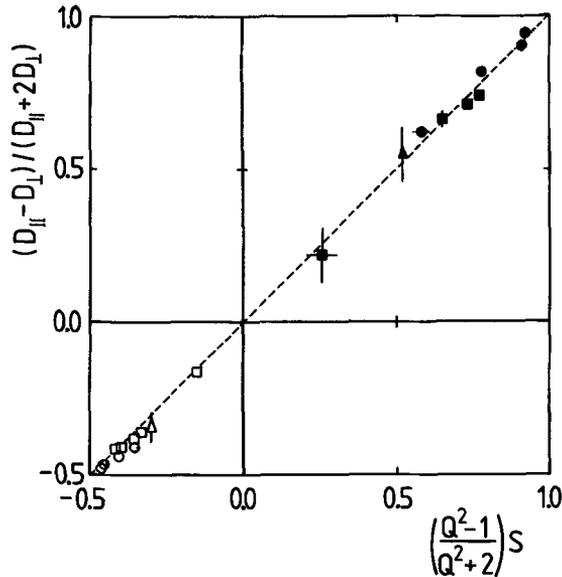


Figure 1. The anisotropy of the diffusion coefficient as a function of the shape scaled order parameter. ●, $Q = 10$; ■, $Q = 5$; ▲, $Q = 3$; △, $Q = \frac{1}{3}$; □, $Q = \frac{1}{3}$; ○, $Q = \frac{1}{10}$. The dashed line is the theoretical prediction.

coefficients D_0 were calculated using Speedy's formula [11] which is based on a re-analysis of a wide range of simulation results [12]. The values of D_0 are given in table 1 for completeness; we have not attempted to correct for system-size dependence, but the precise values quoted are not crucial for our purposes. However, the values of D_0 at $\rho/\rho_{cp} = 0.75$ correspond to the metastable region of the hard sphere fluid, and should be treated with caution.

From the table we can see that the ratio R indeed approaches the 'ideal' value $(Q^2 - 1)/(Q^2 + 2)$ for each shape as the order parameter $S \rightarrow 1$. These 'ideal' values are also given in the table. However, the ratio clearly depends on S . It is plotted against the shape-scaled order parameter $S(Q^2 - 1)/(Q^2 + 2)$ in figure 1. According to (23), these results should all lie on a single straight line. We see good agreement, both with the predicted linear dependence on S and with the coefficient of this linear dependence, which has been absorbed into the shape factor $(Q^2 - 1)/(Q^2 + 2)$. This is the principal result of this paper: the modified affine transformation model accurately reproduces the anisotropy of the diffusion tensor in the nematic phase, for a wide range of molecular axis ratios, both prolate and oblate, over a wide range of S .

A second test is the comparison of the individual values D_{\parallel} and D_{\perp} , or the average diffusion coefficient \bar{D} , with the equivalent hard sphere value D_0 . Equation (24) for the mean diffusion coefficient suggests that \bar{D}/D_0 should depend in a universal way on the shape scaled order parameter, and this is plotted in figure 2(a). (In view of the uncertainty both in our own results and in the reference values of D_0 for the metastable hard sphere fluid, the data for $Q = \frac{1}{3}, 3$ are omitted from this and the following plots.) We see that the general features of the ideal curve are correctly reproduced. In particular, the spectacular enhancement of \bar{D}/D_0 at both extremes of the range is well represented by the affine transformation model. The ratio of the simulation results to the theoretical prediction is given in figure 2(b). The observed level of agreement is

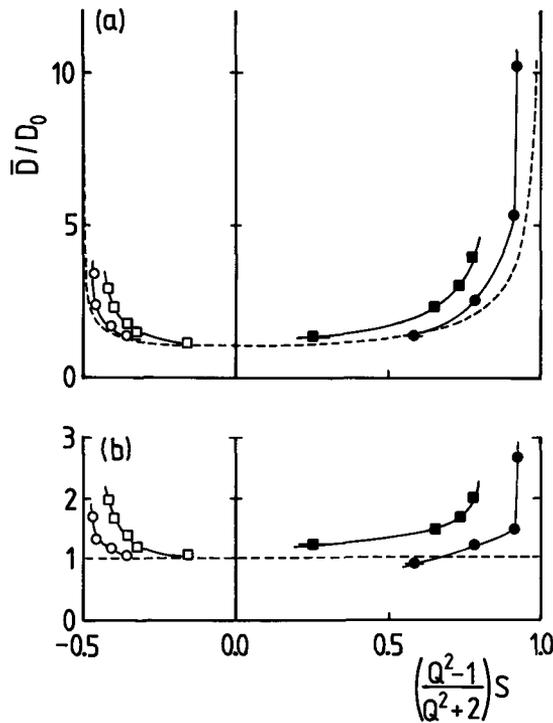


Figure 2. (a) The average diffusion coefficient \bar{D} relative to that of a hard sphere fluid at the same density, as a function of the shape-scaled order parameter. ●, $Q = 10$; ■, $Q = 5$; □, $Q = \frac{1}{2}$; ○, $Q = \frac{1}{10}$. The dashed line is the theoretical prediction, (24); the solid lines are to guide the eye. Data for $Q = 3, \frac{1}{3}$ are not plotted. (b) The same data, normalized by the theoretical prediction (24).

quite satisfactory, bearing in mind the crude approximation made in the derivation. It is also clear, however, that some systematic differences between different values of Q have not been taken into account. An even simpler comparison is to look at the deviation of the observed values of \bar{D}/D_0 , from the theoretical value of unity. This is plotted in figure 3. The deviations are not large, and it is noticeable that \bar{D} is more sensitive to statistical errors in the data, but again systematic dependence on shape can be seen. This shows that the basic identification of the two systems (partially

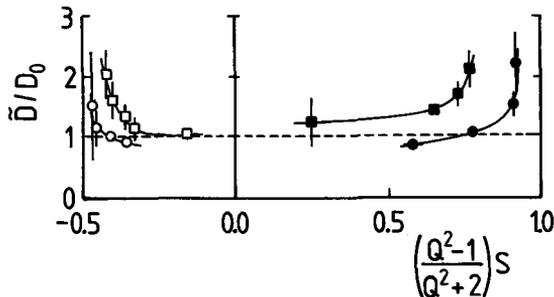


Figure 3. The geometric mean diffusion coefficient \tilde{D} relative to that of a hard sphere fluid at the same density, as a function of the shape-scaled order parameter. Notation as for figure 2.

aligned ellipsoids of axial ratio Q and hard spheres at the same density) is not quite correct.

Finally, we mention an alternative theory, due to Chu and Moroi [13], which relates D_{\parallel} and D_{\perp} to the shape and order parameter. When applied to ellipsoidal shapes, this theory predicts that (in our notation)

$$\begin{aligned} D_{\parallel}/D_0 &= 1 + 2 \left(\frac{Q-1}{Q+2} \right) S \\ D_{\perp}/D_0 &= 1 - \left(\frac{Q-1}{Q+2} \right) S, \end{aligned} \quad (25)$$

and

$$R = \frac{D_{\parallel} - D_{\perp}}{D_{\parallel} + 2D_{\perp}} = S \left(\frac{Q-1}{Q+2} \right). \quad (26)$$

Our simulations do not support these equations. In particular, most of the observed values of R in table 1 are significantly larger in magnitude than the maximum ($S \rightarrow 1$) values permitted by (26) for the appropriate shapes. Moreover, (25) suggests that the scaled *arithmetic* mean value \bar{D}/D_0 should be approximately independent of Q and S , whereas we see quite dramatic variation in this quantity.

6. Conclusion

The modified affine transformation model accounts very well for the anisotropy of the diffusion tensor, as measured by $(D_{\parallel} - D_{\perp})/(D_{\parallel} + 2D_{\perp})$, in hard ellipsoid nematic liquid crystals, for a wide range of axial ratios Q . This anisotropy is accurately predicted by the shape scaled order parameter $S(Q^2 - 1)/(Q^2 + 2)$. An approximate relation holds between the average diffusion tensor \bar{D} and that of a hard sphere system of the same molecular volume and density D_0 . Some systematic, shape dependent, differences are seen here, indicating that the simple mapping between a partially aligned ellipsoid system and a spherical system is not completely correct. These differences can also be seen in the ratio \bar{D}/D_0 , where \bar{D} is the geometric mean of the diagonal components of the diffusion tensor. Nonetheless, the main features of \bar{D}/D_0 , are reproduced quite well by the theory.

Partial financial support by the Deutsche Forschungsgemeinschaft via the SFB 335 'Anisotrope Fluide' is gratefully acknowledged (by SH). This work is part of the research program of FOM (Foundation for Fundamental Research of Matter) and was made possible by financial support from the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO). Computer time was provided by the Science and Engineering Research Council. Travel grants from NATO and The Royal Society are also gratefully acknowledged.

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