Enskog-Boltzmann-Equation for a Fluid of Nonspherical Particles

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The Enskog-Boltzmann-equation is generalized to fluids of nonsperical particles with fixed orientation, i.e. for overdamped rotational motion. General relations between the interparticle position vector at the instant of contact, the impact parameter and the differential cross section are derived. The dependence of these quantities of the orientations of the colliding particles is studied for the special case of hard ellipsoids.

Introduction

The density dependence of transport coefficients (heat conductivity, viscosity) as evaluated from Enskog's version of the Boltzmann equation for hard spheres [1–3] agrees with measured values over a surprisingly large range of densities [2, 4, 5]. Thus it seems worthwhile and desirable to extend the ,,Enkog-theory'' to fluids of nonspherical particles. In contradistinction to earlier theories for dense gases of rotating particles [6–8], the present analysis is concerned with fluids of nonspherical particles where the rotational motion is overdamped. More specifically, the generalized nonlocal Enskog-Boltzmann collision operator is derived for the case where the orientation of the two colliding particles remains constant during the scattering process. This should be a good approximation for nematic liquid crystals or a liquid of nonspherical particles whose orientation is fixed by an external (magnetic or electric) field. Without an applied field, the approximation should still be reasonable for a dense fluid where the rotation is hindered strongly by steric effects.

This article proceeds as follows. In Sect. 1, the generalized Enskog-Boltzmann equation is formulated. Its collision term involves the vector $\boldsymbol{R}$ connecting the centers of mass of the colliding particles at the instance of contact and the differential cross section σ. Both quantities depend on the orientation of the colliding particles. A general relation between $\boldsymbol{R}$, the impact parameter $\boldsymbol{b}$ and the differential cross section for (convex) non-spherical particles is derived in Section 2. Then, in Sect. 3, these quantities are evaluated for hard ellipsoids.

1. Formulation of the Generalized Enskog-Boltzmann Equation

The nonequilibrium state of a fluid of (axisymmetric) particles is characterized by the one particle distribution function

$$f = f(t, \boldsymbol{r}, \boldsymbol{c}, \boldsymbol{u}), \tag{1.1}$$

where t, $\boldsymbol{r}$, $\boldsymbol{c}$ are the time, position and velocity variables. The unit vector $\boldsymbol{u}$ which is parallel to the figure axis of a particle specifies its orientation. With the normalization

$$\int f \, \mathrm{d}^3 c \, \mathrm{d}^2 u = n(t, \boldsymbol{r}), \tag{1.2}$$

where n is the number density of the fluid, the local average $\langle \Psi \rangle$ of a quantity $\Psi = \Psi(\boldsymbol{c}, \boldsymbol{u})$, is, as usual, given by

$$n \langle \Psi \rangle = \int \Psi f \, \mathrm{d}^3 c \, \mathrm{d}^2 u \,. \tag{1.3}$$

The distribution function f is assumed to obey a kinetic equation of the form

$$\partial / \partial t f + \boldsymbol{c} \cdot \boldsymbol{\nabla} f + C(f) + \cdots = 0 , \tag{1.4}$$

where $-C(f)$ is the Enskog-Boltzmann collision term and the dots stand for terms describing orientational changes [9, 10] which, however, are not considered here. The second term of (1.4) is the usual flow term of the Boltzmann equation.

For the following discussion of the Enskog-Boltzmann collision operator, it is convenient to label the two colliding particles by "1" and "2", and to denote their velocities and orientation vectors by $\boldsymbol{c}_i$, $\boldsymbol{u}_i$, $i = 1, 2$.

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Momentum and energy conservation in a collision imply

$$c_s \equiv \tfrac{1}{2}(c_1 + c_2) = c_s' \equiv \tfrac{1}{2}(c_1' + c_2'),$$
$$g = g', \qquad (1.5)$$

where g is the magnitude of the relative velocity

$$\boldsymbol{g} = \boldsymbol{c}_1 - \boldsymbol{c}_2 = g\,\boldsymbol{e}; \qquad (1.6)$$

$\boldsymbol{e}$ is a unit vector. In (1.5), primed variables refer to the precollisional state. Thus one has

$$\boldsymbol{c}_{1,2} = \boldsymbol{c}_s \pm \tfrac{1}{2} g\,\boldsymbol{e}, \quad \boldsymbol{c}_{1,2}' = \boldsymbol{c}_s \pm \tfrac{1}{2} g\,\boldsymbol{e}'. \qquad (1.7)$$

With $\boldsymbol{c} \equiv \boldsymbol{c}_1$, $\boldsymbol{u} \equiv \boldsymbol{u}_1$, the generalized Enskog-Boltzmann collision term occurring in (2.4) can be written as

$$C_1(f) = \int \mathrm{d}^2 u_2 \int \mathrm{d}^3 c_2 \int \mathrm{d}^2 e'\, g\, \sigma(\boldsymbol{e}, \boldsymbol{e}') \qquad (1.8)$$
$$\cdot\, \chi[f_1(\boldsymbol{r})\, f_2(\boldsymbol{r} + \boldsymbol{R}) - f_1'(\boldsymbol{r})\, f_2'(\boldsymbol{r} - \boldsymbol{R})],$$

where the differential cross section

$$\sigma(\boldsymbol{e}, \boldsymbol{e}') = \sigma(\boldsymbol{e}', \boldsymbol{e})$$

and the interparticle distance vector $\boldsymbol{R}$, cf. Fig. 1, are functions of the orientation vectors $\boldsymbol{u}_1, \boldsymbol{u}_2$ which will be determined next. In (1.8), the abbreviations $f_i \equiv f(\boldsymbol{c}_i, \boldsymbol{u}_i)$ and $f_i' = f(\boldsymbol{c}_i', \boldsymbol{u}_i)$, $i = 1, 2$ have been used. Notice that the first and second terms of (1.8) are associated with loss and gain collisions, respectively. The spatial and orientational dependence of the shielding factor χ is disregarded here.

In the next sections, a general relation between $\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{e}, \boldsymbol{e}', \boldsymbol{u}_1, \boldsymbol{u}_2)$, the impact parameter $\boldsymbol{b}$ and the pertaining differential cross section

$$\sigma = \sigma(\boldsymbol{e}, \boldsymbol{e}', \boldsymbol{u}_1, \boldsymbol{u}_2)$$

is established and then rigid ellipsoids are considered as a specific example.

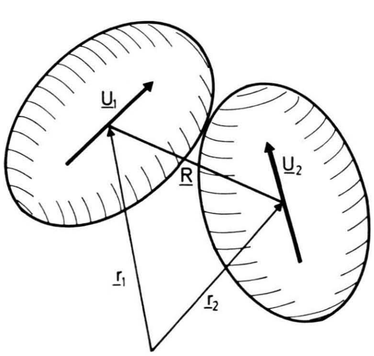

Fig. 1. Two nonspherical particles at the instant of contact; $\boldsymbol{r}_1$, $\boldsymbol{r}_2$ are the position vectors for the centers of mass of particles "1" and "2", $\boldsymbol{u}_{1,2}$ are unit vectors parallel to their figure axes.

2. Classical Cross Section for Nonspherical Particles

For the derivation of a connection between the differential cross section $\sigma(\boldsymbol{e}, \boldsymbol{e}')$ and the impact parameter vector $\boldsymbol{b}$ firstly consider Fig. 2 which shows an "impact parameter element" of the incoming particles (in the center of mass system) and the solid angle element

$$\mathrm{d}\boldsymbol{\Omega} = \boldsymbol{e}\, \mathrm{d}\Omega \qquad (2.1)$$

into which the (detected) particles are scattered. Since we are concerned with the scattering of nonspherical particles, there is no azimuthal symmetry around the $\boldsymbol{e}'$ direction which falicitates the evaluation of the cross section for spherical particles. Now let $\mathrm{d}\boldsymbol{b}_1$ and $\mathrm{d}\boldsymbol{b}_2$ be increments of $\boldsymbol{b}$, as indicated in Fig. 2, parallel and perpendicular to $\boldsymbol{b}$ and let $\mathrm{d}\boldsymbol{e}_1$ and $\mathrm{d}\boldsymbol{e}_2$ be the resulting changes of $\boldsymbol{e}$; here the labels "1" and "2" should not be confused with the previously used labeling of particles. Thus, one has by definition

$$\boldsymbol{b}(\boldsymbol{e}) + \mathrm{d}\boldsymbol{b}_i = \boldsymbol{b}(\boldsymbol{e} + \mathrm{d}\boldsymbol{e}_i); \quad i = 1, 2. \qquad (2.2)$$

Expansion on the right hand side of (2.2) and neglect of higher order terms yields

$$\mathrm{d}\boldsymbol{b}_i = (\partial \boldsymbol{b}/\partial \boldsymbol{e}) \cdot \mathrm{d}\boldsymbol{e}_i, \qquad (2.3)$$

notice that $\boldsymbol{e} \cdot \mathrm{d}\boldsymbol{e}_i = 0$ for $i = 1, 2$.

From the conservation of the number of particles and the definition of the cross section $\mathrm{d}\sigma$, cf. Fig. 2, one infers

$$\mathrm{d}\sigma = -(\mathrm{d}\boldsymbol{b}_1 \times \mathrm{d}\boldsymbol{b}_2) \cdot \boldsymbol{e}'$$
$$= -\left(\frac{\partial \boldsymbol{b}}{\partial \boldsymbol{e}} \cdot \mathrm{d}\boldsymbol{e}_1 \times \frac{\partial \boldsymbol{b}}{\partial \boldsymbol{e}} \cdot \mathrm{d}\boldsymbol{e}_2\right) \cdot \boldsymbol{e}'$$
$$= -\,\varepsilon_{\alpha\beta\gamma} \frac{\partial b_\alpha}{\partial e_\mu} \frac{\partial b_\beta}{\partial e_\nu}\, e_\gamma'\, \mathrm{d}e_{1\mu}\, \mathrm{d}e_{2\nu}. \qquad (2.4)$$

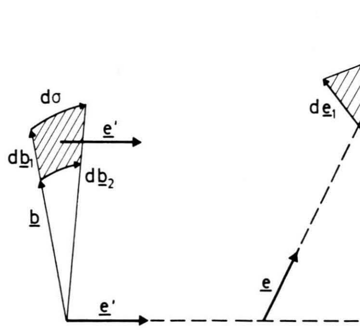

Fig. 2. Schematic diagram of the impact parameter element and the scattering solid angle. Unit vectors parallel to the incident flux and the detected scattered particles are denoted by $\boldsymbol{e}'$ and $\boldsymbol{e}$, respectively. The area $\mathrm{d}\sigma$ spanned by the vectors $\mathrm{d}\boldsymbol{b}_1$ and $\mathrm{d}\boldsymbol{b}_2$ is perpendicular to $\boldsymbol{e}'$; the vectors $\mathrm{d}\boldsymbol{e}_1$ and $\mathrm{d}\boldsymbol{e}_2$ are perpendicular to $\boldsymbol{e}$.

Cartesian component notation has been used in the second line of (2.4). Notice that the exchange $\mu \leftrightarrow \nu$, $\alpha \leftrightarrow \beta$ reproduces the expression (2.4) but now with $\varepsilon_{\beta\alpha\gamma} = -\varepsilon_{\alpha\beta\gamma}$ instead of $\varepsilon_{\alpha\beta\gamma}$; thus $\mathrm{d}e_{1\mu}\mathrm{d}e_{2\nu}$ in (2.4) can be replaced by $\frac{1}{2}(\mathrm{d}e_{1\mu}\mathrm{d}e_{2\nu} - \mathrm{d}e_{1\nu}\mathrm{d}e_{2\mu})$. On the other hand, one has for the solid angle element $\mathrm{d}\boldsymbol{\Omega}$:

$$\varepsilon_{\mu\nu\lambda}\,\mathrm{d}\Omega_\lambda \equiv \mathrm{d}\Omega\, e_\lambda\, \varepsilon_{\lambda\mu\nu} = \mp(\mathrm{d}e_{1\mu}\mathrm{d}e_{2\nu} - \mathrm{d}e_{1\nu}\mathrm{d}e_{2\nu}), \qquad (2.5)$$

where the sign depends on whether $\boldsymbol{e}$, $\mathrm{d}\boldsymbol{e}_1$, $\mathrm{d}\boldsymbol{e}_2$ are a right or left hand system. Thus (2.4) and (2.5) lead to

$$\frac{\mathrm{d}\sigma}{\mathrm{d}\Omega} \equiv \sigma(\boldsymbol{e}, \boldsymbol{e}') = \frac{1}{2}\left|\varepsilon_{\alpha\beta\gamma}\,\varepsilon_{\mu\nu\lambda}\, e'_\gamma\, e_\lambda \frac{\partial b_\alpha}{\partial e_\mu}\frac{\partial b_\beta}{\partial e_\nu}\right|. \qquad (2.6)$$

Due to (2.6), the dependence of the differential cross section $\sigma(\boldsymbol{e}, \boldsymbol{e}')$ on the orientation vectors $\boldsymbol{u}_1$, $\boldsymbol{u}_2$ of the colliding partners can be inferred from the orientation dependence of the impact parameter $\boldsymbol{b}$ or, practically equivalently, of the vector $\boldsymbol{R}$ joining the centers of mass of the two colliding particles. Inspection of Fig. 3 shows that $\boldsymbol{b}$ is related to $\boldsymbol{R}$ by

$$b_\mu = (\delta_{\mu\nu} - e'_\mu e'_\nu)\, R_\nu\,. \qquad (2.7)$$

Thus for given $\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{e}, \boldsymbol{e}'; \boldsymbol{u}_1, \boldsymbol{u}_2)$ the pertaining differential cross section is determined by

$$\sigma(\boldsymbol{e}, \boldsymbol{e}', \boldsymbol{u}_1, \boldsymbol{u}_2) = \frac{1}{2}\left|\varepsilon_{\alpha\beta\gamma}\,\varepsilon_{\mu\nu\lambda}\, e'_\gamma\, e_\lambda \frac{\partial R_\alpha}{\partial e_\mu}\frac{\partial R_\beta}{\partial e_\nu}\right|. \qquad (2.8)$$

To obtain the desired dependence of $\boldsymbol{R}$ on $\boldsymbol{e}$, $\boldsymbol{e}'$ for particles with a specific geometry, it is firstly noticed, cf. Fig. 3, that

$$\boldsymbol{R} = \boldsymbol{R}_2 - \boldsymbol{R}_1\,, \qquad (2.9)$$

where $\boldsymbol{R}_{1,2}$ are the vectors from the centers of mass of particles 1, 2 to the point of contact. From the shape of the particles a relation between $\boldsymbol{R}_1$, $\boldsymbol{R}_2$ and the normal vectors $\boldsymbol{n}_{1,2}$ and

$$\boldsymbol{n} \equiv \boldsymbol{n}_2 = -\boldsymbol{n}_1 \qquad (2.10)$$

can be established. On the other hand, for the elastic collisions of hard and smooth particles one has $\boldsymbol{e} - \boldsymbol{e}' \sim \boldsymbol{n}$ and consequently

$$\boldsymbol{n} = \frac{\boldsymbol{e} - \boldsymbol{e}'}{|\boldsymbol{e} - \boldsymbol{e}'|} = (\boldsymbol{e} - \boldsymbol{e}')\,[2(1 - \boldsymbol{e}\cdot\boldsymbol{e}')]^{-1/2}\,. \qquad (2.11)$$

Thus the cross section $\sigma(\boldsymbol{e}, \boldsymbol{e}')$ can be calculated according to (2.8) when (2.11) is inserted into the functional relation between $\boldsymbol{R}$ and normal vector $\boldsymbol{n}$ which can be inferred from geometric considerations. Before this point is discussed in some detail for the collision of hard ellipsoids it is noticed that (2.8) is equivalent to

$$\sigma(\boldsymbol{e}, \boldsymbol{e}', \boldsymbol{u}_1, \boldsymbol{u}_2) = \tfrac{1}{4}(1 - \boldsymbol{e}\cdot\boldsymbol{e}')^{-1} \cdot \left|\varepsilon_{\alpha\beta\gamma}\,\varepsilon_{\mu\nu\lambda}\, e'_\gamma\, e'_\lambda \frac{\partial R_\alpha}{\partial n_\mu}\frac{\partial R_\beta}{\partial n_\nu}\right|, \qquad (2.12)$$

where $\boldsymbol{R}$ is now differentiated with respect to the components of the unit vector $\boldsymbol{n}$. Furthermore, due to (2.9, 10) one has

$$\frac{\partial R_\alpha}{\partial n_\mu} = \frac{\partial R_{1\alpha}}{\partial n_{1\mu}} + \frac{\partial R_{2\alpha}}{\partial n_{2\mu}} \equiv R^{(1)}_{\alpha\mu} + R^{(2)}_{\alpha\mu}, \qquad (2.13)$$

where the tensor $R^{(i)}_{\alpha\mu}$ can be obtained from an analysis of the shape of one particle.

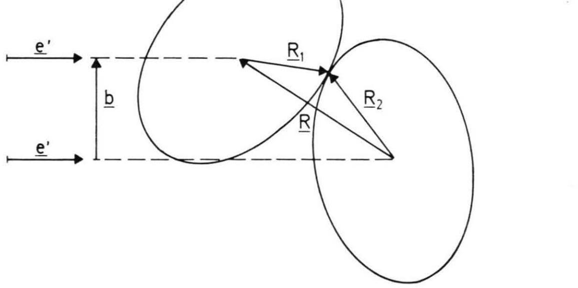

Fig. 3. Schematic diagram of two colliding nonspherical particles at the instant of contact. The vectors $\boldsymbol{R}_1$ and $\boldsymbol{R}_2$ point from the centers of mass to the point of contact, $\boldsymbol{b}$ is the impact parameter vector.

Scattering of Hard Ellipsoids

An ellipsoid of revolution with the semi axes $a = b$ and c, cf. Fig. 4, is described by the relation

$$F(\mathbf{R}) \equiv R^2 - \lambda(\boldsymbol{u}\cdot\mathbf{R})^2 - a^2 = 0\,, \qquad (3.1)$$

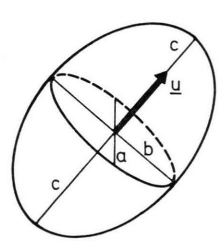

Fig. 4. One ellipsoidal particle with semi axes a, b, c and unit vector $\boldsymbol{u}$ parallel to the c-axis.

where $\boldsymbol{R}$ is the vector pointing from the center of mass of the ellipsoid to its surface, $\boldsymbol{u}$ is a unit vector parallel to the figure axis (c-axis) and λ given by

$$\lambda = 1 - a^2/c^2 . \tag{3.2}$$

Notice that one has $\lambda > 0$ ($\lambda < 0$) for prolate (oblate) particles and $\lambda = 0$ for a sphere. The numerical eccentricity ε is related to λ by $\varepsilon^2 = \lambda$ for $\lambda > 0$.

The vector normal to the surface is proportional to $\partial F/\partial R_\mu$. Thus (3.1) leads to

$$\boldsymbol{n} \sim \boldsymbol{R} - \lambda \boldsymbol{R} \cdot \boldsymbol{u}\boldsymbol{u} = \boldsymbol{R}^\perp + (1-\lambda)\boldsymbol{R}'' , \tag{3.3}$$

where $\boldsymbol{R}^\perp = \boldsymbol{R} - \boldsymbol{u} \cdot \boldsymbol{R}\boldsymbol{u}$ and $\boldsymbol{R}'' = \boldsymbol{u}\boldsymbol{u} \cdot \boldsymbol{R}$ are the components of $\boldsymbol{R}$ perpendicular and parallel to $\boldsymbol{u}$. Relation (3.3) can be inverted for $\boldsymbol{R} = \boldsymbol{R}(\boldsymbol{n})$, viz.

$$\boldsymbol{R} \sim \boldsymbol{n}^\perp + (1-\lambda)^{-1}\boldsymbol{n}'' = \boldsymbol{n} + \beta \boldsymbol{n}'' \tag{3.4}$$

with

$$\beta = (1-\lambda)^{-1} - 1 = \lambda(1-\lambda)^{-1} = c^2/a^2 - 1 . \tag{3.5}$$

The proportionality factor needed in (3.4) is obtained by inserting (3.4) into (3.1). The result is

$$\boldsymbol{R} = \alpha a(\boldsymbol{n} + \beta \boldsymbol{u} \cdot \boldsymbol{n}\boldsymbol{u}) \tag{3.6}$$

with

$$\alpha = [1 + \beta(\boldsymbol{n}\cdot\boldsymbol{u})^2]^{-1/2} . \tag{3.7}$$

So far, one ellipsoid has been considered. For the scattering of two ellipsoid labelled by 1, 2, the vector $\boldsymbol{R}$ occurring in (2.9) and (2.13) is given by, cf. (2.10)

$$R_\mu(\boldsymbol{n}) = \sum_i \tilde{a}_i A^i_{\mu\nu} n_\nu , \tag{3.8}$$

with

$$\tilde{a}_i = \alpha_i a_i , \quad A^i_{\mu\nu} = \delta_{\mu\nu} + \beta_i u^i_\mu u^i_\nu , \tag{3.9}$$

$i = 1, 2$; α_i is given by (3.7) with $\boldsymbol{u}$ replaced by $\boldsymbol{u}^i$. For equal ellipsoids one has $a_1 = a_2$, $\beta_1 = \beta_2$ but $\boldsymbol{u}^1 \neq \boldsymbol{u}^2$, in general.

The tensor $R_{\alpha\mu} = \partial R_\alpha/\partial n_\mu$, cf. (2.13) needed for the evaluation of the differential cross section according to (2.12) can now be calculated from (3.8). The result is written as

$$R_{\alpha\mu} = \sum_i \tilde{a}_i \tilde{A}^i_{\alpha\sigma} n_{\sigma\mu} \tag{3.10}$$

with

$$\tilde{A}^i_{\alpha\sigma} = \delta_{\alpha\sigma} + \tilde{\beta}_i u^i_\alpha u^i_\sigma , \quad \tilde{\beta}_i = \alpha_i^2 \beta_i , \tag{3.11}$$

$$n_{\sigma\mu} = \partial n_\sigma/\partial n_\mu = \delta_{\sigma\mu} - n_\mu n_\sigma . \tag{3.12}$$

Clearly $\tilde{A}$ ... equals A ... apart from the fact that β_i has been replaced by $\tilde{\beta}_i$, cf. (3.11).

Before $R_{\alpha\mu}$ and the corresponding expression for $R_{\beta\nu}$ are inserted into (3.12), it is noted that

$$\varepsilon_{\mu\nu\lambda} e_\lambda n_{\sigma\mu} n_{\tau\nu} = \tfrac{1}{2} \varepsilon_{\sigma\tau\lambda}(e_\lambda - e'_\lambda) ,$$

and consequently one has

$$\sigma(\boldsymbol{e}, \boldsymbol{e}') = \tfrac{1}{8}(1 - \boldsymbol{e}\cdot\boldsymbol{e}')^{-1} \cdot \left| \varepsilon_{\alpha\beta\gamma}\, \varepsilon_{\mu\nu\lambda}\, e'_\gamma (e_\lambda - e'_\lambda)\, C_{\alpha\mu,\,\beta\nu} \right| , \tag{3.13}$$

where C ..,.. stands for

$$C_{\alpha\sigma,\,\beta\tau} = \sum_i \sum_j \tilde{a}_i \tilde{A}^i_{\alpha\sigma} \tilde{a}_j \tilde{A}^j_{\beta\tau} . \tag{3.14}$$

The differential cross section $\sigma(\boldsymbol{e}, \boldsymbol{e}')$ as given by (3.13) is not symmetric under the exchange $\boldsymbol{e}, \boldsymbol{e}' \to \boldsymbol{e}', \boldsymbol{e}$. It can be decomposed into its symmetric and antisymmetric parts σ^{s} and σ^{a} according to

$$\sigma = \sigma^{\mathrm{s}} + \sigma^{\mathrm{a}} ,$$
$$\sigma^{\mathrm{s,a}}(\boldsymbol{e}, \boldsymbol{e}') = \tfrac{1}{2}[\sigma(\boldsymbol{e}, \boldsymbol{e}') \pm \sigma(\boldsymbol{e}', \boldsymbol{e})] . \tag{3.15}$$

It is conjectured that the differential cross section occurring in the Enskog-Boltzmann collision term (1.8) is identified with the symmetric cross section

$$\sigma^{\mathrm{s}}(\boldsymbol{e}, \boldsymbol{e}') = \tfrac{1}{8} \left| \varepsilon_{\alpha\beta\gamma}\, \varepsilon_{\mu\nu\lambda}\, n_\gamma n_\lambda C_{\alpha\mu,\,\beta\nu} \right| . \tag{3.16}$$

Now insertion of (3.14) with (3.11) into (3.16) leads to

$$\sigma^{\mathrm{s}} = \tfrac{1}{4} \sum_i \sum_j [\tilde{a}_i \tilde{a}_j + \tilde{a}_i \tilde{a}_j \tilde{\beta}_j (\boldsymbol{n} \times \boldsymbol{u}^j) \cdot (\boldsymbol{n} \times \boldsymbol{u}^j)] + \tfrac{1}{4} \tilde{a}_1 \tilde{a}_2 \tilde{\beta}_1 \tilde{\beta}_2 [\boldsymbol{n} \cdot (\boldsymbol{u}_1 \times \boldsymbol{u}_2)]^2 . \tag{3.17}$$

For the collision of equal ellipsoids with $a_1 = a_2 = a$, (3.17) becomes

$$\sigma^{\mathrm{s}} = \tfrac{1}{4} a^2 \{(\alpha_1 + \alpha_2)^2 + \beta(\alpha_1 + \alpha_2) \cdot [\alpha_1^3 (\boldsymbol{n} \times \boldsymbol{u}_1) \cdot (\boldsymbol{n} \times \boldsymbol{u}_2) + \alpha_2^3 (\boldsymbol{n} \times \boldsymbol{u}_2) \cdot (\boldsymbol{n} \times \boldsymbol{u}_2)] + \alpha_1^3 \alpha_2^3 \beta^2 [\boldsymbol{n} \cdot (\boldsymbol{u}_1 \times \boldsymbol{u}_2)]^2\} . \tag{3.18}$$

Notice that the term $(\boldsymbol{n} \times \boldsymbol{u}^i)^2$ occurring in the term linear in β in (3.17, 18) can be written as

$$(\boldsymbol{n} \times \boldsymbol{u}_i)^2 = 1 - (\boldsymbol{n} \cdot \boldsymbol{u}_i)^2 = \tfrac{2}{3} - \overline{n_\mu n_\nu}\, \overline{u_{i\mu} u_{i\nu}} , \tag{3.19}$$

where the symbol $\overline{\ldots}$ refers to the symmetric traceless part of a tensor, i.e. $\overline{u_\mu u_\nu} = u_\mu u_\nu - \tfrac{1}{3}\delta_{\mu\nu}$.

In the special case $\boldsymbol{u}^1 = \boldsymbol{u}^2 = \boldsymbol{u}$ which is approximately realized in the presence of a strong orienting field or in the nematic phase of a liquid crystal, (3.18) reduces to

$$\sigma^{\mathrm{s}} = a^2 \alpha^2 [1 + \beta \alpha^2 (\boldsymbol{n} \times \boldsymbol{u})^2] = a^2 (1 + \beta) \alpha^4 , \tag{3.20}$$

for α see (3.9).

Note that the result $\sigma = a^2$ for the scattering of hard spheres with radius a follows, as it should, from (3.13), (3.17), (3.18) with $\beta_1 = \beta_2 = 0$.

Concluding Remarks

In this article, a generalized Enskog-Boltzmann equation has been formulated and expressions for the interparticle vector $\boldsymbol{R}$ as well as for the differential cross section σ have been derived for nonspherical particles with fixed orientation. This case of overdamped rotational motion is in a certain sense the opposite limiting case of the practically free rotational motion encountered in dilute gases where both classical [7, 11] and quantum mechanical [12] kinetic equations have been applied to a great variety of nonequilibrium phenomena, cf. [13 to 15] and references given in [3]. The differential cross section (3.17) is also of importance for the scattering of rotationg ellipsoids where, however, the dynamic raltions (1,5—7), (2.11) have to be modified appropriately [6—8].

For molecular liquids and liquid crystals where one has a strong damping of the rotational motion, the kinetic equation (1.8) with (3.8, 9) and (3.17) can be applied to transport process using the moment method solution procedure [3]. Some promising results have already been obtained for particles with small nonsphericity [16]. For liquid crystals, the somewhat more subtle limiting case of large nonsphericity should be analysed. Furthermore, to treat nonequilibrium alignment phenomena, e.g. flow alignment [9, 10, 17], the terms indicated by the dots in Eq. (1.4) which describe the dynamics of the molecular orientation have to be taken into account, e.g. along the lines indicated in [9, 10]. It should be possible to infer the torque excerted on a particle in a nonequilibrium situation, e.g. viscous flow or heat conduction, from the antisymmetric part of the pressure tensor. In this way the magnitude of the well-known flow birefringence and of the heat flow birefringence which has, so far, only been calculated [18] and detected [19] formolecular gases, could also be obtained for a (model) liquid of nonspherical particles.

Acknowledgements

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