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Computation of Collision Integral of Single Kind Bio molecular Particles

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We introduce a theoretical method for analyzing the thermo dynamical behavior of multi non spherical particle system composed of a single kind. We explained the collision integral term constituting the Boltzmann equation. We defining the translational rotational velocities, energies and utilizing the collision vectors and principal inertial moments. By converting the variables, transformation, we the collision integrals are deduced to be analytic one. Applying the rotational matrix transformation and supporting function, the collision integral can be simplified to those of the principal radius of curvature of the surface of the colliding particles. We computed the shear, bulk viscosity and thermal conductivity of the sphere-cylindrical particles. The present method we introduced will be available for evaluating the systemic behavior of a single kind bio particles.

Boltzmann equation, Translation, Rotatina, Principal inertial moment, Collisoin integral.

単一種の生体分子における衝突積分解析

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単一種類の多数存在する生体分子系の挙動を熱力学的に解析するため、Muckenfuss, Curtiss らが提唱した、非球状粒子の運動理論を利用し、 系の粘性(shear viscosity, bulk viscosity)，系の熱伝導性 thermal conductivity を計算した。ボルツマン方程式に含まれる衝突積分を計算する過程を詳術した。粒子の並進、回転運動速度、エネルギーを衝突ヴェクトル、主慣性モーメントなどを用いて記述した。衝突積分は種々の変数変換、を行い解析的に求められる形式まで還元した。衝突微分断面に関する積分では系の回転マトリックス変換、および Curtiss (1956) の Supporting function を利用して、粒子表面の主曲率半径の積分関数として記述できた。 本方法を両端が半球でその連結部が円柱である粒子に応用して、系の粘性．系の熱伝導性を計算した。本研究は複数の単一生体粒子の振る舞いを一つの系として解析するうえで有用である。

ボルツマン方程式． 並進、回転運動速度、エネルギー．主慣性モーメント．衝突微分断面

1. Introduction.

The ultimate process of biochemical and bio molecular reaction start from the physical encounter of the participant molecules. From the thermodaynamical stand point, the classical mechanical approach is still available for evaluating the total behaviors of the system as a whole from statistical analysis. For these problems, Curtis and Muckenfuss have challenged to analyze the kinetic behavior of the dilute solution (mainly for the non uniform Gas). Such analysis was stared from Chapman (1916, 17, 22, 35) and Enskog (1922) by solving the Boltzmann equations for Dilute and Dense Gas on the basis of rigorous mathematical and physical analysis. Curtis and Muckenfuss (J. Chemical Physics. vol 26. No 6.pp 1619, 1957) applied Chapmann's method for analysis of thermo dynamical and statistical behaviors of non spherical molecules. Particularly they confined attention for the Eulerian components and inertial, angular moments. In the present technical report, we introduce their method for application of collision theory to non spherical molecules of single kind.

2. Mathematical method.

"brace expressions,"

$$\{S_{nn'}^{(\nu)}\mathbf{W}^{(\nu)};S_{mm'}^{(\nu)}\mathbf{W}^{(\nu)}\}$$

$$=\frac{1}{8\pi^2 n}\int\int n_2^*\sin\beta_1\Big[[S_{1,nn'}^{(\nu)}\mathbf{W}_1^{(\nu)};S_{1,mm'}^{(\nu)}\mathbf{W}_1^{(\nu)}]_{12}+[S_{2,nn'}^{(\nu)}\mathbf{W}_2^{(\nu)};S_{1,mm'}^{(\nu)}\mathbf{W}_1^{(\nu)}]_{12}\Big]d\alpha_1 d\alpha_2. \quad (0\text{-}9)$$

The $S_{nn'}^{(\nu)}$ (and $S_{1,nn'}^{(\nu)}$ and $S_{2,nn'}^{(\nu)}$) are products of Sonine polynomials depending on the index ν defined by Eqs. (4-12) to (4-18) of reference 1, and the $\mathbf{W}^{(\nu)}$ (and $\mathbf{W}_1^{(\nu)}$ and $\mathbf{W}_2^{(\nu)}$) are certain vectors and tensors also depending on the index ν defined by Eq. (4-4) of reference 1. The integrations on the right are over all orientations of both molecules, n_2^* is the number density of molecules of orientation α_2 and β_1 is the second Eulerian angle of the rotation α_1. The "square bracket integrals" in the integrand are defined by

$$[\mathbf{G};\mathbf{H}]_{12}=\frac{1}{n_1^* n_2^*}\int\cdots\int[\mathbf{G}^+:(\mathbf{H}'-\mathbf{H})]$$

$$\times f_1^{(0)}f_2^{(0)}(\mathbf{k}\cdot\mathfrak{g})S(\mathbf{k})d\mathbf{k}d\mathbf{v}_1 d\omega_1 d\mathbf{v}_2 d\omega_2. \quad (0\text{-}10)$$

This integration is over all collisions of molecules of specified orientations, α_1 and α_2. Here, $\mathbf{k}$ is the unit vector normal to the plane of contact of the collision, $\mathbf{v}_1$ and $\mathbf{v}_2$ are the linear velocities, and ω_1 and ω_2 the angular velocities of the colliding molecules. The $^+$ indicates the transpose of a tensor, and the prime on $\mathbf{H}'$ indicates the value before a collision in which the unprimed values are the values after the collision. Also, $S(\mathbf{k})$ and $\mathfrak{g}$ are the cross section of the collision and the relative velocity of the points of contact.

1. REDUCTION OF THE SQUARE BRACKET INTEGRALS

The integrands of the various square bracket integrals, defined by Eq. (0-10), depend upon the dynamics of the collisions as expressed by the dependence of the primed variables on the unprimed variables. For convenience in describing this dependence, we define several new variables. First, we define $\mathbf{G}$ as the velocity of the center of mass of the pair of colliding molecules,

$$\mathbf{G}=\tfrac{1}{2}(\mathbf{V}_2+\mathbf{V}_1) \quad (1\text{-}1)$$

and $\mathbf{g}$ as the relative velocity of the pair

$$\mathbf{g}=\mathbf{V}_2-\mathbf{V}_1. \quad (1\text{-}2)$$

The corresponding dimensionless variables are then

$$\mathfrak{G}=\left(\frac{m}{kT}\right)^{\frac{1}{2}}\mathbf{G} \qquad \gamma=\left(\frac{m}{4kT}\right)^{\frac{1}{2}}\mathbf{g}$$

$$\mathbf{W}_1=(\mathfrak{G}-\gamma)/\sqrt{2} \quad (1\text{-}5) \qquad \mathbf{W}_2=(\mathfrak{G}+\gamma)/\sqrt{2} \quad (1\text{-}6)$$

We now define the dimensionless vector related to the change in linear momentum of one of the molecules.

$$\kappa=\frac{1}{\sqrt{2}}(\mathbf{W}_1'-\mathbf{W}_1) \quad (1\text{-}7) \qquad \mathbf{W}_1'=\mathbf{W}_1+\sqrt{2}\kappa \quad (1\text{-}8)$$

and from the conservation of linear momentum

$$\mathbf{W}_2'=\mathbf{W}_2-\sqrt{2}\kappa. \quad (1\text{-}9)$$

Then from Eqs. (1-3) and (4), we find that

$$\mathfrak{G}'=\mathfrak{G}, \quad (1\text{-}10) \qquad \gamma'=\gamma-2\kappa. \quad (1\text{-}11)$$

The vector κ may be evaluated from considerations of the dynamics of the binary collisions. It may be

$$\kappa=\xi(\mathbf{k}\cdot\Gamma)\mathbf{k} \quad (1\text{-}12) \qquad \Gamma=\left(\frac{m}{4kT}\right)^{\frac{1}{2}}\mathfrak{g} \quad (1\text{-}13)$$

is the dimensionless relative velocity of the points of contact, and

$$\frac{1}{\xi}=1+\frac{m}{2}[\sigma_1\times\mathbf{k}]\cdot\mu_1\cdot[\sigma_1\times\mathbf{k}]+\frac{m}{2}[\sigma_2\times\mathbf{k}]\cdot\mu_2\cdot[\sigma_2\times\mathbf{k}]. \quad (1\text{-}14)$$

In these expressions, $\mathbf{k}$ is a unit vector normal to the plane of contact of the collision, σ_i is the radius vector from the center of molecule i to the point of contact, μ_i is the reciprocal of the moment of inertia tensor of molecule i in the space fixed coordinate system, a function of the orientation of the molecule, and

$$\mathfrak{g}=\mathbf{g}-\mathbf{g}_0 \quad (1\text{-}15)$$

where

$$\mathbf{g}_0=(\omega_1\times\sigma_1)-(\omega_2\times\sigma_2). \quad (1\text{-}16)$$

It is also convenient to define a dimensionless relative angular velocity,

$$\mathbf{w}_i=\frac{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}{(2kT)^{\frac{1}{2}}}\Omega_i \quad (1\text{-}17)$$

where Γ_1, Γ_2, and Γ_3 are the principal moments of inertia of a molecule. Then the expressions for the angular momenta before the collision in terms of those

$$\mathbf{I}_1\cdot\mathbf{w}_1'=\mathbf{I}_1\cdot\mathbf{w}_1+(2m)^{\frac{1}{2}}(\Gamma_1\Gamma_2\Gamma_3)^{1/6}[\sigma_1\times\kappa], \quad (1\text{-}18)$$

$$\mathbf{I}_2\cdot\mathbf{w}_2'=\mathbf{I}_2\cdot\mathbf{w}_2-(2m)^{\frac{1}{2}}(\Gamma_1\Gamma_2\Gamma_3)^{1/6}[\sigma_2\times\kappa]. \quad (1\text{-}19)$$

The dimensionless translational kinetic energies [see Eq. (0-11)] before a collision are obtained from Eqs. (1-8) and (1-9), and are

$$\epsilon_1^{(t)\prime}=\epsilon_1^{(t)}+2\sqrt{2}(\kappa\cdot\mathbf{W}_1)+2\kappa^2, \quad (1\text{-}20)$$

$$\epsilon_2^{(t)\prime}=\epsilon_2^{(t)}-2\sqrt{2}(\kappa\cdot\mathbf{W}_2)+2\kappa^2. \quad (1\text{-}21)$$

In a similar manner, one finds from Eqs. (1-18) and (1-19) that

$$\epsilon_1^{(r)\prime}=\epsilon_1^{(r)}+\frac{2(2m)^{\frac{1}{2}}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}\mathbf{w}_1\cdot[\sigma_1\times\kappa]$$

$$+2m[\sigma_1\times\kappa][\sigma_1\times\kappa]:\mu_1, \quad (1\text{-}22)$$

$$\epsilon_2^{(r)\prime}=\epsilon_2^{(r)}-\frac{2(2m)^{\frac{1}{2}}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}\mathrm{w}_2\cdot[\sigma_2\times\kappa]+2m[\sigma_2\times\kappa][\sigma_2\times\kappa]:\mu_2. \quad (1\text{-}23)$$

consider the sum of the square bracket integrals appearing in the expression for the viscosity, Eq. (0-24). From the definition, Eq. (0-10), and the symmetry relation[1] it is seen that

$$[\mathrm{W}_1;\ \mathrm{W}_1]_{12}+[\mathrm{W}_1;\ \mathrm{W}_2]_{12}=-\frac{1}{2n_1^*n_2^*}\int\cdots\int(\mathrm{W}_1'-\mathrm{W}_1):\times(\mathrm{W}_1'+\mathrm{W}_2'-\mathrm{W}_1-\mathrm{W}_2)f_1^{(0)}f_2^{(0)}(\mathbf{k}\cdot\mathbf{g})\times S(\mathbf{k})d\mathbf{k}d\mathrm{v}_1d\omega_1d\mathrm{v}_2d\omega_2. \quad (1\text{-}27)$$

Then introducing the equilibrium distribution functions and the dimensionless velocity variables we find that

$$[\mathrm{W}_1;\ \mathrm{W}_1]_{12}+[\mathrm{W}_1;\ \mathrm{W}_2]_{12}=-\frac{1}{\pi^6}\left(\frac{kT}{m}\right)^{\frac{1}{2}}\int\cdots\int[(\mathrm{W}_1'-\mathrm{W}_1):\times(\mathrm{W}_1'+\mathrm{W}_2'-\mathrm{W}_1-\mathrm{W}_2)]\times\exp(-\epsilon_1^{(t)}-\epsilon_2^{(t)}-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathbf{k}\cdot\Gamma)\times S(\mathbf{k})d\mathbf{k}d\mathrm{W}_1d\mathrm{W}_2d\mathrm{w}_1d\mathrm{w}_2. \quad (1\text{-}28)$$

The quantity in brackets, in the integrand may be expressed in terms of the unprimed variables and the vector κ by means of Eqs. (1-4), (1-8), and (1-9) and we find that

$$(\mathrm{W}_1'-\mathrm{W}_1):(\mathrm{W}_1'+\mathrm{W}_2'-\mathrm{W}_1-\mathrm{W}_2)=-\frac{4\sqrt{2}}{3}(\kappa\cdot\gamma)(\kappa\cdot\mathrm{W}_1)-4\sqrt{2}\kappa^2(\gamma\cdot\mathrm{W}_1)+\frac{16\sqrt{2}}{3}\kappa^2(\kappa\cdot\mathrm{W}_1)-\frac{16}{3}\kappa^2(\kappa\cdot\gamma)+\frac{16}{3}\kappa^4. \quad (1\text{-}29)$$

We now change integration variables from W_1 and W_2 to $\mathfrak{G}$ and γ. The Jacobian of the transformation is unity and

$$\epsilon_1^{(t)}+\epsilon_2^{(t)}=\mathfrak{G}^2+\gamma^2. \quad (1\text{-}30)$$

Thus after integration over $\mathfrak{G}$,

$$[\mathrm{W}_1;\ \mathrm{W}_1]_{12}+[\mathrm{W}_1;\ \mathrm{W}_2]_{12}=-\frac{4}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\cdots\int[\kappa^2\gamma^2+\tfrac{1}{3}(\kappa\cdot\gamma)^2-(8/3)\kappa^2(\kappa\cdot\gamma)+\tfrac{4}{3}\kappa^4]\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})\times(\mathbf{k}\cdot\Gamma)S(\mathbf{k})d\mathbf{k}d\gamma d\mathrm{w}_1d\mathrm{w}_2. \quad (1\text{-}31)$$

It is convenient to define the following functions of $\mathbf{k}$ and the orientation of both molecules:

$$J_{\nu\nu'}^{(r)}=\iiint(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}\times\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})d\gamma d\mathrm{w}_1d\mathrm{w}_2, \quad (1\text{-}32$$

$$\gamma_0=(m/4kT)^{\frac{1}{2}}\mathrm{g}_0. \quad (1\text{-}33)$$

$$[\mathrm{W}_1;\ \mathrm{W}_1]_{12}+[\mathrm{W}_1;\ \mathrm{W}_2]_{12}=-\frac{4}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int S(\mathbf{k})d\mathbf{k} \quad (1\text{-}34)$$
$$[\xi^2(J_{30}^{(1)}-3J_{21}^{(1)}+3J_{12}^{(1)}-J_{03}^{(1)})+\tfrac{1}{3}\xi^2(1-8\xi+4\xi^2)J_{50}^{(0)}-\tfrac{1}{3}\xi^2(3-32\xi+20\xi^2)J_{41}^{(0)}+\tfrac{1}{3}\xi^2(3-48\xi+40\xi^2)J_{32}^{(0)}-\tfrac{1}{3}\xi^2(1-32\xi+40\xi^2)J_{23}^{(0)}-\tfrac{4}{3}\xi^3(2-5\xi)J_{14}^{(0)}-\tfrac{4}{3}\xi^4J_{05}^{(0)}]$$

2. INTEGRATION OVER THE VELOCITIES

Let us now consider the six sets of integrals over the velocities, $J_{\nu\nu'}^{(r)}$, $K_{\nu\nu'}^{(r)}$, $L_{\nu\nu'}^{(r)}$, $M_{\nu\nu'}^{(r)}$, $N_{\nu\nu'}^{(r)}$, $Q_{\nu\nu'}^{(r)}$. We consider first the integration over γ. In all six cases this involves the evaluation of the integral,

$$I_\nu^{(r)}=\int(\mathbf{k}\cdot\gamma)^\nu\gamma^{2r}\exp(-\gamma^2)d\gamma,\quad \mathbf{k}\cdot\gamma<\mathbf{k}\cdot\gamma_0. \quad (2\text{-}1)$$

The range of integration is restricted to those values of γ for which the impulse is positive. This integral depends parametrically on vector $\mathbf{k}$ and scalar $(\mathbf{k}\cdot\gamma_0)$. Since the integral is a scalar, it depends only on the square of the single vector, $\mathbf{k}$ which is unity. So integral $I_\nu^{(r)}$ can be expressed as a function of the single scalar, $(\mathbf{k}\cdot\gamma_0)$. To obtain $(\mathbf{k}\cdot\gamma_0)$ we evaluate by using coordinate system in which $\mathbf{k}$ lies along the positive z axis. Then

$$I_\nu^{(r)}=\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\gamma_3^\nu(\gamma_1^2+\gamma_2^2+\gamma_3^2)^r\times\exp(-\gamma_1^2-\gamma_2^2-\gamma_3^2)d\gamma_1d\gamma_2d\gamma_3, \quad (2\text{-}2)$$

and on carrying out the integration we find that

$$I_\nu^{(0)}=\pi\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}x^\nu\exp(-x^2)dx, \quad (2\text{-}3)$$

$$I_\nu^{(1)}=\pi\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}x^\nu(1+x^2)\exp(-x^2)dx=I_\nu^{(0)}+I_{\nu+2}^{(0)}. \quad (2\text{-}4)$$

To carry out the integration over w_1 and w_2, we change variables to the new set of six,

$$\epsilon_i^{(r)}=\frac{\mathrm{w}_i\cdot\mathrm{I}_i\cdot\mathrm{w}_i}{(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}},\quad i=1,2 \quad (2\text{-}5)$$

$$\gamma_0^{(i)}=\mathrm{w}_i\cdot(\sigma_i\times\mathbf{k}),\quad i=1,2 \quad (2\text{-}6)$$

$$\varphi^{(i)}=\mathrm{w}_i\cdot(\sigma_i\times[\sigma_i\times\mathbf{k}]).\quad i=1,2. \quad (2\text{-}7)$$

Hence let us consider the Jacobian

Let

$$\mathrm{a}_i=\sigma_i\times\mathbf{k},\quad i=1,2 \quad (2\text{-}8)$$

$$\mathrm{b}_i=\sigma_i\times[\sigma_i\times\mathbf{k}],\qquad \mathrm{c}_i=\mathrm{a}_i\times\mathrm{b}_i. \quad (2\text{-}10)$$

Then clearly the Jacobian of the transformation from w_{i1}, w_{i2}, w_{i3} to $\epsilon_i^{(r)}$, $\gamma_0^{(i)}$, $\varphi^{(i)}$ is

$$\frac{\partial(\epsilon_i^{(r)},\gamma_0^{(i)},\varphi^{(i)})}{\partial(w_{i1},w_{i2},w_{i3})}=2\frac{\mathrm{c}_i\cdot\mathrm{I}_i\cdot\mathrm{w}_i}{(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}}. \quad (2\text{-}11)$$

To evaluate this expression in terms of the new variables, it is necessary to solve Eqs. (2-5), (2-6), and (2-7) for the components of w_i in terms of the new variables. That

$$\omega_i=\frac{\mathrm{S}_i\times(\mathrm{c}_i\cdot\mathrm{I}_i)\pm A_i\mathrm{c}_i}{\mathrm{c}_i\cdot\mathrm{I}_i\cdot\mathrm{c}_i}, \quad (2\text{-}12)$$

where

$$\mathrm{S}_i=\gamma_0^{(i)}\mathrm{b}_i-\varphi^{(i)}\mathrm{a}_i \quad (2\text{-}13)$$

and

$$A_i^2=\epsilon_i^{(r)}(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}(\mathrm{c}_i\cdot\mathrm{I}_i\cdot\mathrm{c}_i)-(\Gamma_1\Gamma_2\Gamma_3)(\mathrm{S}_i\cdot\mu_i\cdot\mathrm{S}_i) \quad (2\text{-}14)$$

First, since

$$\mathbf{a}_i\cdot\mathbf{c}_i=0 \quad (2\text{-}15) \qquad \mathbf{a}_i\times\mathbf{S}_i=\gamma_0^{(i)}\mathbf{c}_i, \quad (2\text{-}16)$$

it follows on direct substitution that the solution, Eq. (2-12), satisfies Eq. (2-6). Also since

$$\mathbf{b}_i\cdot\mathbf{c}_i=0 \quad (2\text{-}17) \qquad \mathbf{b}_i\times\mathbf{S}_i=\varphi^{(i)}\mathbf{c}_i \quad (2\text{-}18)$$

it follows on direct substitution that Eq. (2-7) is also satisfied. The proof that Eq. (2-5) is also satisfied depends upon the identity

$$\mathbf{I}_i\cdot[\mathbf{S}_i\times(\mathbf{c}_i\cdot\mathbf{I}_i)]=(\Gamma_1\Gamma_2\Gamma_3)(\boldsymbol{\mu}_i\cdot\mathbf{S}_i)\times\mathbf{c}_i, \quad (2\text{-}19)$$

which may be proved by expansion in terms of components. It then follows upon direct substitution of Eq. (2-12) into Eq. (2-5) and use of known vector identities that Eq. (2-5) is also satisfied. Thus Eq. (2-12) gives $\mathbf{w}_i$ in terms of the new variables.

Upon substitution of Eq. (2-12) into Eq. (2-11), we find that the Jacobian of the transformation is

$$\frac{\partial(\epsilon_i^{(r)},\gamma_0^{(i)},\varphi^{(i)})}{\partial(w_{i1},w_{i2},w_{i3})}=\frac{2A_i}{(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}}. \quad (2\text{-}20)$$

The range of integration of $\mathbf{w}_i$ is from $-\infty$ to $+\infty$ on each of the three components. It may be shown that the equivalent range of integration of the new variables consists of those values for which A_i^2, Eq. (2-14), is positive. The transformation, however, is two to one, so that it is necessary to integrate over this range of the new variables twice. This is equivalent to using as the Jacobian a value half that given by Eq. (2-20).

Since the integrands in which we are interested are independent of $\varphi^{(i)}$, we now consider the integral,

$$(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}\int\frac{1}{A_i}d\varphi^{(i)}. \quad (2\text{-}21)$$

From the definition, Eq. (2-14), it follows that A_i^2 is quadratic in $\varphi^{(i)}$ and may be written in the form

$$A_i^2=(\Gamma_1\Gamma_2\Gamma_3)(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)(\varphi_+^{(i)}-\varphi^{(i)})(\varphi^{(i)}-\varphi_-^{(i)}) \quad (2\text{-}22)$$

where $\varphi_+^{(i)}$ and $\varphi_-^{(i)}$ are the upper and lower roots of the quadratic. Thus the integral of Eq. (2-21) is

$$\frac{1}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)^{\frac{1}{2}}}\int_{\varphi_-^{(i)}}^{\varphi_+^{(i)}}\frac{d\varphi^{(i)}}{(\varphi_+^{(i)}-\varphi^{(i)})^{\frac{1}{2}}(\varphi^{(i)}-\varphi_-^{(i)})^{\frac{1}{2}}}.$$

This integral is a standard integral, (2-23)

$$(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}\int\frac{d\varphi^{(i)}}{A_i}=\frac{\pi}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)^{\frac{1}{2}}}. \quad (2\text{-}24)$$

From Eq. (2-14) it is clear that the roots are

$$\varphi_\pm^{(i)}=\frac{\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{b}_i}{\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i}\gamma_0^{(i)}$$

$$\pm\frac{1}{\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i}\begin{bmatrix}[(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{b}_i)^2-(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)(\mathbf{b}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{b}_i)]\gamma_0^{(i)^2}\\+(\Gamma_1\Gamma_2\Gamma_3)^{-\frac{1}{2}}(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)(\mathbf{c}_i\cdot\mathbf{I}_i\cdot\mathbf{c}_i)\epsilon_i^{(r)}\end{bmatrix} \quad (2\text{-}25)$$

$$(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{b}_i)^2-(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)(\mathbf{b}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{b}_i)=-\frac{\mathbf{c}_i\cdot\mathbf{I}_i\cdot\mathbf{c}_i}{\Gamma_1\Gamma_2\Gamma_3} \quad (2\text{-}26)$$

$$\varphi_\pm^{(i)}=$$

$$(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{b}_i)\gamma_0^{(i)}\pm\frac{(\mathbf{c}_i\cdot\mathbf{I}_i\cdot\mathbf{c}_i)^{\frac{1}{2}}}{(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}}[(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)\epsilon_i^{(r)}-\gamma_0^{(i)^2}]^{\frac{1}{2}}$$

$$\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i \quad (2\text{-}27)$$

$$\gamma_0^{(i)^2}/(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i) \quad (2\text{-}28)$$

to infinity and that then the integration over $\gamma_0^{(i)}$ is taken from -oo to + oo.

$$\eta_i=(\Gamma_1\Gamma_2\Gamma_3)^{1/6}(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)^{\frac{1}{2}}. \quad (2\text{-}29)$$

From Eq(1-32), the expression for $I_\nu^{(0)}$ Eq 92-3) and the result of integration over $\phi^{(i)}$Eq(2-24), it follows that

$$J_{\nu\nu'}^{(0)}=\frac{\pi^3}{\eta_1\eta_2}\int_{-\infty}^{\infty}\int_{\infty}^{\infty}\int_{\gamma_0^{(1)2}/\eta_1^2}^{\infty}\int_{\gamma_0^{(2)2}/\eta_2^2}^{\infty}\int_{-\infty}^{\mathbf{k}\cdot\boldsymbol{\gamma}_0}x^\nu(\mathbf{k}\cdot\boldsymbol{\gamma}_0)^{\nu'}$$

$$\exp(-x^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})dx\,d\epsilon_2^{(r)}d\epsilon_1^{(r)}d\gamma_0^{(1)}d\gamma_0^{(2)} \quad (2\text{-}30)$$

Then after integration over $\epsilon_1^{(r)}$ and $\epsilon_2^{(r)}$ we find that

$$J_{\nu\nu'}^{(0)}=\frac{\pi^3}{\eta_1\eta_2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\mathbf{k}\cdot\boldsymbol{\gamma}_0}x^\nu(\mathbf{k}\cdot\boldsymbol{\gamma}_0)^{\nu'}$$

$$\exp\left(-x^2-\frac{\gamma_0^{(1)^2}}{\eta_1^2}-\frac{\gamma_0^{(2)^2}}{\eta_2^2}\right)dx\,d\gamma_0^{(1)}d\gamma_0^{(2)}, \quad (2\text{-}31)$$

From the definitions, Eqs. (1-33) and (2-6), it follows

$$\left(\frac{m}{kT}\right)^{\frac{1}{2}}\boldsymbol{\omega}_i\cdot(\boldsymbol{\sigma}_i\times\mathbf{k})$$

$$=\frac{(2m)^{\frac{1}{2}}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}\gamma_0^{(i)}+\left(\frac{m}{kT}\right)^{\frac{1}{2}}\boldsymbol{\omega}_0\cdot(\boldsymbol{\sigma}_i\times\mathbf{k}) \quad (2\text{-}35)$$

$$\mathbf{k}\cdot\boldsymbol{\gamma}_0=\frac{(m)^{\frac{1}{2}}}{\sqrt{2}(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}(\gamma_0^{(1)}-\gamma_0^{(2)})$$

$$+\left(\frac{m}{4kT}\right)^{\frac{1}{2}}(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2)\cdot(\mathbf{k}\times\boldsymbol{\omega}_0). \quad (2\text{-}36)$$

Now since we are considering only the special case in which $\boldsymbol{\omega}_0=0$, we transform to new coordinates defined

$$u=\frac{1}{\eta}(\mathbf{k}\cdot\boldsymbol{\gamma}_0)=\frac{\gamma_0^{(1)}-\gamma_0^{(2)}}{(\eta_1^2+\eta_2^2)^{\frac{1}{2}}} \quad (2\text{-}37) \qquad v=\frac{\eta_2^2\gamma_0^{(1)}+\eta_1^2\gamma_0^{(2)}}{\eta_1\eta_2(\eta_1^2+\eta_2^2)^{\frac{1}{2}}} \quad (2\text{-}38)$$

$$\eta=\left(\frac{m}{2}\right)^{\frac{1}{2}}\frac{(\eta_1^2+\eta_2^2)^{\frac{1}{2}}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}},$$

$$\gamma_0^{(1)}=\frac{\eta_1^2u+\eta_1\eta_2v}{(\eta_1^2+\eta_2^2)^{\frac{1}{2}}}, \quad (2\text{-}39) \qquad \gamma_0^{(2)}=\frac{-\eta_2^2u+\eta_1\eta_2v}{(\eta_1^2+\eta_2^2)^{\frac{1}{2}}}, \quad (2\text{-}40)$$

and the Jacobian of the transformation is

$$\frac{\partial(\gamma_0^{(1)},\gamma_0^{(2)})}{\partial(u,v)}=\eta_1\eta_2. \quad (2\text{-}41)$$

The integrals of Eqs. (2-31) to (2-34) are then of the form

$$\pi^3\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{\eta u}(\quad)dx\,du\,dv. \quad (2\text{-}42)$$

The integral over v may thus be carried out next. The integrals over v are complete integrals and may be carried out explicitly. The results are

$$J_{\nu\nu'}^{(0)}=\pi^{7/2}\eta^{\nu'}\int_{-\infty}^{+\infty}\int_{-\infty}^{\eta u}x^\nu u^{\nu'}\exp(-x^2-u^2)dx\,du, \quad (2\text{-}43)$$

Then as a final change of variables we let

$$x=r\cos\vartheta, \quad (2\text{-}49)$$

$$u=r\sin\vartheta. \quad (2\text{-}50)$$

The Jacobian of the transformation is clearly

$$\partial(x,u)/\partial(r,\vartheta)=r. \quad (2\text{-}51)$$

The limits of integration on r are from 0 to ∞, while ϑ goes from ϑ_0 to $\vartheta_0+\pi$ where

$$\tan\vartheta_0=1/\eta. \tag{2-52}$$

We now define

$$\Lambda_{\nu\nu'}=\int_{\vartheta_0}^{\vartheta_0+\pi}\cos^{\nu}\vartheta\,\sin^{\nu'}\vartheta d\vartheta. \tag{2-53}$$

Then after carrying out the integration over r we find that

$$J_{\nu\nu'}{}^{(0)}=\tfrac{1}{2}\pi^{7/2}\eta^{\nu'}\Gamma\left(\frac{\nu+\nu'}{2}+1\right)\Lambda_{\nu\nu'}, \tag{2-54}$$

From the definition of ξ, Eq. (1-14), and the definitions of this section, it follows that

$$\frac{1}{\xi}=1+\frac{m(\eta_1{}^2+\eta_2{}^2)}{2(\Gamma_1\Gamma_2\Gamma_3)^{1/2}}=1+\eta^2. \tag{2-60}$$

Thus

$$\xi=\sin^2\vartheta_0. \tag{2-61}$$

The evaluation of the $\Lambda_{\nu\nu'}$ may be carried out by straightforward methods.
Then from Eq. (1-42) we find that

$$[S_{3/2}^{1}(\epsilon_1{}^{(t)})\mathrm{W}_1;S_{3/2}^{1}(\epsilon_1{}^{(r)})\mathrm{W}_1]_{12}+[S_{3/2}^{1}(\epsilon_1{}^{(t)})\mathrm{W}_1;S_{3/2}^{1}(\epsilon_2{}^{(r)})\mathrm{W}_2]_{12}$$
$$=-\frac{5}{2}\left(\frac{kT}{\pi m}\right)^{1/2}\int\xi^{1/2}(1-\xi)S(\mathbf{k})d\mathbf{k}+\text{antisymmetric terms} \tag{2-65}$$

and from Eq. (1-48) that

$$[S_{3/2}^{1}(\epsilon_1{}^{(r)})\mathrm{W}_1;S_{3/2}^{1}(\epsilon_1{}^{(r)})\mathrm{W}_1]_{12}+[S_{3/2}^{1}(\epsilon_1{}^{(r)})\mathrm{W}_1;S_{3/2}^{1}(\epsilon_2{}^{(r)})\mathrm{W}_2]_{12}$$
$$=\frac{1}{2}\left(\frac{kT}{\pi m}\right)^{1/2}\int\Big[\xi^{1/2}(5-2\xi)+\frac{27}{4}\xi^{1/2}(1-\xi)^2$$
$$+\frac{m^2\eta_1{}^2\eta_2{}^2}{(\Gamma_1\Gamma_2\Gamma_3)^{1/2}}\xi^{1/2}\left(3-\frac{27}{4}\xi\right)\Big]S(\mathbf{k})d\mathbf{k}+\text{antisymmetric terms.} \tag{2-66}$$

3. THE INTEGRATION OVER k AND THE ORIENTATIONS

We now consider the final integrations to be performed in the evaluation of the transport coefficients. From Eq. (0-9) and the definition of n_2^*, it follows that if $\omega_0=0$,

$$\{S_{nn'}{}^{(\nu)}\mathrm{W}^{(\nu)};S_{mm'}{}^{(\nu)}\mathrm{W}^{(\nu)}\}=$$
$$\frac{1}{(8\pi^2)^2}\int\int\Big[[S_{1,nn'}{}^{(\nu)}\mathrm{W}_1{}^{(\nu)};S_{1,mm'}{}^{(\nu)}\mathrm{W}_1{}^{(\nu)}]_{12}$$
$$+[S_{1,nn'}{}^{(\nu)}\mathrm{W}_1{}^{(\nu)};S_{2,mm'}{}^{(\nu)}\mathrm{W}_2{}^{(\nu)}]_{12}\Big]$$
$$\sin\beta_1\sin\beta_2 d\alpha_1 d\alpha_2. \tag{3-1}$$

The square brackets have been reduced to an integration over $\mathbf{k}$. Thus the problem is reduced to an eightfold integration over the two angles (ϑ,φ) of $\mathbf{k}$ and the six Eulerian angles $(\alpha_i, \beta_i, \gamma_i)$ specifying the orientations of the two molecules.

To carry out the eightfold integration, we change variables to a new set of angles. Let K_{ij}, $R_{ij}{}^{(1)}$, and $R_{ij}{}^{(2)}$ be the elements of rotation matrices associated with the sets of angles $(\varphi, \vartheta, 0)$, $(\alpha_1, \beta_1, \gamma_1)$, and $(\alpha_2, \beta_2, \gamma_2)$, respectively. We then define the angles ϑ_1', φ_1', ϑ_2', and φ_2' by the relations

$$K_{3i}{}^{(1)'}=\textstyle\sum_j K_{3j}R_{ij}{}^{(1)}, \tag{3-2}$$

$$K_{3i}{}^{(2)'}=\textstyle\sum_j K_{3j}R_{ij}{}^{(2)}, \tag{3-3}$$

where the $K_{ij}{}^{(1)'}$ and $K_{ij}{}^{(2)'}$ are elements of rotation matrices associated with the rotations $(\varphi_1', \vartheta_1', 0)$ and $(\varphi_2', \vartheta_2', 0)$, respectively. Geometrically, the angles ϑ_1' and φ_1' are the polar angles of the point of contact in a coordinate system fixed in body 1. Similar considerations apply to ϑ_2' and φ_2'. We next define the angle ψ by the relations

$$\sin\psi=Q_{11}{}^{(1)}Q_{21}{}^{(2)}-Q_{21}{}^{(1)}Q_{11}{}^{(2)}, \tag{3-4}$$

$$\cos\psi=Q_{11}{}^{(1)}Q_{11}{}^{(2)}+Q_{21}{}^{(1)}Q_{21}{}^{(2)}, \tag{3-5}$$

where

$$Q_{ij}{}^{(1)}=\sum_{k,l}K_{jk}{}^{(1)'}R_{kl}{}^{(1)}K_{il}, \tag{3-6}$$

$$Q_{ij}{}^{(2)}=\sum_{k,l}K_{jk}{}^{(2)'}R_{kl}{}^{(2)}K_{il}. \tag{3-7}$$

The angle ψ is an azimuthal angle which, along with ϑ_1', φ_1', ϑ_2', and φ_2', specifies the relative orientation of the two bodies.

We now consider a change of variables from the set

$$\vartheta,\ \varphi,\ \alpha_1,\ \beta_1,\ \gamma_1 \tag{3-8}$$

to the set

$$\vartheta_1',\ \varphi_1',\ \vartheta_2',\ \varphi_2',\ \psi. \tag{3-9}$$

$$\left|\frac{\partial(\vartheta_1',\varphi_1',\vartheta_2',\varphi_2',\psi)}{\partial(\vartheta,\varphi,\alpha_1,\beta_1,\gamma_1)}\right|=\frac{\sin\vartheta\sin\beta_1}{\sin\vartheta_1'\sin\vartheta_2'}. \tag{3-10}$$

Thus from Eq. (2-62) and Eq. (3-1), it follows that

$$\{\mathrm{W};\ \mathrm{W}\}=\frac{1}{96\pi^4}\left(\frac{kT}{\pi m}\right)^{1/2}\int\xi^{1/2}(5-2\xi)S(\mathbf{k})\sin\vartheta_1'$$
$$\times\sin\vartheta_2'\sin\beta_2 d\vartheta_1' d\varphi_1' d\vartheta_2' d\varphi_2' d\psi d\alpha_2 d\beta_2 d\gamma_2, \tag{3-11}$$

with similar expressions applying to the other brace expressions.

In all of the integrals of the type given in the last equation the integrand is independent of the Eulerian angles α_2, β_2, and γ_2. Thus we can carry out the integration over these angles and obtain,

$$\{\mathrm{W};\ \mathrm{W}\}=\frac{1}{12\pi^2}\left(\frac{kT}{\pi m}\right)^{1/2}\int\xi^{1/2}(5-2\xi)S(\mathbf{k})$$
$$\times\sin\vartheta_1'\sin\vartheta_2' d\vartheta_1' d\varphi_1' d\vartheta_2' d\varphi_2' d\psi. \tag{3-12}$$

The shape of the rigid ovaloids is conveniently described by means of the supporting functions,[2] $H^{(1)}(\vartheta_1',\varphi_1')$ and $H^{(2)}(\vartheta_2',\varphi_2')$. Since the two bodies are assumed to be identical the two functions must be of the same functional form. Furthermore, since the center of mass is assumed to be a center of symmetry the function must be of such a form that

$$H^{(1)}(\pi-\vartheta_1',\ \varphi_1'\pm\pi)=H^{(1)}(\vartheta_1',\ \varphi_1'). \tag{3-13}$$

In terms of the supporting functions and the present coordinates, it can be shown[2] that the element of surface is

$$S(\mathbf{k})=\mathcal{R}^{(1)'}\mathcal{T}^{(1)'}-\mathcal{S}^{(1)'}\mathcal{S}^{(1)'}+\mathcal{R}^{(2)'}\mathcal{T}^{(2)'}-\mathcal{S}^{(2)'}\mathcal{S}^{(2)'}$$
$$+\cos^2\psi(\mathcal{R}^{(1)'}\mathcal{T}^{(2)'}+\mathcal{T}^{(1)'}\mathcal{R}^{(2)'}-2\mathcal{S}^{(1)'}\mathcal{S}^{(2)'})$$
$$+\sin^2\psi(\mathcal{R}^{(1)'}\mathcal{R}^{(2)'}+\mathcal{T}^{(1)'}\mathcal{T}^{(2)'}+2\mathcal{S}^{(1)'}\mathcal{S}^{(2)'})$$
$$+2\sin\psi\cos\psi[\mathcal{S}^{(1)'}(\mathcal{R}^{(2)'}-\mathcal{T}^{(2)'})$$
$$-(\mathcal{R}^{(1)'}-\mathcal{T}^{(1)'})\mathcal{S}^{(2)'}], \tag{3-14}$$

$$\mathcal{R}^{(i)\prime}=H^{(i)}+\frac{\partial^2 H^{(i)}}{\partial\vartheta_i^{\prime 2}}, \tag{3-15}$$

$$\mathcal{S}^{(i)\prime}=\frac{\partial}{\partial\vartheta_i'}\left(\frac{1}{\sin\vartheta_i'}\frac{\partial H^{(i)}}{\partial\varphi_i'}\right), \tag{3-16}$$

$$\mathcal{T}^{(i)\prime}=H^{(i)}+\frac{\cos\vartheta_i'}{\sin\vartheta_i'}\frac{\partial H^{(i)}}{\partial\vartheta_i'}+\frac{1}{\sin^2\vartheta_i'}\frac{\partial^2 H^{(i)}}{\partial\vartheta_i^{\prime 2}}. \tag{3-17}$$

The integrands in which we are interested depend on the angle ψ only through the element of surface, Eq. (3-14). Thus we integrate $S(\mathbf{k})$ over ψ to obtain

$$\int S(\mathbf{k})d\psi=2\pi\left[\begin{array}{c}\mathcal{R}^{(1)\prime}\mathcal{T}^{(1)\prime}+\mathcal{R}^{(2)\prime}\mathcal{T}^{(2)\prime}\\ +\tfrac{1}{2}(\mathcal{R}^{(1)\prime}+\mathcal{T}^{(1)\prime})(\mathcal{R}^{(2)\prime}+\mathcal{T}^{(2)\prime})\\ -\mathcal{S}^{(1)\prime}\mathcal{S}^{(1)\prime}-\mathcal{S}^{(2)\prime}\mathcal{S}^{(2)\prime}\end{array}\right]. \tag{3-18}$$

The remaining portion of the integrands depend upon the remaining angles through the η_i, Eq. (2-29), both explicitly and through ξ, Eq. (2-60).
in terms of the supporting function,

$$(\sigma_1\times\mathbf{k})_i=-\frac{\partial H^{(1)}}{\partial\vartheta_1'}\sum_j K_{2j}^{(1)\prime}R_{ji}^{(1)}+\frac{1}{\sin\vartheta_1'}\frac{\partial H^{(1)}}{\partial\vartheta_1'}\sum_j K_{1j}^{(1)\prime}R_{ji}^{(1)}, \tag{3-19}$$

$$(\sigma_2\times\mathbf{k})_i=-\frac{\partial H^{(2)}}{\partial\vartheta_2'}\sum_j K_{2j}^{(2)\prime}R_{ji}^{(2)}+\frac{1}{\sin\vartheta_2'}\frac{\partial H^{(2)}}{\partial\varphi_2'}\sum_j K_{1j}^{(2)\prime}R_{ji}^{(2)}. \tag{3-20}$$

The second expression applies only if the center of mass is a center of symmetry so that the supporting function satisfies the identity, Eq. (3-13). If the body fixed system is such that the moment of inertia tensor is diagonal (principal axes) then

$$\sum_{k,l}R_{ik}^{(\nu)}\mu_{kl}^{(\nu)}R_{jl}^{(\nu)}=\frac{\delta_{ij}}{\Gamma_i}. \tag{3-21}$$

From Eq. (2-29) it is seen that

$$\eta_\nu^2=(\Gamma_1\Gamma_2\Gamma_3)^{1/3}\sum_{k,l}(\sigma_\nu\times\mathbf{k})_k\mu_{kl}^{\nu}(\sigma_\nu\times\mathbf{k})_l. \tag{3-22}$$

$$\eta_\nu^2=\sum_i\left(\frac{\partial H^{(\nu)}}{\partial\vartheta_\nu'}K_{2i}^{(\nu)\prime}-\frac{1}{\sin\vartheta_\nu'}\frac{\partial H^{(\nu)}}{\partial\varphi_\nu'}K_{1i}^{(\nu)\prime}\right)^2\frac{(\Gamma_1\Gamma_2\Gamma_3)^{1/3}}{\Gamma_i} \tag{3-23}$$

From Eqs. (3-12) and (3-18), it follows that

$$\{\mathrm{W};\ \mathrm{W}\}=\frac{1}{6\pi}\left(\frac{kT}{\pi m}\right)^{1/2}\int\xi^{1/2}(5-2\xi)\times\left[\begin{array}{c}(\mathcal{R}^{(1)\prime}\mathcal{T}^{(1)\prime}-\mathcal{S}^{(1)\prime}\mathcal{S}^{(1)\prime})\\ +(\mathcal{R}^{(2)\prime}\mathcal{T}^{(2)\prime}-\mathcal{S}^{(2)\prime}\mathcal{S}^{(2)\prime})\\ +\tfrac{1}{2}(\mathcal{R}^{(1)\prime}+\mathcal{T}^{(1)\prime})(\mathcal{R}^{(2)\prime}+\mathcal{T}^{(2)\prime})\end{array}\right]\times\sin\vartheta_1'\sin\vartheta_2'd\vartheta_1'd\varphi_1'd\vartheta_2'd\varphi_2'.$$

Let $g_1^{(i)}$ and $g_2^{(i)}$ be the principal radii of curvature of the surface of body i. Then it may be shown that

$$\mathcal{R}^{(i)\prime}\mathcal{T}^{(i)\prime}-\mathcal{S}^{(i)\prime}\mathcal{S}^{(i)\prime}=g_1^{(i)}g_2^{(i)}$$

$$\mathcal{R}^{(i)\prime}+\mathcal{T}^{(i)\prime}=g_1^{(i)}+g_2^{(i)}.$$

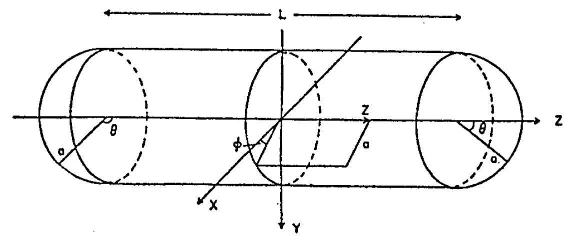
$$(\mathcal{R}^{(i)\prime}\mathcal{T}^{(i)\prime}-\mathcal{S}^{(i)\prime}\mathcal{S}^{(i)\prime})\sin\vartheta_i'd\vartheta_i'd\varphi_i'=dS_i$$

is an element of surface of the ovaloid. Thus

$$\{\mathrm{W};\ \mathrm{W}\}=\frac{1}{6\pi}\left(\frac{kT}{\pi m}\right)^{1/2}\int\xi^{1/2}(5-2\xi)\times\left[\begin{array}{c}\dfrac{1}{g_1^{(1)}g_2^{(1)}}+\dfrac{1}{g_1^{(2)}g_2^{(2)}}\\ +\dfrac{1}{2}\left(\dfrac{1}{g_1^{(1)}}+\dfrac{1}{g_2^{(1)}}\right)\left(\dfrac{1}{g_1^{(2)}}+\dfrac{1}{g_2^{(2)}}\right)\end{array}\right]dS_1dS_2$$

4. THE SPHEROCYLINDICAL MODEL

The spherocylindrical model and the coordinates used to parameterize the surface are indicated in Fig. 1. The axis of the cylinder is an axis of symmetry of the body. The cylinder is of length L and of radius a.



A point on the cylinder is described by the coordinate z $[-(L/2)\leq z\leq(L/2)]$ and the azimuthal angle $\varphi(0\leq\varphi\leq2\pi)$. A point on the hemispherical caps is described by the polar angle $\vartheta(0\leq\vartheta\leq\pi/2$, on the upper cap, and $(\pi/2)\leq\vartheta\leq\pi$, on the lower cap) and the azimuthal angle $\varphi(0\leq\varphi\leq2\pi)$.

The radius vector to a point on the surface in the body fixed coordinate system is

$\sigma=(a\cos\varphi,\ a\sin\varphi,\ z)$, cylindrical section

$\sigma=[a\sin\vartheta\cos\varphi,\ a\sin\vartheta\sin\varphi,\ \pm(L/2)+a\cos\vartheta]$, spherical caps (4-1)

and the unit normal to the surface is

$\mathbf{k}=(\cos\varphi,\ \sin\varphi,\ 0)$, cylindrical section

$\mathbf{k}=(\cos\varphi\sin\vartheta,\ \sin\varphi\sin\vartheta,\ \cos\vartheta)$. spherical caps (4-2)

Thus

$(\sigma\times\mathbf{k})=(-z\sin\varphi,\ z\cos\varphi,\ 0)$, cylindrical section

$(\sigma\times\mathbf{k})=[\mp(L/2)\sin\vartheta\sin\varphi,\ \pm(L/2)\sin\vartheta\cos\varphi,\ 0]$. spherical caps. (4-3)

Then if the geometrical symmetry axis is a principal axis of the mass distribution, and $\Gamma_1=\Gamma_2=\Gamma$,

$$\frac{m\eta_i^2}{2(\Gamma_1\Gamma_2\Gamma_3)^{1/3}}=\frac{4\alpha}{L^2}z_i^2,\quad\text{cylindrical section}$$

$$=\alpha\sin^2\vartheta_i,\quad\text{spherical caps} \tag{4-4}$$

where

$$\alpha=mL^2/8\Gamma \tag{4-5}$$

is a measure of the relative importance of the geometrical asymmetry and the mass distribution. Finally, the principal radii of curvature of the surface are

$$g_1^{(i)}=a, \quad g_2^{(i)}=\infty, \quad \text{cylindrical section}$$
$$g_1^{(i)}=a, \quad g_2^{(i)}=a. \quad \text{spherical caps.} \tag{4-6}$$

When these results are combined with the results of the previous section, we find that

$$\frac{1}{(8\pi^2)^2}\int\int\int \xi^{\nu/2}S(\mathrm{k})\sin\beta_1\sin\beta_2 d\mathrm{k}\,d\alpha_1 d\alpha_2 = U_{11}^{(\nu)}+2U_{12}^{(\nu)}+U_{22}^{(\nu)}, \tag{4-7}$$

where

$$U_{11}^{(\nu)}=4\pi a^2\int_0^\pi\int_0^\pi(1+\alpha\sin^2\vartheta_1+\alpha\sin^2\vartheta_2)^{-\nu/2} \times\sin\vartheta_1\sin\vartheta_2 d\vartheta_1 d\vartheta_2, \tag{4-8}$$

$$U_{12}^{(\nu)}=2\pi a\int_0^\pi\int_{-L/2}^{L/2}\left(1+\frac{4\alpha}{L^2}z_1^2+\alpha\sin^2\vartheta_2\right)^{-\nu/2}\sin\vartheta_2 dz_1 d\vartheta_2, \tag{4-9}$$

$$U_{22}^{(\nu)}=\frac{\pi}{2}\int_{-L/2}^{L/2}\int_{-L/2}^{L/2}\left[1+\frac{4\alpha}{L^2}(z_1^2+z_2^2)\right]^{-\nu/2}dz_1 dz_2 \tag{4-10}$$

and

$$\frac{1}{(8\pi^2)^2}\int\int\int\frac{m^2\eta_i^2\eta_j^2}{4(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}}\xi^{\nu/2}S(\mathrm{k})\sin\beta_1\sin\beta_2 d\mathrm{k}\,d\alpha_1 d\alpha_2 = V_{11}^{(\nu)}+2V_{12}^{(\nu)}+V_{22}^{(\nu)}, \tag{4-11}$$

where

$$V_{11}^{(\nu)}=4\pi a^2\alpha^2\int_0^\pi\int_0^\pi(1+\alpha\sin^2\vartheta_1+\alpha\sin^2\vartheta_2)^{-\nu/2} \times\sin^3\vartheta_1\sin^3\vartheta_2 d\vartheta_1 d\vartheta_2, \tag{4-12}$$

$$V_{12}^{(\nu)}=\frac{8\pi a\alpha^2}{L^2}\int_0^\pi\int_{-L/2}^{L/2}\left(1+\frac{4\alpha}{L^2}z_1^2+\alpha\sin^2\vartheta_2\right)^{-\nu/2} \times\sin^3\vartheta_2 z_1^2 dz_1 d\vartheta_2, \tag{4-13}$$

$$V_{22}^{(\nu)}=\frac{8\pi\alpha^2}{L^4}\int_{-L/2}^{L/2}\int_{-L/2}^{L/2}\left[1+\frac{4\alpha}{L^2}(z_1^2+z_2^2)\right]^{-\nu/2} \times z_1^2 z_2^2 dz_1 dz_2. \tag{4-14}$$

The problem is thus reduced to the evaluation of six sets of integrals. It is convenient to define the "rigid sphere" cross section,

$$A=4\pi(2a)^2=16\pi a^2,$$

and a parameter β which is a measure of the geometrical asymmetry

$$\beta=L/2a.$$

On making the appropriate changes of variables we find that

$$U_{11}^{(\nu)}=A\int_0^1\int_0^1[1+\alpha(2-x^2-y^2)]^{-\nu/2}dxdy,$$

$$U_{12}^{(\nu)}=\tfrac{1}{2}A\beta\int_0^1\int_0^1[1+\alpha(1+x^2-y^2)]^{-\nu/2}dxdy,$$

$$U_{22}^{(\nu)}=\tfrac{1}{8}A\beta^2\int_0^1\int_0^1[1+\alpha(x^2+y^2)]^{-\nu/2}dxdy,$$

$$V_{11}^{(\nu)}=A\alpha^2\int_0^1\int_0^1(1-x^2)(1-y^2) \times[1+\alpha(2-x^2-y^2)]^{-\nu/2}dxdy,$$

$$V_{12}^{(\nu)}=\tfrac{1}{2}A\alpha^2\beta\int_0^1\int_0^1 x^2(1-y^2)[1+\alpha(1+x^2-y^2)]^{-\nu/2}dxdy,$$

$$V_{22}^{(\nu)}=\tfrac{1}{8}A\alpha^2\beta^2\int_0^1\int_0^1 x^2y^2[1+\alpha(x^2+y^2)]^{-\nu/2}dxdy.$$

The transport coefficients are given in terms of the brace expressions by Eqs. (0-24) to (0-26). The resulting expressions for the shear and bulk viscosity are

$$\eta=\frac{15(kT\pi m)^{\frac{1}{2}}}{64\pi a^2}\left\{\frac{10}{\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{7+10\alpha}{\alpha(1+2\alpha)^{\frac{1}{2}}}\times\sin^{-1}\frac{\alpha}{1+\alpha}+\beta\left[\frac{5}{\alpha^{\frac{1}{2}}}\sinh^{-1}\alpha^{\frac{1}{2}}+\frac{5}{\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac{1}{2}}-\frac{7+5\alpha}{2\alpha(1+\alpha)^{\frac{1}{2}}}\ln(1+2\alpha)\right]+\beta^2\left[\frac{5}{4\alpha^{\frac{1}{2}}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{7}{8\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}\right]\right\}^{-1}, \tag{4-15}$$

$$\kappa=\frac{(\pi mkT)^{\frac{1}{2}}}{32\pi a^2}\left\{\frac{2}{\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{2(1+\alpha)}{\alpha(1+2\alpha)^{\frac{1}{2}}}\sin^{-1}\frac{\alpha}{1+\alpha}+\beta\left[\frac{1}{\alpha^{\frac{1}{2}}}\sinh^{-1}\alpha^{\frac{1}{2}}+\frac{1}{\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac{1}{2}}-\frac{2+\alpha}{2\alpha(1+\alpha)^{\frac{1}{2}}}\ln(1+2\alpha)\right]+\beta^2\left[\frac{1}{4\alpha^{\frac{1}{2}}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{1}{4\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}\right]\right\}^{-1}. \tag{4-16}$$

$$\{S_{\frac{1}{2}}^1(\epsilon^{(t)})\mathrm{W};S_{\frac{1}{2}}^1(\epsilon^{(r)})\mathrm{W}\} =-\frac{5A}{2}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\left\{\frac{2}{\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{2(1+\alpha)}{\alpha(1+2\alpha)^{\frac{1}{2}}}\sin^{-1}\frac{\alpha}{1+\alpha}+\beta\left[\frac{1}{\alpha^{\frac{1}{2}}}\sinh^{-1}\alpha^{\frac{1}{2}}+\frac{1}{\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac{1}{2}}-\frac{(2+\alpha)}{2\alpha(1+\alpha)^{\frac{1}{2}}}\ln(1+2\alpha)\right]+\beta^2\left[\frac{1}{4\alpha^{\frac{1}{2}}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{1}{4\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}\right]\right\},$$

$$\{S_{\frac{1}{2}}^1(\epsilon^{(r)})\mathrm{W};S_{\frac{1}{2}}^1(\epsilon^{(r)})\mathrm{W}\}=\frac{A}{2}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\left\{\frac{47+32\alpha}{2\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{(12+36\alpha+20\alpha^2)}{\alpha(1+2\alpha)^{\frac{1}{2}}}\sin^{-1}\frac{\alpha}{1+\alpha}-\frac{8\alpha+17}{2(1+\alpha)}+\beta\left[\frac{47+32\alpha}{4\alpha^{\frac{1}{2}}}\sinh^{-1}\alpha^{\frac{1}{2}}+\frac{47+16\alpha}{4\alpha^{\frac{1}{2}}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac{1}{2}}-\frac{(48+172\alpha+79\alpha^2)}{8\alpha(1+\alpha)^{\frac{1}{2}}}\ln(1+2\alpha)-\frac{8\alpha+17}{2(1+\alpha)^{\frac{1}{2}}}\right]+\beta^2\left[-\frac{3}{2\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}+\frac{47+16\alpha}{16\alpha^{\frac{1}{2}}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac{1}{2}}-\frac{(17+42\alpha+16\alpha^2)}{16(1+\alpha)(1+2\alpha)^{\frac{1}{2}}}\right]\right\}.$$

after integration over $\mathfrak{G}$, that

$$[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)});S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})]_{12}+[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)});S_{\frac{1}{2}}^{1}(\epsilon_2^{(t)})]_{12}$$

$$=-\frac{8}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\cdots\int(\kappa^2-\kappa\cdot\gamma)^2\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathrm{k}\cdot\Gamma)S(\mathrm{k})d\mathrm{k}d\gamma d\mathrm{w}_1d\mathrm{w}_2$$

$$=-\frac{8}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\left[\xi^2(1-2\xi+\xi^2)J_{50}^{(0)}-\xi^2(3-8\xi+5\xi^2)J_{41}^{(0)}+\xi^2(3-12\xi+10\xi^2)J_{32}^{(0)}-\xi^2(1-8\xi+10\xi^2)J_{23}^{(0)}-\xi^3(2-5\xi)J_{14}^{(0)}-\xi^4J_{05}^{(0)}\right]S(\mathrm{k})d\mathrm{k}.$$

It then follows from the conservation of energy expression, Eq. (1-26), that if $\omega_0=0$,

$$[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)});S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})]_{12}+[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)});S_{\frac{1}{2}}^{1}(\epsilon_2^{(r)})]_{12}=-[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)});S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})]_{12}-[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)});S_{\frac{1}{2}}^{1}(\epsilon_2^{(t)})]_{12}.$$

We now consider the three square bracket expressions which enter into the expression for the thermal con ductivity, Eq. (0-26).

$$[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1]_{12}+[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_2^{(t)})\mathrm{W}_2]_{12}$$

$$=-\frac{6}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\cdots\int[\tfrac{2}{3}\kappa^2\gamma^2+3(\kappa\cdot\gamma)^2-(22/3)\kappa^2(\kappa\cdot\gamma)+(11/3)\kappa^4]\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathrm{k}\cdot\Gamma)S(\mathrm{k})d\mathrm{k}d\gamma d\mathrm{w}_1d\mathrm{w}_2$$

$$=-\frac{6}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\begin{bmatrix}\tfrac{2}{3}\xi^2(J_{30}^{(1)}-3J_{21}^{(1)}+3J_{12}^{(1)}-J_{03}^{(1)})+\xi^2[3-22\xi+(11/3)\xi^2]J_{50}^{(0)}\\ -\xi^2[9-(88/3)\xi+(55/3)\xi^2]J_{41}^{(0)}+\xi^2[9-44\xi+(110/3)\xi^2]J_{32}^{(0)}\\ -\xi^2[3-(88/3)\xi+(110/3)\xi^2]J_{23}^{(0)}-\xi^3[(22/3)-(55/3)\xi]J_{14}^{(0)}-(11/3)\xi^4J_{05}^{(0)}\end{bmatrix}S(\mathrm{k})d\mathrm{k}.$$

To evaluate the next sum of square brackets, we use the unsymmetrized form,

$$[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1]_{12}+[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_2^{(r)})\mathrm{W}_2]_{12}$$

$$=\frac{1}{n_1^*n_2^*}\int\cdots\int[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)\prime})\mathrm{W}_1'-S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1]\cdot[S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1+S_{\frac{1}{2}}^{1}(\epsilon_2^{(r)})\mathrm{W}_2]\times f_1^{(0)}f_2^{(0)}(\mathrm{k}\cdot\mathrm{g})S(\mathrm{k})d\mathrm{k}d\mathrm{v}_1d\mathrm{v}_2d\omega_1d\omega_2$$

which after integration over $\mathfrak{G}$ is

$$\frac{2}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\cdots\int\begin{bmatrix}(\epsilon_1^{(r)}-\epsilon_2^{(r)})[(5/4)(\kappa\cdot\gamma)-\tfrac{3}{2}\gamma^2(\kappa\cdot\gamma)+2(\kappa\cdot\gamma)^2+\kappa^2\gamma^2-2\kappa^2(\kappa\cdot\gamma)]\\ +\tfrac{5}{2}(3-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\kappa\cdot\gamma-\kappa^2)\end{bmatrix}\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathrm{k}\cdot\Gamma)S(\mathrm{k})d\mathrm{k}d\gamma d\mathrm{w}_1d\mathrm{w}_2.$$

We now introduce two additional sets of integrals similar to the $J_{\nu\nu'}^{(r)}$,

$$K_{\nu\nu'}^{(r)}=\int\int\int(\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathrm{k}\cdot\gamma)^{\nu}(\mathrm{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})d\gamma d\mathrm{w}_1d\mathrm{w}_2,$$

$$L_{\nu\nu'}^{(r)}=\int\int\int(3-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathrm{k}\cdot\gamma)^{\nu}(\mathrm{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})d\gamma d\mathrm{w}_1d\mathrm{w}_2.$$

In terms of these quantities,

$$[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1]_{12}+[S_{\frac{1}{2}}^{1}(\epsilon_1^{(t)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_2^{(r)})\mathrm{W}_2]_{12}$$

$$=\frac{2}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\begin{bmatrix}2\xi^2(1-\xi)K_{50}^{(0)}-2\xi^2(3-4\xi)K_{41}^{(0)}+6\xi^2(1-2\xi)K_{32}^{(0)}-2\xi^2(1-4\xi)K_{23}^{(0)}\\ -2\xi^3K_{14}^{(0)}+(5/4)\xi K_{30}^{(0)}-\tfrac{5}{2}\xi K_{21}^{(0)}+(5/4)\xi K_{12}^{(0)}-\xi(\tfrac{3}{2}-\xi)K_{30}^{(1)}\\ +3\xi(1-\xi)K_{21}^{(1)}-\tfrac{3}{2}\xi(1-2\xi)K_{12}^{(1)}-\xi^2K_{03}^{(1)}+\tfrac{5}{2}\xi(1-\xi)L_{30}^{(0)}\\ -\tfrac{5}{2}\xi(2-3\xi)L_{21}^{(0)}+\tfrac{5}{2}\xi(1-3\xi)L_{12}^{(0)}+\tfrac{5}{2}\xi^2L_{03}^{(0)}\end{bmatrix}S(\mathrm{k})d\mathrm{k}.$$

To evaluate the last sum of square brackets, we use the analogous unsymmetrized form,[1]

$$[S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1]_{12}+[S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_2^{(r)})\mathrm{W}_2]_{12}$$

$$=\frac{1}{n_1^*n_2^*}\int\cdots\int[S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)\prime})\mathrm{W}_1'-S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1]\cdot[S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1+S_{\frac{1}{2}}^{1}(\epsilon_2^{(r)})\mathrm{W}_2]\,f_1^{(0)}f_2^{(0)}(\mathrm{k}\cdot\mathrm{g})S(\mathrm{k})d\mathrm{k}d\mathrm{v}_1d\mathrm{v}_2d\omega_1d\omega_2$$

$$\frac{2}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\cdots\int\begin{bmatrix}(\tfrac{3}{2}-\epsilon_1^{(r)})(\epsilon_1^{(r)}-\epsilon_2^{(r)})(\kappa\cdot\gamma)+[(\epsilon_1^{(r)}-\epsilon_2^{(r)})(\gamma^2-2\kappa\cdot\gamma)-\tfrac{3}{2}(3-\epsilon_1^{(r)}-\epsilon_2^{(r)})]\\ \times[(m/kT)^{\frac{1}{2}}\omega_1\cdot(\sigma_1\times\kappa)+m(\sigma_1\times\kappa)\cdot\mu_1\cdot(\sigma_1\times\kappa)]\end{bmatrix}\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathrm{k}\cdot\Gamma)S(\mathrm{k})d\mathrm{k}d\gamma d\mathrm{w}_1d\mathrm{w}_2.$$

$$M_{\nu\nu'}^{(r)}=\left(\frac{m}{kT}\right)^{\frac{1}{2}}\int\int\int(\epsilon_1^{(r)}-\epsilon_2^{(r)})(\omega_1\cdot[\sigma_1\times\mathrm{k}])(\mathrm{k}\cdot\gamma)^{\nu}(\mathrm{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})d\gamma d\mathrm{w}_1d\mathrm{w}_2,$$

$$N_{\nu\nu'}^{(r)}=\left(\frac{m}{kT}\right)^{\frac{1}{2}}\int\int\int(3-\epsilon_1^{(r)}-\epsilon_2^{(r)})(\omega_1\cdot[\sigma_1\times\mathrm{k}])(\mathrm{k}\cdot\gamma)^{\nu}(\mathrm{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})d\gamma d\mathrm{w}_1d\mathrm{w}_2,$$

$$Q_{\nu\nu'}^{(r)}=\int\int\int(\tfrac{3}{2}-\epsilon_1^{(r)})(\epsilon_1^{(r)}-\epsilon_2^{(r)})(\mathrm{k}\cdot\gamma)^{\nu}(\mathrm{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})d\gamma d\mathrm{w}_1d\mathrm{w}_2.$$

$$\begin{matrix}[S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1]_{12}\\ +[S_{\frac{1}{2}}^{1}(\epsilon_1^{(r)})\mathrm{W}_1;S_{\frac{1}{2}}^{1}(\epsilon_2^{(r)})\mathrm{W}_2]_{12}\end{matrix}=\frac{2}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\begin{bmatrix}\xi Q_{30}^{(0)}-2\xi Q_{21}^{(0)}+\xi Q_{12}^{(0)}+\xi M_{20}^{(1)}-2\xi M_{11}^{(1)}+\xi M_{02}^{(1)}-2\xi^2M_{40}^{(0)}+6\xi^2M_{31}^{(0)}\\ -6\xi^2M_{22}^{(0)}+2\xi^2M_{13}^{(0)}-\tfrac{3}{2}\xi N_{20}^{(0)}+3\xi N_{11}^{(0)}-\tfrac{3}{2}\xi N_{02}^{(0)}+[m(\sigma_1\times\mathrm{k})\cdot\mu_1\cdot(\sigma_1\times\mathrm{k})]\\ \times[\xi^2K_{30}^{(1)}-3\xi^2K_{21}^{(1)}+3\xi^2K_{12}^{(1)}-\xi^2K_{03}^{(1)}-2\xi^3K_{50}^{(0)}+8\xi^3K_{41}^{(0)}-12\xi^3K_{32}^{(0)}\\ +8\xi^3K_{23}^{(0)}-2\xi^3K_{14}^{(0)}-\tfrac{3}{2}\xi^2L_{30}^{(0)}+(9/2)\xi^2L_{21}^{(0)}-(9/2)\xi^2L_{12}^{(0)}+\tfrac{3}{2}\xi^2L_{03}^{(0)}]\end{bmatrix}S(\mathrm{k})d\mathrm{k}.$$