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Analysis of Collision Encounter Integrals of Bio Molecular Particles.

----Molecular Dynamical Computation ---

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We introduced a rigorous physico-chemical theoretical method to determine the shear, bulk viscosity and thermal conductivity of bio molecular particles that has been proposed by Curtiss and Muckenfuss (1957). The Boltzmann equation was solved by the perturbation method by assuming that the system does not deviate excessively from the equilibrium state. The collision integral was expressed by the Sonine Polynomials which was based on the Chapman and Enskog method. We introduced this method on the basis of vector analysis and analytic integration. We computed shear and bulk viscosity and thermal conductivity of sphero-cylindrical particles as functions of parameter that include the principal moment of inertia. The present method will be available for evaluating the gene regulation molecules.

Gene expression. Bio molecular. Thermal conductivity. Boltzmann equation. Collision integral.

生体分子の衝突積分解析

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遺伝子発現の分子生物、物理学的解析を試みた。多数の均一な生体分子が拡散しながら拡がる状況を想定し、分子間の粘性、熱力学的移動度の値を求める方法をCurtiss Muckenfuss (1957)らに基ついて解説した。　ボルツマン方程式の分布関数を角速度、オイラー角を含めた形式とした。系が非平衡からごくわずかしか遷移していないと想定して、漸近近似を行った。　衝突積分は Chapmann-Enskog らの方法をもとに、Sonine の多項式により有限級数として表示した。ヴェクトル解析および解析的積分定理をもちいて、衝突積分を解析的に求める方法を紹介した。具体例として、円筒の両底が半球でおおわれる形状の均一粒子から構成される系の粘性と移動度を、分子の主慣性モメントの関数として計算した。Curtiss Muckenfuss らの方法は遺伝子制御生体分子から構成される系の記述に適している。

遺伝子発現. 生体分子. 熱力学的移動度. ボルツマン方程式. 衝突積分. Sonine の多項式

1. Introduction.

Genetic expression onsets by molecular-molecular interactions between the gene regulating particles - inducer and target bases region in the DNA. We introduce mathematical methods to compute viscosity and conductance of two molecular systems which are firstly proposed by Curtiss and Muckenfuss 1957.

2. Mathematical modeling.

Fig 1a shows trajectories of colliding two molecules. A and B are the centers of the two molecules. g21 and g21' are initial and relative velocities. The trajectory LMN is traced by B. The orientation of the plane LMN about AP' is independent of the velocities. It is specified by the angle ε between the plane LMN and a plane containing AP'. The angle χ through which g21 is deflected depends on the magnitude of g of the initial velocity and on the distance b of A from either of the asymptotes. b is a collision parameter. It has a relation to two diameters (d1 , d2) of

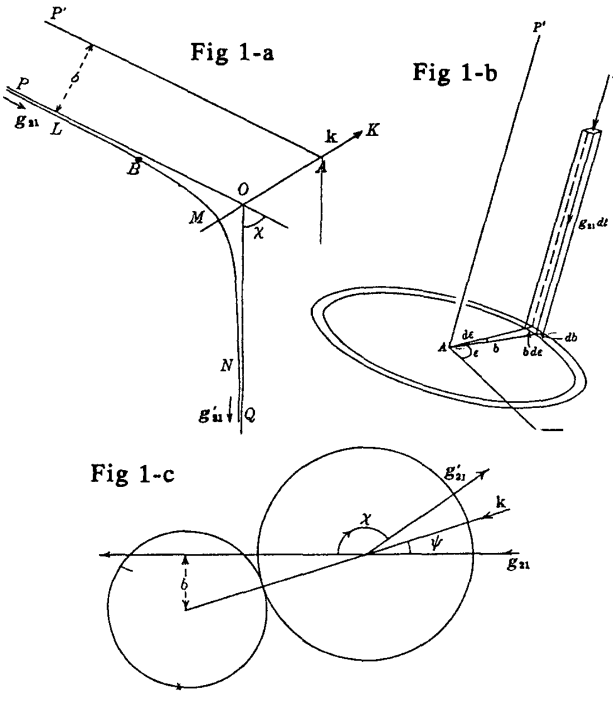


Fig 1-a
Fig 1-b
Fig 1-c

two molecules such that b = (d1 + d2)/2*cos(χ /2) = (d1 + d2)/2*sin(ψ). The most important integral variables for the collision integral is the vector k (collision direction) over the collision cylinder.

we define the "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. These quantities are discussed in detail later.

We now define the reduced relative translational and rotational kinetic energies

$$\epsilon_i^{(t)}=mV_i^2/2kT;\quad i=1,2 \quad (0\text{-}11)$$

$$\epsilon_i^{(r)}=\mathbf{I}_i:\Omega_i\Omega_i/2kT;\quad i=1,2 \quad (0\text{-}12)$$

where

$$\mathbf{V}_i=\mathbf{v}_i-\mathbf{v}_0;\quad i=1,2 \quad (0\text{-}13)$$

is the velocity relative to the local stream velocity, $\mathbf{v}_0$, and

$$\Omega_i=\omega_i-\omega_0;\quad i=1,2 \quad (0\text{-}14)$$

is the angular velocity relative to the local average angular velocity, ω_0. We also define the dimensionless relative velocity

$$\mathbf{W}_i=\left(\frac{m}{2kT}\right)^{\frac{1}{2}}\mathbf{V}_i;\quad i=1,2 \quad (0\text{-}15)$$

and the associated tensor,

$$\mathsf{W}_i=\frac{m}{2kT}(\mathbf{V}_i\mathbf{V}_i-\tfrac{1}{3}V_i^2\mathsf{U});\quad i=1,2 \quad (0\text{-}16)$$

$$\eta=\tfrac{5}{2}kT/\{\mathsf{W};\mathsf{W}\}, \quad (0\text{-}24)$$

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 [see Eq. (0-15)],

$$\mathfrak{G}=\left(\frac{m}{kT}\right)^{\frac{1}{2}}\mathbf{G}=\frac{1}{\sqrt{2}}(\mathbf{W}_2+\mathbf{W}_1), \quad (1\text{-}3)$$

$$\gamma=\left(\frac{m}{4kT}\right)^{\frac{1}{2}}\mathbf{g}=\frac{1}{\sqrt{2}}(\mathbf{W}_2-\mathbf{W}_1). \quad (1\text{-}4)$$

Solving this set of equations we find that

$$\mathbf{W}_1=\frac{1}{\sqrt{2}}(\mathfrak{G}-\boldsymbol{\gamma}), \tag{1-5}$$

$$\mathbf{W}_2=\frac{1}{\sqrt{2}}(\mathfrak{G}+\boldsymbol{\gamma}). \tag{1-6}$$

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

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

and from the conservation of linear momentum

$$\mathbf{W}_2'=\mathbf{W}_2-\sqrt{2}\boldsymbol{\kappa}. \tag{1-9}$$

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

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

The vector $\boldsymbol{\kappa}$ may be evaluated from considerations of the dynamics of the binary collisions. It may be

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

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

$$\frac{1}{\xi}=1+\frac{m}{2}[\boldsymbol{\sigma}_1\times\mathbf{k}]\cdot\boldsymbol{\mu}_1\cdot[\boldsymbol{\sigma}_1\times\mathbf{k}]+\frac{m}{2}[\boldsymbol{\sigma}_2\times\mathbf{k}]\cdot\boldsymbol{\mu}_2\cdot[\boldsymbol{\sigma}_2\times\mathbf{k}]. \tag{1-14}$$

In these expressions, $\mathbf{k}$ is a unit vector normal to the plane of contact of the collision, $\boldsymbol{\sigma}_i$ is the radius vector from the center of molecule i to the point of contact, $\boldsymbol{\mu}_i$ 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

$$\mathfrak{g}=\mathbf{g}-\mathbf{g}_0 \tag{1-15}$$

where

$$\mathbf{g}_0=(\boldsymbol{\omega}_1\times\boldsymbol{\sigma}_1)-(\boldsymbol{\omega}_2\times\boldsymbol{\sigma}_2). \tag{1-16}$$

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

$$\mathbf{w}_i=\frac{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}{(2kT)^{\frac{1}{2}}}\boldsymbol{\Omega}_i \tag{1-17}$$

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 after are

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

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

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

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

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

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

$$\epsilon_1^{(r)\prime}=\epsilon_1^{(r)}+\frac{2(2m)^{\frac{1}{2}}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}\mathbf{w}_1\cdot[\boldsymbol{\sigma}_1\times\boldsymbol{\kappa}] +2m[\boldsymbol{\sigma}_1\times\boldsymbol{\kappa}][\boldsymbol{\sigma}_1\times\boldsymbol{\kappa}]:\boldsymbol{\mu}_1, \tag{1-22}$$

$$\epsilon_2^{(r)\prime}=\epsilon_2^{(r)}-\frac{2(2m)^{\frac{1}{2}}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}\mathbf{w}_2\cdot[\boldsymbol{\sigma}_2\times\boldsymbol{\kappa}] +2m[\boldsymbol{\sigma}_2\times\boldsymbol{\kappa}][\boldsymbol{\sigma}_2\times\boldsymbol{\kappa}]:\boldsymbol{\mu}_2. \tag{1-23}$$

Then from the first pair of equations, Eqs. (1-20) and (1-21), along with the definition of $\boldsymbol{\gamma}$, Eq. (1-4), we

$$\epsilon_1^{(t)\prime}+\epsilon_2^{(t)\prime}=\epsilon_1^{(t)}+\epsilon_2^{(t)}-4(\boldsymbol{\kappa}\cdot\boldsymbol{\gamma})+4\kappa^2, \tag{1-24}$$

and from the last pair, Eqs. (1-22) and (1-23), along with the relations, Eqs. (1-12 to 16), we find that

$$\epsilon_1^{(r)\prime}+\epsilon_2^{(r)\prime}=\epsilon_1^{(r)}+\epsilon_2^{(r)}+4(\boldsymbol{\kappa}\cdot\boldsymbol{\gamma}_0) +4\xi(1-\xi)(\boldsymbol{\kappa}\cdot\boldsymbol{\Gamma})^2 -2(m/kT)^{\frac{1}{2}}(\boldsymbol{\kappa}\times\boldsymbol{\omega}_0)\cdot(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2). \tag{1-25}$$

When the last two relations are combined and use is made of the expression for $\boldsymbol{\kappa}$, Eq. (1-12), we obtain

$$\epsilon_1^{(t)\prime}+\epsilon_2^{(t)\prime}+\epsilon_1^{(r)\prime}+\epsilon_2^{(r)\prime}=\epsilon_1^{(t)}+\epsilon_2^{(t)}+\epsilon_1^{(r)}+\epsilon_2^{(r)} -2(m/kT)^{\frac{1}{2}}(\boldsymbol{\kappa}\times\boldsymbol{\omega}_0)\cdot(\boldsymbol{\sigma}_1-\boldsymbol{\sigma}_2), \tag{1-26}$$

which is, of course for the case in which $\omega_0=0$, the statement of conservation of energy.

Let us now 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

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

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

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

The quantity in brackets, in the integrand may be expressed in terms of the unprimed variables and the vector $\boldsymbol{\kappa}$ by means of Eqs. (1-4), (1-8), and (1-9)

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

We now cnange integration variables from $\mathbf{W}_1$ and $\mathbf{W}_2$ to $\mathfrak{G}$ and $\boldsymbol{\gamma}$. The Jacobian of the transformation is unity and

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

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

$$[W_1;\ W_1]_{12}+[W_1;\ W_2]_{12}$$
$$=-\frac{4}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\cdots\int[\kappa^2\gamma^2+\tfrac{1}{3}(\kappa\cdot\gamma)^2$$
$$-(8/3)\kappa^2(\kappa\cdot\gamma)+\tfrac{4}{3}\kappa^4]\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})$$
$$\times(\mathbf{k}\cdot\Gamma)S(\mathbf{k})d\mathbf{k}d\gamma dw_1dw_2. \quad (1\text{-}31)$$

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

$$J_{\nu\nu'}{}^{(r)}=\int\int\int(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}$$
$$\times\exp(-\gamma^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})d\gamma dw_1dw_2, \quad (1\text{-}32)$$

where

$$\gamma_0=(m/4kT)^{\frac{1}{2}}g_0. \quad (1\text{-}33)$$

Then introducing the expression for κ, Eq. (1-12), and the expression for Γ, Eqs. (1-13) and (1-15) into Eq. (1-31) we find that the sum of square brackets may be written as a sum of integrals of the $J_{\nu\nu'}{}^{(r)}$ in the follow-

$$[W_1;\ W_1]_{12}+[W_1;\ W_2]_{12}=-\frac{4}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\Big|S(\mathbf{k})d\mathbf{k}\quad(1\text{-}34)$$
$$[\xi^2(J_{30}{}^{(1)}-3J_{21}{}^{(1)}+3J_{12}{}^{(1)}-J_{03}{}^{(1)})+\tfrac{1}{3}\xi^2(1-8\xi+4\xi^2)J_{50}{}^{(0)}$$
$$-\tfrac{1}{3}\xi^2(3-32\xi+20\xi^2)J_{41}{}^{(0)}+\tfrac{1}{3}\xi^2(3-48\xi+40\xi^2)J_{32}{}^{(0)}$$
$$-\tfrac{1}{3}\xi^2(1-32\xi+40\xi^2)J_{23}{}^{(0)}-\tfrac{4}{3}\xi^3(2-5\xi)J_{14}{}^{(0)}-\tfrac{4}{3}\xi^4J_{05}{}^{(0)}]$$

To evaluate the next sum of square brackets.

$$[S_{\frac{1}{2}}{}^1(\epsilon_1{}^{(i)})W_1;\ S_{\frac{1}{2}}{}^1(\epsilon_1{}^{(r)})W_1]_{12}+[S_{\frac{1}{2}}{}^1(\epsilon_1{}^{(i)})W_1;\ S_{\frac{1}{2}}{}^1(\epsilon_2{}^{(r)})W_2]_{12}$$
$$=\frac{1}{n_1{}^*n_2{}^*}\int\cdots\int$$
$$[S_{\frac{1}{2}}{}^1(\epsilon_1{}^{(i)\prime})W_1'-S_{\frac{1}{2}}{}^1(\epsilon_1{}^{(i)})W_1]\cdot[S_{\frac{1}{2}}{}^1(\epsilon_1{}^{(r)})W_1+S_{\frac{1}{2}}{}^1(\epsilon_2{}^{(r)})W_2]$$
$$\times f_1{}^{(0)}f_2{}^{(0)}(\mathbf{k}\cdot\mathbf{g})S(\mathbf{k})d\mathbf{k}d\mathbf{v}_1d\mathbf{v}_2d\omega_1d\omega_2 \quad (1\text{-}38)$$

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

$$\frac{2}{\pi^4}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\cdots\int\Big[(\epsilon_1{}^{(r)}-\epsilon_2{}^{(r)})$$
$$[(5/4)(\kappa\cdot\gamma)-\tfrac{3}{2}\gamma^2(\kappa\cdot\gamma)+2(\kappa\cdot\gamma)^2+\kappa^2\gamma^2-2\kappa^2(\kappa\cdot\gamma)]$$
$$+\tfrac{5}{2}(3-\epsilon_1{}^{(r)}-\epsilon_2{}^{(r)})(\kappa\cdot\gamma-\kappa^2)\Big]$$
$$\times\exp(-\gamma^2-\epsilon_1{}^{(r)}-\epsilon_2{}^{(r)})(\mathbf{k}\cdot\Gamma)S(\mathbf{k})d\mathbf{k}d\gamma dw_1dw_2. \quad (1\text{-}39)$$

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

$$K_{\nu\nu'}{}^{(r)}=\int\int\int(\epsilon_1{}^{(r)}-\epsilon_2{}^{(r)})(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}$$
$$\exp(-\gamma^2-\epsilon_1{}^{(r)}-\epsilon_2{}^{(r)})d\gamma dw_1dw_2, \quad (1\text{-}40)$$
$$L_{\nu\nu'}{}^{(r)}=\int\int\int(3-\epsilon_1{}^{(r)}-\epsilon_2{}^{(r)})(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}\gamma^{2r}$$
$$\exp(-\gamma^2-\epsilon_1{}^{(r)}-\epsilon_2{}^{(r)})d\gamma dw_1dw_2. \quad (1\text{-}41)$$

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

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

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

Similar recursion relations for higher values of r may also be easily obtained, but only the values 0 and 1 occur in the discussion of Sec. 1. Since each of the six sets of integrals mentioned above are integrals of $I_{\nu}{}^{(r)}$, it is clear that similar recursion relations apply to each of the six. In the remaining portion of this section, we consider the evaluation of the sets of integrals for the case of $r=0$.

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

$$\epsilon_i{}^{(r)}=\frac{w_i\cdot I_i\cdot w_i}{(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}},\quad i=1,2 \quad (2\text{-}5)$$
$$\gamma_0{}^{(i)}=w_i\cdot(\sigma_i\times\mathbf{k}),\quad i=1,2 \quad (2\text{-}6)$$
$$\varphi^{(i)}=w_i\cdot(\sigma_i\times[\sigma_i\times\mathbf{k}]).\quad i=1,2. \quad (2\text{-}7)$$

Hence let us consider the Jacobian

Let
$$a_i=\sigma_i\times\mathbf{k},\quad i=1,2 \quad (2\text{-}8)$$
$$b_i=\sigma_i\times[\sigma_i\times\mathbf{k}],\qquad c_i=a_i\times b_i. \quad (2\text{-}10)$$

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

$$\frac{\partial(\epsilon_i{}^{(r)},\gamma_0{}^{(i)},\varphi^{(i)})}{\partial(w_{i1},w_{i2},w_{i3})}=2\frac{c_i\cdot I_i\cdot w_i}{(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}}. \quad (2\text{-}11)$$

ɔ 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

$$\omega_i=\frac{S_i\times(c_i\cdot I_i)\pm A_ic_i}{c_i\cdot I_i\cdot c_i}, \quad (2\text{-}12)$$

where

$$S_i=\gamma_0{}^{(i)}b_i-\varphi^{(i)}a_i \quad (2\text{-}13)$$

and

$$A_i{}^2=\epsilon_i{}^{(r)}(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}(c_i\cdot I_i\cdot c_i)-(\Gamma_1\Gamma_2\Gamma_3)(S_i\cdot\mu_i\cdot S_i) \quad (2\text{-}14)$$

First, since

$$a_i\cdot c_i=0 \quad (2\text{-}15)\qquad a_i\times S_i=\gamma_0{}^{(i)}c_i, \quad (2\text{-}16)$$

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

$$b_i\cdot c_i=0 \quad (2\text{-}17)\qquad b_i\times S_i=\varphi^{(i)}c_i \quad (2\text{-}18)$$

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

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

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,

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

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

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

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

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

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

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

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

$$\varphi_\pm^{(i)}=\frac{(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{b}_i)\gamma_0^{(i)}\pm\dfrac{(\mathbf{c}_i\cdot\mathbf{I}_i\cdot\mathbf{c}_i)^{1/2}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/2}}[(\Gamma_1\Gamma_2\Gamma_3)^{1/2}(\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i)\epsilon_i^{(r)}-\gamma_0^{(i)^2}]^{1/2}}{\mathbf{a}_i\cdot\boldsymbol{\mu}_i\cdot\mathbf{a}_i} \quad (2\text{-}27)$$

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

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

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

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

$$J_{\nu\nu'}^{(0)}=\frac{\pi^3}{\eta_1\eta_2}\int_{-\infty}^{\infty}\int_{\infty}^{\infty}\int_{\gamma_0^{(1)2}/\eta_1^2}^{\infty}\int_{\gamma_0^{(2)2}/\eta_2^2}^{\infty}\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}x^\nu(\mathbf{k}\cdot\gamma_0)^{\nu'}$$
$$\exp(-x^2-\epsilon_1^{(r)}-\epsilon_2^{(r)})dx\,d\epsilon_2^{(r)}d\epsilon_1^{(r)}d\gamma_0^{(1)}d\gamma_0^{(2)} \quad (2\text{-}30)$$

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

$$J_{\nu\nu'}^{(0)}=\frac{\pi^3}{\eta_1\eta_2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}x^\nu(\mathbf{k}\cdot\gamma_0)^{\nu'}\exp\left(-x^2-\frac{\gamma_0^{(1)^2}}{\eta_1^2}-\frac{\gamma_0^{(2)^2}}{\eta_2^2}\right)dx\,d\gamma_0^{(1)}d\gamma_0^{(2)}, \quad (2\text{-}31)$$

$$K_{\nu\nu'}^{(0)}=\frac{\pi^3}{\eta_1\eta_2}\int_{-\infty}^{\infty}\int_{\infty}^{\infty}\int_{\infty}^{\mathbf{k}\cdot\gamma_0}x^\nu\left(\frac{\gamma_0^{(1)^2}}{\eta_1^2}-\frac{\gamma_0^{(2)^2}}{\eta_2^2}\right)(\mathbf{k}\cdot\gamma_0)^{\nu'}\exp\left(-x^2-\frac{\gamma_0^{(1)^2}}{\eta_1^2}-\frac{\gamma_0^{(2)^2}}{\eta_2^2}\right)dx\,d\gamma_0^{(1)}d\gamma_0^{(2)}, \quad (2\text{-}32)$$

$$L_{\nu\nu'}^{(0)}=\frac{\pi^3}{\eta_1\eta_2}\int_{\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}x^\nu\left(1-\frac{\gamma_0^{(1)^2}}{\eta_1^2}-\frac{\gamma_0^{(2)^2}}{\eta_2^2}\right)(\mathbf{k}\cdot\gamma_0)^{\nu'}\exp\left(-x^2-\frac{\gamma_0^{(1)^2}}{\eta_1^2}-\frac{\gamma_0^{(2)^2}}{\eta_2^2}\right)dx\,d\gamma_0^{(1)}d\gamma_0^{(2)}. \quad (2\text{-}33)$$

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

$$\left(\frac{m}{kT}\right)^{1/2}\omega_i\cdot(\sigma_i\times\mathbf{k})=\frac{(2m)^{1/2}}{(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}\gamma_0^{(i)}+\left(\frac{m}{kT}\right)^{1/2}\omega_0\cdot(\sigma_i\times\mathbf{k}) \quad (2\text{-}35)$$

$$\mathbf{k}\cdot\gamma_0=\frac{(m)^{1/2}}{\sqrt{2}(\Gamma_1\Gamma_2\Gamma_3)^{1/6}}(\gamma_0^{(1)}-\gamma_0^{(2)})+\left(\frac{m}{4kT}\right)^{1/2}(\sigma_1-\sigma_2)\cdot(\mathbf{k}\times\omega_0). \quad (2\text{-}36)$$

Now since we are considering only the special case in which $\omega_0=0$, we transform to new coordinates defined

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

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

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

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 integrals over v are complete integrals

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

$$K_{\nu\nu'}^{(0)}=\pi^{7/2}\eta^{\nu'}\frac{\eta_1^2-\eta_2^2}{\eta_1^2+\eta_2^2}\int_{-\infty}^{+\infty}\int_{-\infty}^{\eta u}(u^2-\tfrac{1}{2})x^\nu u^{\nu'}\times\exp(-x^2-u^2)dx\,du, \quad (2\text{-}44)$$

$$L_{\nu\nu'}{}^{(0)}=\pi^{7/2}\eta^{\nu'}\int_{-\infty}^{+\infty}\int_{-\infty}^{\eta u}(\tfrac{1}{2}-u^2)x^{\nu}u^{\nu'}\times\exp(-x^2-u^2)dxdu, \quad (2\text{-}45)$$

$$M_{\nu\nu'}{}^{(0)}=\pi^{7/2}\eta^{\nu'}\frac{2\eta\eta_1^2}{(\eta_1^2+\eta_2^2)^2}\int_{-\infty}^{+\infty}\int_{-\infty}^{\eta u}[(\eta_1^2-\eta_2^2)u(u^2-\tfrac{1}{2})+2\eta_2^2u]\times x^{\nu}u^{\nu'}\exp(-x^2-u^2)dxdu, \quad (2\text{-}46)$$

$$N_{\nu\nu'}{}^{(0)}=\pi^{7/2}\eta^{\nu'}\frac{2\eta\eta_1^2}{\eta_1^2+\eta_2^2}\int_{-\infty}^{+\infty}\int_{-\infty}^{\eta u}u(\tfrac{1}{2}-u^2)x^{\nu}u^{\nu'}\times\exp(-x^2-u^2)dxdu, \quad (2\text{-}47)$$

Then as a final change of variables we let

$u=r\sin\vartheta$. (2-49) $\qquad x=r\cos\vartheta$ (2-50)

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

$$\tan\vartheta_0=1/\eta. \quad (2\text{-}52)$$

We now define

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

Then after carrying out the integration over r we find

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

$$L_{\nu\nu'}{}^{(0)}=\tfrac{1}{2}J_{\nu\nu'}{}^{(0)}-\frac{1}{\eta^2}J_{\nu,\nu'+2}{}^{(0)}, \quad (2\text{-}56) \qquad K_{\nu\nu'}{}^{(0)}=-\frac{\eta_1^2-\eta_2^2}{\eta_1^2+\eta_2^2}L_{\nu\nu'}{}^{(0)} \quad (2\text{-}55)$$

$$M_{\nu\nu'}{}^{(0)}=\frac{2\eta_1^2}{(\eta_1^2+\eta_2^2)^2}\left[(\tfrac{5}{2}\eta_2^2-\tfrac{1}{2}\eta_1^2)J_{\nu,\nu'+1}{}^{(0)}+\frac{\eta_1^2-\eta_2^2}{\eta^2}J_{\nu,\nu'+3}{}^{(0)}\right] \quad (2\text{-}57)$$

$$N_{\nu\nu'}{}^{(0)}=\frac{2\eta_1^2}{\eta_1^2+\eta_2^2}\left[\tfrac{1}{2}J_{\nu,\nu'+1}{}^{(0)}-\frac{1}{\eta^2}J_{\nu,\nu'+3}{}^{(0)}\right], \quad (2\text{-}58)$$

$$Q_{\nu\nu'}{}^{(0)}=-\left[1+\frac{\eta_1^2-\eta_2^2}{4(\eta_1^2+\eta_2^2)}-\frac{3\eta_2^2(\eta_1^2-\eta_2^2)}{4(\eta_1^2+\eta_2^2)^2}\right]J_{\nu\nu'}{}^{(0)}$$
$$+\left[\frac{\eta_1^2-\eta_2^2}{2(\eta_1^2+\eta_2^2)}+\frac{(\eta_1^2-\eta_2^2)^2-8\eta_1^2\eta_2^2}{2(\eta_1^2+\eta_2^2)^2}\right]\frac{1}{\eta^2}J_{\nu,\nu'+2}{}^{(0)}$$
$$-\frac{\eta_1^2(\eta_1^2-\eta_2^2)}{\eta^4(\eta_1^2+\eta_2^2)^2}J_{\nu,\nu'+4}{}^{(0)}. \quad (2\text{-}59)$$

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

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

Thus

$$\xi=\sin^2\vartheta_0. \quad (2\text{-}61)$$

The evaluation of the $\Lambda_{\nu\nu'}$ may be carried out by straightforward methods. The expressions for the $J_{\nu\nu'}{}^{(0)}$ obtained by substituting the results into Eq. (2-54)

The expressions for the various sets of integrals derived in the foregoing may be used in the expressions for the square bracket integrals derived in the previous section. Thus we find from Eq. (1-34) that

$$[\mathbf{W}_1;\mathbf{W}_1]_{12}+[\mathbf{W}_1;\mathbf{W}_2]_{12}=\frac{2}{3}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\xi^{\frac{1}{2}}(5-2\xi)S(\mathbf{k})d\mathbf{k} \quad (2\text{-}62)$$

from Eq. (1-35) that

$$[S_{\frac{3}{2}}{}^1(\epsilon_1{}^{(t)});S_{\frac{3}{2}}{}^1(\epsilon_1{}^{(t)})]_{12}+[S_{\frac{3}{2}}{}^1(\epsilon_1{}^{(t)});S_{\frac{3}{2}}{}^1(\epsilon_2{}^{(t)})]_{12}=2\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\xi^{\frac{1}{2}}(1-\xi)S(\mathbf{k})d\mathbf{k} \quad (2\text{-}63)$$

and from Eq. (1-37) that

$$[S_{\frac{3}{2}}{}^1(\epsilon_1{}^{(t)})\mathbf{W}_1;S_{\frac{3}{2}}{}^1(\epsilon_1{}^{(t)})\mathbf{W}_1]_{12}+[S_{\frac{3}{2}}{}^1(\epsilon_1{}^{(t)})\mathbf{W}_1;S_{\frac{3}{2}}{}^1(\epsilon_2{}^{(t)})\mathbf{W}_2]_{12}=\frac{1}{2}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\xi^{\frac{1}{2}}(15-11\xi)S(\mathbf{k})d\mathbf{k}. \quad (2\text{-}64)$$

Then from Eq. (1-42) we find that

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

and from Eq. (1-48) that

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

In the latter two expressions we have not written down the terms which are antisymmetric with respect to an interchange of 1 and 2 since these terms do not contribute to the brace expression defined by Eq. (0-9) in the case under consideration in which $\omega_0=0$.

3. THE INTEGRATION OVER k AND THE ORIENTATIONS

From Eq. (0-9) and the definition of n_2^*, if $\omega_0=0$,

$$\{S_{nn'}{}^{(\nu)}\mathbf{W}^{(\nu)};S_{mm'}{}^{(\nu)}\mathbf{W}^{(\nu)}\}=\frac{1}{(8\pi^2)^2}\int\int[[S_{1,nn'}{}^{(\nu)}\mathbf{W}_1{}^{(\nu)};S_{1,mm'}{}^{(\nu)}\mathbf{W}_1{}^{(\nu)}]_{12}+[S_{1,nn'}{}^{(\nu)}\mathbf{W}_1{}^{(\nu)};S_{2,mm'}{}^{(\nu)}\mathbf{W}_2{}^{(\nu)}]_{12}]\sin\beta_1\sin\beta_2 d\alpha_1 d\alpha_{\cdot} \quad (3\text{-}1)$$

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

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

$$K_{3i}{}^{(2)\prime}=\textstyle\sum_j K_{3j}R_{ij}{}^{(2)}, \quad (3\text{-}3)$$

where the $K_{ij}{}^{(1)\prime}$ and $K_{ij}{}^{(2)\prime}$ 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

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

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

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

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

It is shown in Appendix B that the Jacobian of the transformation is

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

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

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

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,

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

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

$$\begin{aligned} S(\mathbf{k}) = {} & \mathcal{R}^{(1)\prime}\mathcal{T}^{(1)\prime} - \mathcal{S}^{(1)\prime}\mathcal{S}^{(1)\prime} + \mathcal{R}^{(2)\prime}\mathcal{T}^{(2)\prime} - \mathcal{S}^{(2)\prime}\mathcal{S}^{(2)\prime} \\ & + \cos^2\psi(\mathcal{R}^{(1)\prime}\mathcal{T}^{(2)\prime} + \mathcal{T}^{(1)\prime}\mathcal{R}^{(2)\prime} - 2\mathcal{S}^{(1)\prime}\mathcal{S}^{(2)\prime}) \\ & + \sin^2\psi(\mathcal{R}^{(1)\prime}\mathcal{R}^{(2)\prime} + \mathcal{T}^{(1)\prime}\mathcal{T}^{(2)\prime} + 2\mathcal{S}^{(1)\prime}\mathcal{S}^{(2)\prime}) \\ & + 2\sin\psi\cos\psi[\mathcal{S}^{(1)\prime}(\mathcal{R}^{(2)\prime} - \mathcal{T}^{(2)\prime}) \\ & \qquad - (\mathcal{R}^{(1)\prime} - \mathcal{T}^{(1)\prime})\mathcal{S}^{(2)\prime}], \end{aligned} \tag{3-14}$$

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

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

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

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

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

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).

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

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

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

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

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

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

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

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

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

and

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

Furthermore,

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

is an element of surface of the ovaloid. Thus

$$\{\mathrm{W};\ \mathrm{W}\} = \frac{1}{6\pi}\left(\frac{kT}{\pi m}\right)^{\frac{1}{2}}\int\xi^{\frac{1}{2}}(5-2\xi) \left[\frac{1}{g_1^{(1)}g_2^{(1)}} + \frac{1}{g_1^{(2)}g_2^{(2)}} + \frac{1}{2}\left(\frac{1}{g_1^{(1)}} + \frac{1}{g_2^{(1)}}\right)\left(\frac{1}{g_1^{(2)}} + \frac{1}{g_2^{(2)}}\right)\right] dS_1 dS_2$$

We have computed following coefficients

$$\eta=\tfrac{5}{2}kT/\{\mathrm{W};\mathrm{W}\},$$

$$\kappa=\frac{\tfrac{1}{2}kT}{[\{S_{\frac12}^{1}(\epsilon^{(t)});S_{\frac12}^{1}(\epsilon^{(t)})\}-\{S_{\frac12}^{1}(\epsilon^{(t)});S_{\frac12}^{1}(\epsilon^{(r)})\}]}.$$

$$\lambda=\frac{3k^2T}{8m}\frac{\left[\begin{array}{l}9\{S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W}\}-15\{S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W}\}\\ -15\{S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W}\}+25\{S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W}\}\end{array}\right]}{\left[\begin{array}{l}\{S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W}\}\{S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W}\}\\ \qquad -\{S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W}\}\{S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W}\}\end{array}\right]}$$

$$\begin{aligned}\{\mathrm{W};\mathrm{W}\}=\frac{2A}{3}\left(\frac{kT}{\pi m}\right)^{\frac12}\Bigg\{&\frac{10}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{7+10\alpha}{\alpha(1+2\alpha)^{\frac12}}\sin^{-1}\frac{\alpha}{1+\alpha}\\ &+\beta\left[\frac{5}{\alpha^{\frac12}}\sinh^{-1}\alpha^{\frac12}+\frac{5}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac12}-\frac{7+5\alpha}{2\alpha(1+\alpha)^{\frac12}}\ln(1+2\alpha)\right]\\ &+\beta^2\left[\frac{5}{4\alpha^{\frac12}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{7}{8\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}\right]\Bigg\}\end{aligned}$$

$$\begin{aligned}\{S_{\frac12}^{1}(\epsilon^{(t)});S_{\frac12}^{1}(\epsilon^{(t)})\}=2A\left(\frac{kT}{\pi m}\right)^{\frac12}\Bigg\{&\frac{2}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{2(1+\alpha)}{\alpha(1+2\alpha)^{\frac12}}\sin^{-1}\frac{\alpha}{1+\alpha}\\ &+\beta\left[\frac{1}{\alpha^{\frac12}}\sinh^{-1}\alpha^{\frac12}+\frac{1}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac12}-\frac{(2+\alpha)}{2\alpha(1+\alpha)^{\frac12}}\ln(1+2\alpha)\right]\\ &+\beta^2\left[\frac{1}{4\alpha^{\frac12}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{1}{4\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}\right]\Bigg\}\end{aligned}$$

$$\begin{aligned}\{S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W}\}=\frac{A}{2}\left(\frac{kT}{\pi m}\right)^{\frac12}\Bigg\{&\frac{30}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{30\alpha+26}{\alpha(1+2\alpha)^{\frac12}}\sin^{-1}\frac{\alpha}{1+\alpha}\\ &+\beta\left[\frac{15}{\alpha^{\frac12}}\sinh^{-1}\alpha^{\frac12}+\frac{15}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac12}-\frac{15\alpha+26}{2\alpha(1+\alpha)^{\frac12}}\ln(1+2\alpha)\right]\\ &+\beta^2\left[\frac{15}{4\alpha^{\frac12}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{13}{4\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}\right]\Bigg\}\end{aligned}$$

$$\begin{aligned}\{S_{\frac12}^{1}(\epsilon^{(t)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W}\}=-\frac{5A}{2}\left(\frac{kT}{\pi m}\right)^{\frac12}\Bigg\{&\frac{2}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{2(1+\alpha)}{\alpha(1+2\alpha)^{\frac12}}\sin^{-1}\frac{\alpha}{1+\alpha}\\ &+\beta\left[\frac{1}{\alpha^{\frac12}}\sinh^{-1}\alpha^{\frac12}+\frac{1}{\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac12}-\frac{(2+\alpha)}{2\alpha(1+\alpha)^{\frac12}}\ln(1+2\alpha)\right]\\ &+\beta^2\left[\frac{1}{4\alpha^{\frac12}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{1}{4\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}\right]\Bigg\}\end{aligned}$$

$$\begin{aligned}\{S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W};S_{\frac12}^{1}(\epsilon^{(r)})\mathrm{W}\}=\frac{A}{2}\left(\frac{kT}{\pi m}\right)^{\frac12}\Bigg\{&\frac{47+32\alpha}{2\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{(12+36\alpha+20\alpha^2)}{\alpha(1+2\alpha)^{\frac12}}\\ &\sin^{-1}\frac{\alpha}{1+\alpha}-\frac{8\alpha+17}{2(1+\alpha)}\\ &+\beta\Bigg[\frac{47+32\alpha}{4\alpha^{\frac12}}\sinh^{-1}\alpha^{\frac12}+\frac{47+16\alpha}{4\alpha^{\frac12}}\sin^{-1}\left(\frac{\alpha}{1+2\alpha}\right)^{\frac12}\\ &-\frac{(48+172\alpha+79\alpha^2)}{8\alpha(1+\alpha)^{\frac12}}\ln(1+2\alpha)-\frac{8\alpha+17}{2(1+\alpha)^{\frac12}}\Bigg]\\ &+\beta^2\left[-\frac{3}{2\alpha}\sin^{-1}\frac{\alpha}{1+\alpha}+\frac{47+16\alpha}{16\alpha^{\frac12}}\sinh^{-1}\left(\frac{\alpha}{1+\alpha}\right)^{\frac12}-\frac{(17+42\alpha+16\alpha^2)}{16(1+\alpha)(1+2\alpha)^{\frac12}}\right]\Bigg\}\end{aligned}$$

η shear viscosity , κ bulk viscosity , λ thermal conductivity

Fig 2-a

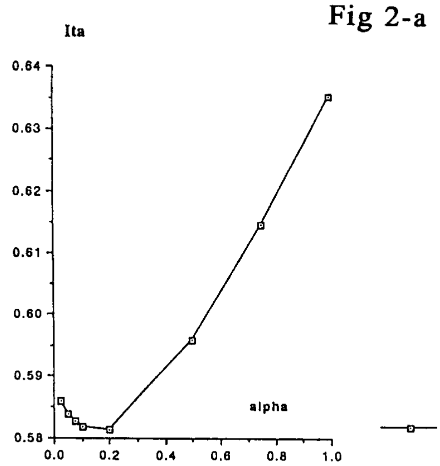


Fig 2-b

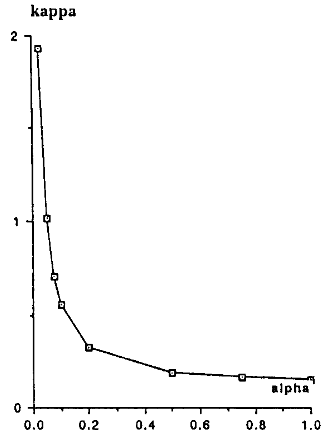
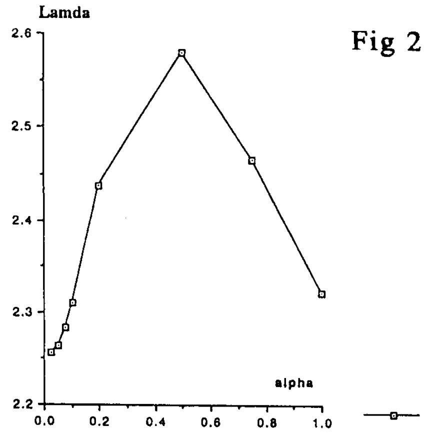


Fig 2-c



3. Results.

Fig 2 shows shear viscosity η * (kT)/A, bulk viscosity κ *kT /A and thermal conductivity λ *8/3(k^2T) as functions of α = m L^2 /(8Γ) where Γ is principal moment of inertia. β = sqr (Γ/m a^{2}* 2 α). We set for simplicity beta =1 and m =1. η and λ showed definite peak values. There was significant discrepancy between the shear viscosity and bulk viscosity.

4. Discussion.

We introduced mathematical method for only a simple kind particles. An extended version will provide molecular collision for mixed kind particles.

5. References

1. Curtiss C F and Muckenfuss C. J.. Chemical Physics. vol 26. No 6. 1957.