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Collision Integral for Non Spherical Bio Particles and Characterization of Bio Physical Reaction Field.

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A theoretical method was introduced to describe the bio physical reaction field around the gene regulation protein particle, repressor. The method basis on the statistical molecular thermo dynamical approach developed by Curtiss CF and Muckenfuss (1957). The system was described by the Boltamann equation including the angular and linear velocities. The solution for the collision integral was expressed by the series expansion of Sonine Polynomials. For the practical use, we introduced a sphere cylinder model that mimics the slender bio molecular particle. These three bio physical quantities changed as functions of number density, the ratio of radius and length of the sphero cylinder. The present method when extended will be available for evaluating the molecular thermo dynamical behavior of the gene regulation protein particle.

Gene regulating particle. Molecular thermo dynamics. Boltzmann equation. Collision integral.

非球状生体粒子の衝突積分と局所物理場の特性解析

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遺伝子制御蛋白粒子レプレッサーが標的遺伝子領域に接近する場合の生体粒子が形成する物理的反応場を記述する目的で、統計熱分子力学的解析方法をCurtiss Muckenfuss (1957)らに基ついて紹介した。系はボルツマン方程式から出発し角速度を含めた複雑な方程式群で記述した。生体粒子に近い形状を想定するため、円筒の両端が半球になっている形状の粒子の局所 shear viscosity, bulk viscosity, thermal conductivity を計算した。さらにこれらの物理的特性が粒子の形状によってどのように変動するかを分析するため、　密度係数(density number)半球径対円筒長比を種々に変化させてそれらの局所的物理場の特性を推定した。　本研究を発展させることより、遺伝子発現における分子熱力学的特性を推定することが可能であると考えられる。

遺伝子制御蛋白粒子.　統計熱分子力学.　ボルツマン方程式.　物理的反応場.

1. Introduction.

Expression and inhibition of gene are controlled by the protein particles that are specific for particular region of the gene molecule. In the present paper, we introduce a statistical molecular thermo dynamical approach developed by Curtiss and Muckenfuss (1957,58) for the characterization of bio physical reaction field around the gene regulating protein particle.

2. Mathematical method.

We examine the behavior of representative points in a typical volume element and calculate, using a Taylor series expansion, the net rate at which molecules of kind i join the group in the volume element in a time interval dt. In this way we obtain

$$\mathfrak{D}_i f_i = J_i = \sum_j J_{ij}, \qquad (1.2)$$

$$\mathfrak{D}_i = \frac{\partial}{\partial t} + \frac{\partial}{\partial \mathbf{r}}\cdot \mathbf{v}_i + \frac{\partial}{\partial \mathbf{v}_i}\cdot\frac{\mathbf{F}_i}{m_i} + \frac{\partial}{\partial \alpha_i}\cdot\dot{\alpha}_i + \frac{\partial}{\partial \omega_i}\cdot\dot{\omega}_i,$$

and $\mathbf{F}_i$ is the external force on a molecule of kind i whose mass is m_i. The term J_i is then related to the net number of molecules of kind i which enter the volume element resulting from collisions with molecules of all other kinds.

$$J_{ij} = -\int (f_i' f_j' - f_i f_j)\mathbf{k}\cdot \mathfrak{g}_{ji} S(\mathbf{k}) d\mathbf{k} d\mathbf{v}_j d\alpha_j d\omega_j. \qquad (1.7)$$

In this equation the primed velocities are functions of the unprimed velocities through the dynamics of collisions of rigid convex bodies

where $\mathfrak{g}_{ji}$ is the relative velocity of the points of contact before the encounter,

$$\mathfrak{g}_{ji} = \mathbf{v}_j - \mathbf{v}_i + \omega_j \times \mathfrak{d}_j - \omega_i \times \mathfrak{d}_i, \qquad (1.4)$$

and $S(\mathbf{k})d\mathbf{k}$ is the element of surface of the volume from which the center of molecule j is excluded when the molecules are in contact. The radius vector from the center of a molecule to the point of contact is denoted by $\mathfrak{d}$ and the sense of $\mathbf{k}$ is taken from molecule i to molecule j.

3. SOLUTION OF THE BOLTZMANN EQUATIONS

The equilibrium solutions for the Boltzmann equations are

$$f_i^0 = \frac{n_i^* m_i^{\frac{3}{2}} \Gamma_i^{\frac{1}{2}}}{(2\pi kT)^3}\exp\left(-\frac{m_i V_i^2}{2kT} - \frac{\Omega_i\cdot \mathsf{I}_i\cdot\Omega_i}{2kT}\right), \qquad (3.1)$$

where Γ_i is the determinant of the tensor of inertia of a molecule of kind i and

$$n_i^* = \frac{n_i \sin\beta_i}{Q_i}\exp\left(\frac{\omega_0\cdot \mathsf{I}_i\cdot\omega_0}{2kT}\right). \qquad (3.2)$$

The term Q_i is defined by

$$Q_i = \int \sin\beta_i \exp\left(\frac{\omega_0\cdot \mathsf{I}_i\cdot\omega_0}{2kT}\right) d\alpha_i.$$

If we write

$$f_i = f_i^0(1+\phi_i), \qquad (3.3)$$

the zero-order equations are:

$$\sum_i \int (f_i^{0\prime} f_j^{0\prime} - f_i^0 f_j^0)\mathbf{k}\cdot\mathfrak{g}_{ji} S(\mathbf{k}) d\mathbf{k} d\mathbf{v}_j d\alpha_j d\omega_j = 0. \qquad (3.4)$$

A solution of the zero order equation has been carried out and found to be given by (3.1). In these solutions, ni*, vo, ωo and T are arbitrary functions of the space and time. We choose to let these functions to be local equilibrium values of the corresponding macroscopic functions. This choice imposes the following restrictions on the perturbation functions.

$$\int f_i^0 \phi_i d\mathbf{v}_i d\omega_i = 0, \qquad (3.5)$$

$$\sum_i m_i \int \mathbf{v}_i f_i^0 \phi_i d\mathbf{v}_i d\alpha_i d\omega_i = 0, \qquad (3.6)$$

$$\sum_i \int \mathsf{I}_i\cdot\omega_i f_i^0 \phi_i d\mathbf{v}_i d\alpha_i d\omega_i = 0, \qquad (3.7)$$

and

$$\sum_i \int \left(\tfrac{1}{2} m_i V_i^2 + \tfrac{1}{2}\Omega_i\cdot \mathsf{I}_i\cdot\Omega_i\right) f_i^0 \phi_i d\mathbf{v}_i d\alpha_i d\omega_i = 0. \qquad (3.8)$$

These conditions are necessary and sufficient for a unique solution of the equations for the perturbation functions ϕ_i.

The first-order equations are

$$\mathfrak{D}_i f_i^0 = \sum_j \int \mathfrak{F}_{ij}(\phi) d\alpha_j, \qquad (3.9)$$

$$\mathfrak{F}_{ij}(\phi) = \int (\phi_i' + \phi_j' - \phi_i - \phi_j) f_i^0 f_j^0 \mathbf{k}\cdot\mathfrak{g}_{ji} S(\mathbf{k}) d\mathbf{k} d\mathbf{v}_j d\omega_j.$$

We proceed to evaluate the terms in $\mathfrak{D}_i f_i^0$ in (3.9) by straightforward differentiation of (3.1) with respect to t, $\mathbf{r}$, $\mathbf{v}_i$, α_i, and ω_i. We eliminate the derivatives with respect to t by using the equations of change, assuming that the forces and torques are independent of the linear and angular velocities. Thus we obtain

$$\frac{1}{f_i^0}\mathfrak{D}_i f_i^0 = \left[-\tfrac{1}{3}\left(\frac{m_i V_i^2}{2kT} + \frac{\Omega_i\cdot \mathsf{I}_i\cdot\Omega_i}{2kT}\right)\mathsf{U} + \frac{m_i \mathbf{V}_i\mathbf{V}_i}{kT}\right] : \frac{\partial}{\partial \mathbf{r}}\mathbf{v}_0 + \frac{\mathsf{I}_i\cdot\Omega_i\mathbf{V}_i}{kT} : \frac{\partial}{\partial \mathbf{r}}\omega_0 + \frac{n}{n_i^*}(\mathbf{e}_i\cdot\Omega_i + \mathbf{d}_i\cdot\mathbf{V}_i) - \left(4 - \frac{m_i V_i^2}{2kT} - \frac{\Omega_i\cdot \mathsf{I}_i\cdot\Omega_i}{2kT}\right)\mathbf{V}_i\cdot\frac{\partial \ln T}{\partial \mathbf{r}}, \qquad (3.10)$$

where $\mathbf{d}(\alpha_i)$ and $\mathbf{e}(\alpha_i)$ are defined by

$$\mathbf{d}_i = \frac{\partial}{\partial \mathbf{r}}\left(\frac{n_i^*}{n_i}\right) + \frac{n_i^*}{n}\left(1 - \frac{m_i}{m}\right)\frac{\partial \ln p}{\partial \mathbf{r}} - \frac{n_i^*}{nkT}\left(\mathbf{F}_i - \frac{m_i}{m}\mathbf{F}_i^0\right) \qquad (3.11)$$

$$\mathbf{e}_i = -\frac{n_i^*}{nkT}[\mathbf{G}_i - \mathsf{I}_i\cdot(\mathsf{I}^0)^{-1}\cdot\mathbf{G}_i^0]. \qquad (3.12)$$

In these equations we have used m defined by $mn=\rho$ and the total average force $\mathbf{F}$ defined by

$$n\mathbf{F} = \sum_i n_i \langle\langle \mathbf{F}_i \rangle\rangle.$$

The superscript zero (^{0}) is used to indicate that the relevant average value is calculated by using f_i^0. The definitions of **d**i and **e**i are.

$$\sum_i \int \mathbf{d}_i d\alpha_i = 0 \quad (3.13) \qquad \sum_i \int \mathbf{e}_i d\alpha_i = 0. \quad (3.14)$$

it convenient to partition the orientation space into a large number of cells. The volume of cell l is denoted by τ_l.

Thus Eq. (3.9) is rewritten as

$$\mathfrak{D}_i f_{i,k}{}^0 = \sum_{jl} \tau_l \mathfrak{F}_{ij,kl}(\phi), \qquad (3.15)$$

$$\mathfrak{F}_{ij,kl}(\phi) = \int (\phi_{i,k}{}' + \phi_{j,l}{}' - \phi_{i,k} - \phi_{j,l}) \times f_{i,k}{}^0 f_{j,l}{}^0 \mathrm{k} \cdot \mathrm{g}_{ji} S(\mathrm{k})\, d\mathrm{k} d\mathrm{v}_j d\omega_j.$$

The first pair of indices refer to the two species and the second pair refer to the two cells of orientation space such that the first species index is associated with the first orientation space index and the second species index is associated with the second orientation space index. We also rewrite (3.10) in the following way

$$\mathfrak{D}_i f_{i,k}{}^0 = \mathrm{K}_{i,k}{}^1 \cdot \frac{\partial \ln T}{\partial \mathrm{r}} + \mathrm{K}_{i,k}{}^2 : \frac{\partial}{\partial \mathrm{r}} \mathrm{v}_0 + \mathrm{K}_{i,k}{}^3 : \frac{\partial}{\partial \mathrm{r}} \omega_0 + \mathrm{K}_{i,k}{}^4 \cdot \mathrm{d}_{i,k} + \mathrm{K}_{i,k}{}^5 \cdot \mathrm{e}_{i,k}, \qquad (3.16)$$

where the vectors and tensors $\mathrm{K}_{i,k}{}^\nu$ are easily found by comparing coefficients of similar force terms in (3.10) and (3.16) and evaluating in the appropriate orientation space cell.

In the solution of the set of integral equations (3.15) for $\phi_{i,k}$ we consider the derivatives of v_0, ω_0, T, and all but one of each of the $\mathrm{d}_{i,k}$ and $\mathrm{e}_{i,k}$ as independent parameters. The linear form of the functional $\mathfrak{F}_{ij,kl}$ implies that each of the $\phi_{i,k}$ is linear to these parameters. That is, $\phi_{i,k}$ has the form

$$\phi_{i,k} = \mathrm{A}_{i,k}{}^1 \cdot \frac{\partial \ln T}{\partial \mathrm{r}} + \mathrm{A}_{i,k}{}^2 : \frac{\partial}{\partial \mathrm{r}} \mathrm{v}_0 + \mathrm{A}_{i,k}{}^3 : \frac{\partial}{\partial \mathrm{r}} \omega_0 + \sum_{jl} \tau_l (\mathrm{A}_{i,k}{}^{4j,l} \cdot \mathrm{d}_{j,l} + \mathrm{A}_{i,k}{}^{5j,l} \cdot \mathrm{e}_{j,l}). \qquad (3.17)$$

Inasmuch as the d_i and e_i are not independent, but are related according to Eqs. (3.13) and (3.14) we take $\mathrm{A}_{i,k}{}^{4i,k} = \mathrm{A}_{i,k}{}^{5i,k} = 0$ for all species in all orientation space cells.

Substituting (3.17) into the integral equations (3.15) and equating coefficients of the independent parameters (or "forces") we find

$$\sum_{jl} \tau_l \mathfrak{F}_{ij,kl}(\mathrm{A}^\nu) = \mathrm{K}_{i,k}{}^\nu, \quad \text{for } \nu = 1, 2, \text{ or } 3, \qquad (3.18)$$

$$\sum_{jl} \tau_l \mathfrak{F}_{ij,kl}(\mathrm{A}^{\nu nh',mh}) = \mathrm{K}_{i,k}{}^{\nu nh',mh}, \quad \text{for } \nu = 4 \text{ or } 5, \qquad (3.19)$$

$$\mathrm{K}_{i,k}{}^{\nu nh',mh} = \mathrm{K}_{i,k}{}^\nu \left(\frac{\delta_{km}\delta_{in}}{\tau_m} - \frac{\delta_{kh}\delta_{ih'}}{\tau_h} \right) \qquad (3.20)$$

and

$$\mathrm{A}_{i,k}{}^{\nu nh',mh} = \mathrm{A}_{i,k}{}^{\nu n,m} - \mathrm{A}_{i,k}{}^{\nu h',h}. \qquad (3.21)$$

For convenience in the solution of the integral equations we define:

$$\mathrm{K}_{i,k}{}^{11} = -\left(\tfrac{5}{2} - \frac{m_i V_i^2}{2kT} \right) \mathrm{V}_i f_{i,k}{}^0,$$

$$\mathrm{K}_{i,k}{}^{12} = -\left(\tfrac{3}{2} - \frac{\Omega_i \cdot \mathrm{I}_{i,k} \cdot \Omega_i}{2kT} \right) \mathrm{V}_i f_{i,k}{}^0$$

$$\mathrm{K}_{i,k}{}^{21} = \frac{m_i}{kT} (\mathrm{V}_i \mathrm{V}_i - \tfrac{1}{3} V_i^2 \mathrm{U}) f_{i,k}{}^0$$

$$K_{i,k}{}^{22} = \tfrac{1}{3} \left(\frac{m_i V_i^2}{2kT} - \frac{\Omega_i \cdot \mathrm{I}_{i,k} \cdot \Omega_i}{2kT} \right) f_{i,k}{}^0$$

$$\mathrm{K}_{i,k}{}^1 = \mathrm{K}_{i,k}{}^{11} + \mathrm{K}_{i,k}{}^{12} \qquad \mathrm{K}_{i,k}{}^2 = \mathrm{K}_{i,k}{}^{21} + K_{i,k}{}^{22} \mathrm{U}.$$

$$\mathrm{A}_{i,k}{}^1 = \mathrm{A}_{i,k}{}^{11} + \mathrm{A}_{i,k}{}^{12} \qquad \mathrm{A}_{i,k}{}^2 = \mathrm{A}_{i,k}{}^{21} + A_{i,k}{}^{22} \mathrm{U}$$

where $\mathrm{A}_{i,k}{}^{pq}$ (p, $q = 1$ or 2) are solutions of the integral equations (3.18) with the auxiliary conditions given by Eqs. (3.5)–(3.8). The integral equations are now solved by a variational method.[6] The variational trial functions must, of course, have the proper tensor transformation properties. We use as variational functions, functions of the following form:

$$\mathrm{A}_{i,k}{}^{\nu nh',mh} = A_{i,k}{}^{\nu nh',mh} \mathrm{W}_{i,k}{}^{\nu nh',mh} \qquad (3.22)$$

where $A_{i,k}{}^{\nu nh',mh}$ are scalar functions of the two scalars:

$$\epsilon_i{}^t = \frac{m_i V_i^2}{2kT} \quad \text{and} \quad \epsilon_{i,k}{}^r = \frac{\Omega_i \cdot \mathrm{I}_{i,k} \cdot \Omega_i}{2kT}$$

and

$$\mathrm{W}_{i,k}{}^{11} = \mathrm{W}_{i,k}{}^{12} = \mathrm{W}_{i,k}{}^{4nh',mh} = \mathrm{V}_i,$$

$$\mathrm{W}_{i,k}{}^{21} = \mathrm{V}_i \mathrm{V}_i - \tfrac{1}{3} V_i^2 \mathrm{U}, \qquad W_{i,k}{}^{22} = 1,$$

$$\mathrm{W}_{i,k}{}^3 = (\mathrm{I}_{i,k} \cdot \Omega_i) \mathrm{V}_i, \qquad \cancel{\mathrm{W}_{i,k}{}^{5nh',mh} = \Omega_i.}$$

We approximate the scalar functions $A_{ik}{}^\nu$ by finite series of products of Sonine polynomials.

where for simplicity, we have written ν for all of the superscript indices that we apply. The products of Sonine polynomials are

$$S_{i,k;r'r''}{}^{11} = S_{i,k;r'r''}{}^{12} = S_{i,k;r'r''}{}^{4nh',mh} = S_{\frac{3}{2}}{}^{r'}(\epsilon_i{}^t) S_{\frac{1}{2}}{}^{r''}(\epsilon_{i,k}{}^r),$$

$$S_{i,k;r'r''}{}^{21} = S_{5/2}{}^{r'}(\epsilon_i{}^t) S_{\frac{1}{2}}{}^{r''}(\epsilon_{i,k}{}^r),$$

$$S_{i,k;r'r''}{}^{22} = S_{\frac{1}{2}}{}^{r'}(\epsilon_i{}^t) S_{\frac{1}{2}}{}^{r''}(\epsilon_{i,k}{}^r),$$

$$S_{i,k;r'r''}{}^{3} = S_{\frac{3}{2}}{}^{r'}(\epsilon_i{}^t) S_{\frac{3}{2}}{}^{r''}(\epsilon_{i,k}{}^r),$$

$$S_{i,k;r'r''}{}^{5nh',mh} = S_{\frac{1}{2}}{}^{r'}(\epsilon_i{}^t) S_{\frac{3}{2}}{}^{r''}(\epsilon_{i,k}{}^r).$$

Application of the variational method provided a set of coupled linear algebraic equations for the expansion coefficients

define the following

$$\mathfrak{R}_{i,k;r'r''}{}^\nu = \int S_{i,k;r'r''}{}^\nu \mathrm{W}_{i,k}{}^T : \mathrm{K}_{i,k}{}^\nu d\mathrm{v}_i d\omega_i \qquad (3.24)$$

and

$$\mathrm{Q}_{ij,kl;r'r''m'm''}{}^\nu = \sum_{pq} \frac{\tau_q}{\tau_l} n_{i,k}{}^* n_{p,q}{}^* \times \{ \delta_{ij}\delta_{kl} (\mathrm{W}_{i,k}{}^\nu S_{i,k;r'r''}{}^\nu ;\, \mathrm{W}_{i,k}{}^\nu S_{i,k;m'm''}{}^\nu)_{ip,kq} + \delta_{jp}\delta_{ql} [\mathrm{W}_{i,k}{}^\nu S_{i,k;r'r''}{}^\nu ;\, \mathrm{W}_{i,k}{}^\nu S_{i,k;m'm''}{}^\nu]_{ip,kq} \} \qquad (3.25)$$

where the bracket and parenthesis operators are defined and discussed in Appendix A. We find that the application of the variational method as outlined above yields the following equations:

$$\mathfrak{R}_{i,k;r'r''}{}^\nu = -\sum_{jlm'm''} \tau_l a_{jl;m'm''}{}^\nu \mathrm{Q}_{ij,kl;r'r''m'm''}{}^\nu. \qquad (3.26)$$

The solutions of these equations are subject to constraints implied by Eqs. (3.5)–(3.8).

In reverting to a continuum concept for orientation space, the preceding equation becomes

$$\mathfrak{R}_{i;r'r''}{}^\nu(\alpha_i) = -\sum_{jm'm''} \int \mathrm{Q}_{ij;r'r''m'm''}{}^\nu(\alpha_i, \alpha_j) a_{j;m'm''}{}^\nu(\alpha_j) d\alpha_j. \qquad (3.27)$$

We expand the R's, a's and Q's in terms of the representation coefficients of the three dimensional rotation group; $D^L(\alpha)_{\mu s}$ in the following manner.

$$\mathcal{R}_{i;r'r''}{}^{r} = \sin\beta_i \sum_{L\mu s} R_i^{r}(L\mu s \mid r'r'') D^L(\alpha_i)_{\mu s},$$

$$a_{j;m'm''}{}^{r} = \frac{n_j \sin\beta_j}{n_j^*} \sum_{L\mu s} a_j^{r}(L\mu s \mid m'm'') \bar{D}^L(\alpha_j)_{\mu s},$$

$$\mathcal{Q}_{ij;r'r''m'm''}{}^{r}$$

$$= \frac{n_j \sin\beta_i}{n_i} \sum_{L\mu s L'\mu' s'} Q_{ij}{}^{r}(L\mu s L'\mu' s' | r'r''m'm'') \times D^L(\alpha_i)_{\mu s} D^{L'}(\alpha_j)_{\mu' s'}.$$

The bar above the symbol indicates the complex conjugate. The expansion coefficients here are easily obtained in view of the orthogonality properties of the representation coefficients. The auxiliary conditions (3.5)–(3.8) become:

$$a_j^{22}(L\mu s \mid 00) = 0, \quad (3.28)$$

$$\sum_j n_j a_j^{11}(000 \mid 00) = 0, \quad (3.29)$$

$$\sum_j n_j a_j^{12}(000 \mid 00) = 0, \quad (3.30)$$

$$\sum_j n_j a_j^{4nh',mh}(000 \mid 00) = 0, \quad (3.31)$$

$$\sum_j n_j [a_j^{22}(000 \mid 01) + a_j^{22}(000 \mid 10)] = 0, \quad (3.32)$$

and

$$\sum_j n_j a_j^{5nh',mh}(000 \mid 00) = 0. \quad (3.33)$$

Reverting to a continuum concept for (4.28) substituting these expansions, equating coefficients of $D^L(\alpha_i)_{\mu s}$, dividing by $\sin\beta_i$, and carrying out the integration over α_j using the orthogonality properties of the representation coefficients we find:

$$\sum_{\substack{m'm''j\\ L'\mu' s'}} \frac{n_j}{n_i} a_j^{r}(L'\mu' s' \mid m'm'') Q_{ij}{}^{r}(L\mu s L'\mu' s' \mid r'r''m'm'') = -\frac{2L'+1}{8\pi^2} R_i^{r}(L\mu s \mid r'r''). \quad (3.34)$$

These equations and the equations of constraint (3.28)–(3.33) determine the expansion coefficients $a_j^{r}(L\mu s \mid m'm'')$.

4. Evaluation of the collisional integral.

We introduce following relations for, the expressions for the angular momenta before the collision by using a unit vector normal to the plane of the collision contact k, the radius vector from the center of molecule i to the contact point σ i. We also introduce the dimensionless translational and rotational kinetic energies before a collision are $\varepsilon^{(t)}$ and $\varepsilon^{(r)}$,

$$\mathbf{W}_i' = \mathbf{W}_i + M_i^{-\frac{1}{2}}\kappa, \quad (6.1)$$

$$\mathbf{W}_j' = \mathbf{W}_j - M_j^{-\frac{1}{2}}\kappa, \quad (6.2)$$

$$\mathbf{I}_i \cdot \mathbf{w}_i' = \mathbf{I}_i \cdot \mathbf{w}_i + (\boldsymbol{\sigma}_i \times \mathbf{k}) m_0^{\frac{1}{2}} \Gamma_i^{1/6}, \quad (6.3)$$

$$\mathbf{I}_j \cdot \mathbf{w}_j' = \mathbf{I}_j \cdot \mathbf{w}_j - (\boldsymbol{\sigma}_j \times \mathbf{k}) m_0^{\frac{1}{2}} \Gamma_j^{1/6}, \quad (6.4)$$

$$\epsilon_i^{t\prime} = \epsilon_i^{t} + M_i^{-1}\kappa^2 + 2M_i^{-\frac{1}{2}}\kappa \cdot \mathbf{W}_i, \quad (6.5)$$

$$\epsilon_j^{t\prime} = \epsilon_j^{t} + M_j^{-1}\kappa^2 - 2M_j^{-\frac{1}{2}}\kappa \cdot \mathbf{W}_j, \quad (6.6)$$

$$\epsilon_i^{r\prime} = \epsilon_i^{r} + \frac{2m_0}{\Gamma_i^{1/6}} \mathbf{w}_i \cdot (\boldsymbol{\sigma}_i \times \kappa) + m_0 (\boldsymbol{\sigma}_i \times \kappa) \cdot \mathbf{I}_i^{-1} \cdot (\boldsymbol{\sigma}_i \times \kappa), \quad (6.7)$$

$$\epsilon_j^{r\prime} = \epsilon_j^{r} - \frac{2m_0}{\Gamma_j^{1/6}} \mathbf{w}_j \cdot (\boldsymbol{\sigma}_j \times \kappa) + m_0 (\boldsymbol{\sigma}_j \times \kappa) \cdot \mathbf{I}_j^{-1} \cdot (\boldsymbol{\sigma}_j \times \kappa). \quad (6.8)$$

In these equations we have used the dimensionless peculiar velocities:

$$\mathbf{W}_i = \left(\frac{m_i}{2kT}\right)^{\frac{1}{2}} \mathbf{V}_i \quad \text{and} \quad \mathbf{w}_i = \frac{\Gamma_i \Omega_i}{(2kT)^{\frac{1}{2}}},$$

the vector (κ) associated with the change of linear momentum of one of the molecules during the collision:

$$\kappa = 2\xi_{ij} (\mathbf{k} \cdot \mathbf{\Gamma}) (M_i M_j)^{\frac{1}{2}} \mathbf{k} \quad (6.9)$$

$$\xi_{ij}^{-1} = 1 + \mu_{ij} [(\boldsymbol{\sigma}_i \times \mathbf{k}) \cdot \mathbf{I}_i^{-1} \cdot (\boldsymbol{\sigma}_i \times \mathbf{k}) + (\boldsymbol{\sigma}_j \times \mathbf{k}) \cdot \mathbf{I}_j^{-1} \cdot (\boldsymbol{\sigma}_j \times \mathbf{k}), \quad (6.10)$$

and the dimensionless relative velocity of the points of contact of the collision:

$$\mathbf{\Gamma} = \left(\frac{\mu_{ij}}{2kT}\right)^{\frac{1}{2}} \mathbf{G}_{ij} = \left(\frac{\mu_{ij}}{2kT}\right)^{\frac{1}{2}} (\mathbf{g}_{ji} - \mathbf{g}_0). \quad (6.11)$$

Further, μ_{ij} is the reduced mass of the pair of colliding molecules, m_0 is the total mass of the pair, M_i and M_j are defined by

$$M_i = m_i/m_0 \quad \text{and} \quad M_j = m_j/m_0,$$

and $\mathbf{g}_0$ is defined by

$$\mathbf{g}_0 = (\omega_i \times \boldsymbol{\sigma}_i) - (\omega_j \times \boldsymbol{\sigma}_j).$$

We further define γ, the dimensionless relative velocity of the molecules:

$$\gamma = \left(\frac{\mu_{ij}}{2kT}\right)^{\frac{1}{2}} \mathbf{g}_{ji} = \left(\frac{\mu_{ij}}{2kT}\right)^{\frac{1}{2}} (\mathbf{V}_j - \mathbf{V}_i)$$

$$\gamma_0 = \left(\frac{\mu_{ij}}{2kT}\right)^{\frac{1}{2}} \mathbf{g}_0. \quad (6.12) \qquad \mathbf{k} \cdot \mathbf{\Gamma} = \mathbf{k} \cdot \gamma - \mathbf{k} \cdot \gamma_0. \quad (6.13)$$

In carrying out the integrations over linear velocities we find it convenient to change variables to the reduced relative velocity γ and the reduced velocity of the center of mass of the pair of colliding molecules,

$$\mathfrak{G} = \left(\frac{m_0}{2kT}\right)^{\frac{1}{2}} [M_i \mathbf{V}_i + M_j \mathbf{V}_j].$$

We further note that

$$\mathfrak{G}^2 + \gamma^2 = W_i^2 + W_j^2 = \epsilon_i^{t} + \epsilon_j^{t}.$$

As an example, we consider explicitly the evaluation of $[\mathbf{V}_i; \mathbf{V}_j]_{ij,lk}$ the bracket which contributes to the brace expressions leading to the diffusion coefficient. Similar integrals have been evaluated in the second paper in this series (reference 2). The symmetric form (see Appendix A) for this integral is

$$\frac{-1}{2n_{i,l}{}^{*} n_{j,k}{}^{*}} \int (\mathbf{V}_i' - \mathbf{V}_i) \cdot (\mathbf{V}_j' - \mathbf{V}_j) \mathbf{k} \cdot \mathbf{g}_{ji} f_{i,l}^{0} f_{j,k}^{0} S(\mathbf{k}) d\mathbf{k} d\mathbf{v}_i d\omega_i d\mathbf{v}_j d\omega_j.$$

We introduce Γ for $\mathfrak{g}_{ji}$ (6.11) and (3.1) for the equilibrium distribution functions, changing variables of integration from $\mathbf{v}_i$, ω_i, $\mathbf{v}_j$, and ω_j to $\mathfrak{G}$, γ, $\mathbf{w}_i$, and $\mathbf{w}_j$. Making the appropriate substitutions for the primed variables in terms of the unprimed variables, we find after integrating over $\mathfrak{G}$ that

$$[\mathbf{V}_i;\mathbf{V}_j]_{ij,lk}=\frac{2(2kT)^{3/2}}{(m_im_jm_0)^{\frac{1}{2}}\pi^{9/2}}\int\xi^2(J_{30}{}^0-3J_{21}{}^0+3J_{12}{}^0-J_{03}{}^0)\,S(\mathbf{k})d\mathbf{k}. \tag{6.14}$$

In (6.14) we have introduced the $J_{\nu\nu'}{}^{\zeta}$ integrals, which are defined by:

$$J_{\nu\nu'}{}^{\zeta}=\int(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}(\gamma^2)^{\zeta}\times\exp(-\gamma^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,d\gamma d\mathbf{w}_id\mathbf{w}_j.$$

For simplicity we have dropped the two species indices and the two orientation space cell indices from $J_{\nu\nu'}{}^0$ (and from ξ). In this theory we meet $J_{\nu\nu'}{}^{\zeta}$ for $\zeta=0$, 1, and 2. Integration over two components of γ reveals

$$J_{\nu\nu'}{}^1=J_{\nu\nu'}{}^0+J_{(\nu+2)\nu'}{}^0,$$

$$J_{\nu\nu'}{}^2=2J_{\nu\nu'}{}^0+2J_{(\nu+2)\nu'}{}^0+J_{(\nu+4)\nu'}{}^0,$$

$$J_{\nu\nu'}{}^0=\pi\int d\mathbf{w}_id\mathbf{w}_j\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}dx\,x^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}\times\exp(-x^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r).$$

We see, therefore, that we need consider the integration of only $J_{\nu\nu'}{}^0$. To this end, we change variables in a manner similar to that of the second paper in the series (reference 2), *viz.*, to $\epsilon_{i,l}{}^r$, $\epsilon_{j,k}{}^r$, $\gamma_0{}^{i,l}$, $\gamma_0{}^{j,k}$, $\varphi^{i,l}$, and $\varphi^{j,k}$. After integrating over $\epsilon_{i,l}{}^r$, $\epsilon_{j,k}{}^r$, $\varphi^{i,l}$, and $\varphi^{j,k}$ we find

$$J_{\nu\nu'}{}^0=\frac{\pi^3}{\eta_{i,l}\eta_{j,k}}\int d\gamma_0{}^{i,l}d\gamma_0{}^{j,k}\int_{-\infty}^{\mathbf{k}\cdot\gamma_0}dx\,x^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}\times\exp\left[-x^2-\left(\frac{\gamma_0{}^{i,l}}{\eta_{i,l}}\right)^2-\left(\frac{\gamma_0{}^{j,k}}{\eta_{j,k}}\right)^2\right],$$

where

$$\eta_{i,l}{}^2=\Gamma_i{}^{\frac{1}{3}}(\mathfrak{d}_{i,l}\times\mathbf{k})\cdot\mathbf{I}_i{}^{-1}\cdot(\mathfrak{d}_{i,l}\times\mathbf{k}).$$

To continue the reduction of $J_{\nu\nu'}{}^0$ we define $\eta_{ij,lk}$ by:

$$\eta_{ij,lk}{}^2=\mu_{ij}\left(\frac{\eta_{i,l}{}^2}{\Gamma_i{}^{\frac{1}{3}}}+\frac{\eta_{j,k}{}^2}{\Gamma_j{}^{\frac{1}{3}}}\right)=\xi_{ij,lk}{}^{-1}-1. \tag{6.15}$$

We easily find expressions for $\mathbf{k}\cdot\gamma_0$ and $\omega_i\cdot(\mathfrak{d}_{i,l}\times\mathbf{k})$ in terms of $\gamma_0{}^{i,l}$ (see reference 2).

We next change variables to v and u defined by

$$v=\frac{\Gamma_i{}^{1/6}\gamma_0{}^{i,l}\eta_{j,k}{}^2+\Gamma_j{}^{1/6}\gamma_0{}^{j,k}\eta_{i,l}{}^2}{\eta_{i,l}\eta_{j,k}(\Gamma_j{}^{\frac{1}{3}}\eta_{i,l}{}^2+\Gamma_i{}^{\frac{1}{3}}\eta_{j,k}{}^2)}$$

and

$$\eta_{ij,lk}u=\mathbf{k}\cdot\gamma_0.$$

After making the substitutions and integrating over v we make a final change of variables from x and u to r and θ of plane polar coordinates. Thus we finally obtain

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

where

$$\Lambda_{\nu\nu'}=\int_{\theta_0}^{\theta_0+\pi}d\theta\cos^{\nu}\theta\sin^{\nu'}\theta$$

and $\sin^2\theta_0=\xi_{ij,lk}$. Integration of $\Lambda_{\nu\nu'}$ is trivial and $J_{\nu\nu'}{}^0$ for the ν and ν' values relevant to this theory are given in terms of $\xi_{ij,lk}$ in Appendix A of reference 2. Thus we find

$$[\mathbf{V}_i;\mathbf{V}_j]_{ij,lk}=\frac{-(2kT)^{\frac{1}{2}}}{\mu_{ij}{}^{\frac{1}{2}}m_0\pi^{\frac{1}{2}}}\int\xi_{ij,lk}{}^{\frac{1}{2}}S(\mathbf{k})d\mathbf{k}. \tag{6.16}$$

In evaluating brackets and parentheses for other transport coefficients we meet, instead of $J_{\nu\nu'}{}^0$, linear combinations of $J_{\nu\nu'}{}^0$ and the following integrals:

$$K_{\nu\nu'}{}^{\zeta}=\int(\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}(\gamma^2)^{\zeta}\times\exp(-\gamma^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,d\gamma d\mathbf{w}_id\mathbf{w}_j,$$

$$L_{\nu\nu'}{}^{\zeta}=\int(3-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}(\gamma^2)^{\zeta}\times\exp(-\gamma^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,d\gamma d\mathbf{w}_id\mathbf{w}_j,$$

$$M_{\nu\nu'}{}^{\zeta}=\left(\frac{2\mu_{ij}}{kT}\right)^{\frac{1}{2}}\int(\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,\omega_i\cdot(\mathfrak{d}_{i,l}\times\mathbf{k})\times(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}(\gamma^2)^{\zeta}\exp(-\gamma^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,d\gamma d\mathbf{w}_id\mathbf{w}_j,$$

$$N_{\nu\nu'}{}^{\zeta}=\left(\frac{2\mu_{ij}}{kT}\right)^{\frac{1}{2}}\int(3-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,\omega_i\cdot(\mathfrak{d}_{i,l}\times\mathbf{k})(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}(\gamma^2)^{\zeta}\times\exp(-\gamma^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,d\gamma d\mathbf{w}_id\mathbf{w}_j,$$

$$P_{\nu\nu'}{}^{\zeta}=\int(\tfrac{3}{2}-\epsilon_{i,l}{}^r)(\tfrac{3}{2}-\epsilon_{j,k}{}^r)(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}(\gamma^2)^{\zeta}\times\exp(-\gamma^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,d\gamma d\mathbf{w}_id\mathbf{w}_j$$

$$Q_{\nu\nu'}{}^{\zeta}=\int(\tfrac{3}{2}-\epsilon_{i,l}{}^r)^2(\mathbf{k}\cdot\gamma)^{\nu}(\mathbf{k}\cdot\gamma_0)^{\nu'}(\gamma^2)^{\zeta}\times\exp(-\gamma^2-\epsilon_{i,l}{}^r-\epsilon_{j,k}{}^r)\,d\gamma d\mathbf{w}_id\mathbf{w}_j.$$

We find that these integrals can be reduced to combinations of the same integrals with $\zeta=0$ according to the recursion relations given earlier in this section for $J_{\nu\nu'}{}^{\zeta}$. The integrations are carried out by the same procedure used for $J_{\nu\nu'}{}^0$, and we ultimately find that these integrals can be expressed in terms of $J_{\nu\nu'}{}^0$:

$$K_{\nu\nu'}{}^0=\frac{\Gamma_i{}^{\frac{1}{3}}\eta_{j,k}{}^2-\Gamma_j{}^{\frac{1}{3}}\eta_{i,l}{}^2}{\Gamma_j{}^{\frac{1}{3}}\eta_{i,l}{}^2+\Gamma_i{}^{\frac{1}{3}}\eta_{j,k}{}^2}L_{\nu\nu'}{}^0,$$

$$L_{\nu\nu'}{}^0=\tfrac{1}{2}J_{\nu\nu'}{}^0-\frac{1}{\eta_{ij,lk}{}^2}J_{\nu(\nu'+2)}{}^0,$$

$$M_{\nu\nu'}{}^0=\frac{\mu_{ij}\eta_{i,l}{}^2}{\Gamma_i{}^{2/3}\Gamma_j{}^{1/3}\eta_{ij,lk}{}^4}\left\{\begin{array}{l}(5\Gamma_i{}^{\frac{1}{3}}\eta_{j,k}{}^2-\Gamma_j{}^{\frac{1}{3}}\eta_{i,l}{}^2)\,J_{\nu(\nu'+1)}{}^0+\\ \dfrac{2}{\eta_{ij,lk}{}^2}(\Gamma_j{}^{\frac{1}{3}}\eta_{i,l}{}^2-\Gamma_i{}^{\frac{1}{3}}\eta_{j,k}{}^2)\,J_{\nu(\nu'+3)}{}^0\end{array}\right\},$$

$$N_{\nu\nu'}{}^0=\frac{\mu_{ij}\eta_{i,l}{}^2}{\Gamma_i{}^{\frac{1}{3}}\eta_{ij,lk}{}^2}\left(J_{\nu(\nu'+1)}{}^0-\frac{2}{\eta_{ij,lk}{}^2}J_{\nu(\nu'+3)}{}^0\right),$$

$$P_{\nu\nu'}{}^0=\frac{\mu_{ij}{}^2\eta_{i,l}{}^2\eta_{j,k}{}^2}{(\Gamma_i\Gamma_j)^{\frac{1}{3}}\eta_{ij,lk}{}^4}\left(\tfrac{3}{4}J_{\nu\nu'}{}^0+\frac{1}{\eta_{ij,lk}{}^4}J_{\nu(\nu'+4)}{}^0\right)+\frac{J_{\nu(\nu'+2)}{}^0}{\eta_{ij,lk}{}^2}\left\{-\tfrac{1}{2}+\frac{\mu_{ij}{}^2}{\eta_{ij,lk}{}^4(\Gamma_i\Gamma_j)^{\frac{1}{3}}}\left[\tfrac{1}{2}(\Gamma_j{}^{\frac{1}{3}}\eta_{i,l}{}^2-\Gamma_i{}^{\frac{1}{3}}\eta_{j,k}{}^2)-(\Gamma_i\Gamma_j)^{\frac{1}{3}}\eta_{i,l}{}^2\eta_{j,k}{}^2\right]\right\},$$

$$Q_{\nu\nu'}{}^0=\left(\frac{5}{4}-\frac{\mu_{ij}\eta_{j,k}{}^2}{2\Gamma_j{}^{\frac{1}{3}}\eta_{ij,lk}{}^2}+\frac{3}{4}\frac{\mu_{ij}{}^2\eta_{j,k}{}^4}{\Gamma_j{}^{\frac{2}{3}}\eta_{ij,lk}{}^4}\right)J_{\nu\nu'}{}^0+\frac{J_{\nu(\nu'+2)}{}^0}{\eta_{ij,lk}{}^2}\left(-\frac{\mu_{ij}\eta_{i,l}{}^2}{\eta_{ij,lk}{}^2\Gamma_i{}^{\frac{1}{3}}}+3\frac{\mu_{ij}{}^2\eta_{i,l}{}^2\eta_{j,k}{}^2}{(\Gamma_i\Gamma_j)^{\frac{1}{3}}\eta_{ij,lk}{}^4}\right)+\frac{\mu_{ij}{}^2\eta_{i,l}{}^4}{\Gamma_i{}^{\frac{2}{3}}\eta_{ij,lk}{}^8}J_{\nu(\nu'+4)}{}^0.$$

In evaluating $M_{\nu\nu'}{}^{0}$ and $N_{\nu\nu'}{}^{0}$ with the indices i and j interchanged, we must remember that this permutation changes the sign of $\mathbf{k}$; therefore, we change the sign of the integrand. The other integrals are symmetric with respect to a permutation of i and j.

Thus we have reduced the brackets and parentheses to twofold integrals over $\mathbf{k}$.

We proceed to evaluate the brace expressions. These now involve integrals over two orientations and over $\mathbf{k}$.

We define the following integrals

$$\mathcal{A}_{ij}(\zeta)=\frac{1}{64\pi^4}\int \xi_{ij}{}^{\zeta/2}S(\mathbf{k})\ \sin\beta_i \sin\beta_j d\mathbf{k}\, d\alpha_i d\alpha_j, \qquad (6.17)$$

$$\mathcal{B}_{ij}(\zeta)=\frac{1}{64\pi^4}\int \frac{\mu_{ij}\eta_i{}^2}{\Gamma_i{}^{\frac{1}{2}}}\xi_{ij}{}^{\zeta/2}S(\mathbf{k})\ \sin\beta_i \sin\beta_j d\mathbf{k}\, d\alpha_i d\alpha_j, \qquad (6.18)$$

$$\mathcal{C}_{ij}(\zeta)=\frac{1}{64\pi^4}\int \frac{\mu_{ij}{}^2\eta_i{}^2\eta_j{}^2}{(\Gamma_i\Gamma_j)^{\frac{1}{2}}}\xi_{ij}{}^{\zeta/2}S(\mathbf{k})\ \sin\beta_i \sin\beta_j d\mathbf{k}\, d\alpha_i d\alpha_j, \qquad (6.19)$$

noting that $\mathcal{A}_{ij}(\zeta)$ and $\mathcal{C}_{ij}(\zeta)$ are symmetric with respect to a permutation of i and j and that

$$\mathcal{B}_{ij}(\zeta)+\mathcal{B}_{ji}(\zeta)=\mathcal{A}_{ij}(\zeta-2)-\mathcal{A}_{ij}(\zeta).$$

From the definitions of the brace integrals (5.2), the previous results, and the definitions (6.17) through (6.19) we find that

$$\{\mathrm{W}_i;\mathrm{W}_j\}_{ij}=-\frac{4n_iM_iM_j\epsilon}{3n_j}\mathcal{A}_{ij}(3),$$

$$\{\mathrm{W}_i;\mathrm{W}_i\}_{ii}=-\frac{4\epsilon}{3}\left\{\frac{1}{2}\left(\frac{\mu_{ij}}{\mu_{ii}}\right)^{\frac{1}{2}}[\mathcal{A}_{ii}(3)-\tfrac{5}{2}\mathcal{A}_{ii}(1)]+\frac{n_jM_j}{n_i}[M_j\mathcal{A}_{ij}(3)-\tfrac{5}{2}\mathcal{A}_{ij}(1)]\right\},$$

$$\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{t})\}_{ij}=-\frac{2n_iM_iM_j\epsilon}{n_j}\mathcal{A}_{ij}(3),$$

$$\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t})\}_{ii}=2\epsilon\left\{\left(\frac{\mu_{ij}}{\mu_{ii}}\right)^{\frac{1}{2}}\mathcal{B}_{ii}(3)+\frac{n_j}{n_i}M_iM_j\mathcal{A}_{ij}(3)+\frac{n_jM_j}{n_i}[\mathcal{B}_{ij}(3)+\mathcal{B}_{ji}(3)]\right\},$$

$$\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{t})\}_{ij}=-\frac{2n_iM_i\epsilon}{n_j}\mathcal{B}_{ij}(3),$$

$$\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t})\}_{ii}=\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r})\}_{ii}=-2\epsilon\left[\left(\frac{\mu_{ij}}{\mu_{ii}}\right)^{\frac{1}{2}}\mathcal{B}_{ii}(3)+\frac{n_jM_j}{n_i}\mathcal{B}_{ij}(3)\right],$$

$$\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{r})\}_{ij}=-\frac{2n_iM_j\epsilon}{n_j}\mathcal{B}_{ji}(3),$$

$$\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{r})\}_{ij}=-\frac{2n_i\epsilon}{n_j}\mathcal{C}_{ij}(3),$$

$$\{S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r})\}_{ii}=2\epsilon\left\{\left(\frac{\mu_{ij}}{\mu_{ii}}\right)^{\frac{1}{2}}\mathcal{B}_{ii}(3)+\frac{n_j}{n_i}[\mathcal{B}_{ij}(3)+\mathcal{C}_{ij}(3)]\right\},$$

$$\{\mathrm{V}_i;\mathrm{V}_i\}_{ii}=\frac{n_jM_j\epsilon'}{n_iM_i}\mathcal{A}_{ij}(1),\quad \{\mathrm{V}_i;\mathrm{V}_j\}_{ij}=-\frac{n_i\epsilon'}{n_j}\mathcal{A}_{ij}(1)$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});\mathrm{V}_j\}_{ij}=\frac{M_j}{M_i}\{\mathrm{V}_i;S_{\frac{1}{2}}^{1}(\epsilon_j{}^{t})\mathrm{V}_j\}_{ij}=\frac{n_iM_j\epsilon'}{2n_j}\mathcal{A}_{ij}(3),$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});\mathrm{V}_i\}_{ii}=\{\mathrm{V}_i;S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t})\mathrm{V}_i\}_{ii}=\frac{n_jM_j{}^2\epsilon'}{2n_iM_i}\mathcal{A}_{ij}(3),$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});\mathrm{V}_j\}_{ij}=\frac{n_i\epsilon'}{2n_j}\mathcal{B}_{ij}(3),$$

$$\{\mathrm{V}_i;S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r})\mathrm{V}_i\}_{ii}=\frac{M_i}{M_j}\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});\mathrm{V}_i\}_{ii}=-\frac{n_j\epsilon'}{n_i}\mathcal{B}_{ij}(3),$$

$$\{\mathrm{V}_i;S_{\frac{1}{2}}^{1}(\epsilon_j{}^{r})\mathrm{V}_j\}_{ij}=\frac{n_i\epsilon'}{2n_j}\mathcal{B}_{ji}(3),$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{t})\mathrm{V}_j\}_{ij}=-\frac{27n_iM_i\epsilon'}{4n_j}\mathcal{B}_{ij}(5),$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t})\mathrm{V}_i\}_{ii}=\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r})\mathrm{V}_i\}_{ii}$$
$$=\epsilon'\left\{\frac{n_jM_j{}^{\frac{1}{2}}}{n_iM_i{}^{\frac{1}{2}}}\left[\frac{27}{4}M_j\mathcal{B}_{ij}(5)-5\mathcal{B}_{ij}(3)\right]-\frac{5}{2M_i}\left(\frac{\mu_{ij}}{\mu_{ii}}\right)^{\frac{1}{2}}\mathcal{B}_{ii}(3)\right\},$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{r})\mathrm{V}_j\}_{ij}=-\frac{27n_iM_j\epsilon'}{4n_j}\mathcal{B}_{ji}(5),$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{t})\mathrm{V}_j\}_{ij}=-\frac{27n_iM_iM_j\epsilon'}{4n_j}\mathcal{A}_{ij}(5),$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{t});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{t})\mathrm{V}_i\}_{ii}$$
$$=\frac{\epsilon'}{M_i}\left\{\left(\frac{\mu_{ij}}{\mu_{ii}}\right)^{\frac{1}{2}}[\tfrac{15}{4}\mathcal{A}_{ii}(1)-\tfrac{11}{4}\mathcal{A}_{ii}(3)]+\frac{n_jM_j}{n_i}[\tfrac{27}{4}M_j{}^2\mathcal{A}_{ij}(5)-11M_j\mathcal{A}_{ij}(3)+\tfrac{15}{2}\mathcal{A}_{ij}(1)]\right\},$$

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_j{}^{r})\mathrm{V}_j\}_{ij}=-\frac{27n_i\epsilon'}{4n_j}\mathcal{C}_{ij}(5),$$

and

$$\{\mathrm{V}_iS_{\frac{1}{2}}^{1}(\epsilon_i{}^{r});S_{\frac{1}{2}}^{1}(\epsilon_i{}^{r})\mathrm{V}_i\}_{ii}$$
$$=\frac{\epsilon'}{M_i}\left\{\left(\frac{\mu_{ij}}{\mu_{ii}}\right)^{\frac{1}{2}}[\tfrac{3}{4}\mathcal{A}_{ii}(1)+\tfrac{35}{8}\mathcal{B}_{ii}(3)-\tfrac{27}{8}\mathcal{B}_{ii}(5)+3\mathcal{C}_{ii}(3)-\tfrac{27}{4}\mathcal{C}_{ii}(5)]+\frac{n_j}{n_i}\left[\frac{3M_j}{2}\mathcal{A}_{ij}(1)+(3M_i+\tfrac{23}{4}M_j)\mathcal{B}_{ij}(3)-\tfrac{27}{4}M_j\mathcal{B}_{ij}(5)+3\mathcal{C}_{ij}(3)-\tfrac{27}{4}M_j\mathcal{C}_{ij}(5)\right]\right\}.$$

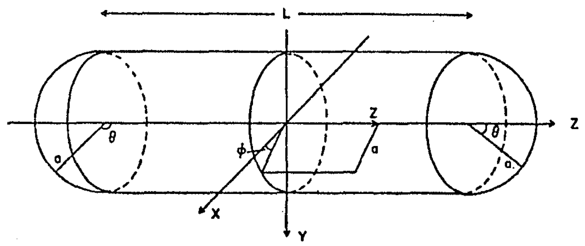
$$\epsilon=\left(\frac{2kT}{\pi\mu_{ij}}\right)^{\frac{1}{2}}\qquad \epsilon'=\frac{(2kT)^{\frac{1}{2}}}{m_0(\pi\mu_{ij})^{\frac{1}{2}}}.$$

Integration of $\mathcal{A}_{ij}(\zeta)$, $\mathcal{B}_{ij}(\zeta)$, and $\mathcal{C}_{ij}(\zeta)$ is carried out as outlined in reference 2; we obtain from (6.17):

$$\mathcal{A}_{ij}(\zeta)=\frac{1}{4\pi}\int \xi_{ij}{}^{\frac{1}{2}}\left[\frac{1}{q_1{}^iq_2{}^i}+\frac{1}{{}_1q^jq_2{}^j}+\frac{1}{2}\left(\frac{1}{q_1{}^i}+\frac{1}{q_2{}^i}\right)\left(\frac{1}{q_1{}^j}+\frac{1}{q_2{}^j}\right)\right]\times dS_idS_j, \qquad (6.20)$$

where dS_i and dS_j are elements of the surfaces of molecules i and j and $q_\lambda{}^i(\lambda=1$, or $2)$ are the two principal radii of curvature of the surface of molecule i. The integrals $\mathcal{B}_{ij}(\zeta)$ and $\mathcal{C}_{ij}(\zeta)$ have the same form as (6.20), differing only by the inclusion of factors $\mu_{ij}\eta_i{}^2/\Gamma_i{}^{\frac{1}{2}}$ and $\mu_{ij}{}^2\eta_i{}^2\eta_j{}^2/(\Gamma_i\Gamma_j)^{\frac{1}{2}}$, respectively, in the integrand.

4. THE SPHEROCYLINDICAL MODEL



cylinder is of length L_i and radius a_i. A point on the cylinder is described by the coordinate z_i and the azimuthal angle φ_i. A point on the hemispherical caps is described by the polar angle θ_i and the azimuthal angle. Thus we find

$$(\sigma_i\times\mathbf{k})=(-z_i\sin\theta_i,\ z_i\cos\varphi_i,\ 0)$$

on the cylinder and

$$(\sigma_i\times\mathbf{k})=\left(\mp\frac{L_i}{2}\sin\varphi_i\sin\theta_i,\ \pm\frac{L_i}{2}\cos\varphi_i\sin\theta_i,\ 0\right)$$

on the caps. Taking the symmetry axis to be a principal axis of the moment of inertia we find that

$$\frac{\mu_{ij}\eta_i^2}{\Gamma_i^{\frac12}}=\frac{4\alpha_i z_i^2}{L_i^2}\qquad\text{on the cylinder}$$

$$\frac{\mu_{ij}\eta_i^2}{\Gamma_i^{\frac12}}=\alpha_i\sin^2\theta_i\qquad\text{on the caps}$$

$$\alpha_i=\mu_{ij}L_i^2/4\Gamma_i$$

and Γ_i is the principal moment of inertia about an axis perpendicular to the symmetry axis. Furthermore, we find that the surface elements are

$$dS_i=a_i d\varphi_i dz_i$$

on the cylinder and

$$dS_i=a_i^2\sin\theta_i d\theta_i d\varphi_i$$

on the caps. Finally the principal radii of curvature of the surfaces are

$$q_1^{\ i}=a_i;\qquad q_2^{\ i}=\infty$$

on the cylinder and

$$q_1^{\ i}=q_2^{\ i}=a_i$$

on the caps.

Combining these results with the definitions of $\mathfrak{A}_{ij}(\zeta)$, $\mathfrak{B}_{ij}(\zeta)$, and $\mathfrak{C}_{ij}(\zeta)$ and integrating over φ_i and φ_j we find that these integrals can be expressed as the sum of four double integrals,

$$\mathfrak{A}_{ij}(\zeta)=\Theta_1^{\ \zeta}(ij)+\Theta_2^{\ \zeta}(ij)+\Theta_3^{\ \zeta}(ij)+\Theta_3^{\ \zeta}(ji),\quad(7.1)$$

$$\mathfrak{B}_{ij}(\zeta)=\Theta_4^{\ \zeta}(ij)+\Theta_5^{\ \zeta}(ij)+\Theta_6^{\ \zeta}(ij)+\Theta_7^{\ \zeta}(ij),\quad(7.2)$$

$$\mathfrak{C}_{ij}(\zeta)=\Theta_8^{\ \zeta}(ij)+\Theta_9^{\ \zeta}(ij)+\Theta_{10}^{\ \zeta}(ij)+\Theta_{10}^{\ \zeta}(ji).\quad(7.3)$$

$$A=4\pi(a_i+a_j)^2,\quad(7.4)$$

α_i, α_j, β_i, and β_j, where β_i is defined by

$$\beta_i=L_i/2a_i.\quad(7.5)$$

APPENDIX B. Θ INTEGRALS

$$\Theta_1^{\ 1}(12)=\tfrac18 A\beta_1\beta_2\left[\frac{1}{\alpha_2^{\frac12}}\sinh^{-1}\left(\frac{\alpha_2}{1+\alpha_1}\right)^{\frac12}+\frac{1}{\alpha_1^{\frac12}}\sinh^{-1}\left(\frac{\alpha_1}{1+\alpha_2}\right)^{\frac12}\right.$$
$$\left.-\frac{1}{(\alpha_1\alpha_2)^{\frac12}}\sin^{-1}\left(\frac{\alpha_1\alpha_2}{1+\alpha_1+\alpha_2+\alpha_1\alpha_2}\right)^{\frac12}\right],$$

$$\Theta_1^{\ 3}(12)=\tfrac18 A\beta_1\beta_2\left[\frac{1}{(\alpha_1\alpha_2)^{\frac12}}\sin^{-1}\left(\frac{\alpha_1\alpha_2}{1+\alpha_1+\alpha_2+\alpha_1\alpha_2}\right)^{\frac12}\right],$$

$$\Theta_1^{\ 5}(12)=\tfrac18 A\beta_1\beta_2\left[\frac{1}{3(\alpha_1\alpha_2)^{\frac12}}\sin^{-1}\left(\frac{\alpha_1\alpha_2}{1+\alpha_1+\alpha_2+\alpha_1\alpha_2}\right)^{\frac12}\right.$$
$$\left.+\frac{2+\alpha_1+\alpha_2}{3(1+\alpha_1+\alpha_2)^{\frac12}(1+\alpha_1+\alpha_2+\alpha_1\alpha_2)}\right],$$

$$\Theta_2^{\ 1}(12)=A\left[\frac{1}{\alpha_1^{\frac12}}\sinh^{-1}\left(\frac{\alpha_1}{1+\alpha_1}\right)^{\frac12}+\frac{1}{\alpha_2^{\frac12}}\sinh^{-1}\left(\frac{\alpha_2}{1+\alpha_2}\right)^{\frac12}\right.$$
$$\left.-\frac{(1+\alpha_1+\alpha_2)^{\frac12}}{(\alpha_1\alpha_2)^{\frac12}}\sin^{-1}\left(\frac{\alpha_1\alpha_2}{1+\alpha_1+\alpha_2+\alpha_1\alpha_2}\right)^{\frac12}\right]$$

$$\Theta_2^{\ 3}(12)=A\left[\frac{1}{(\alpha_1\alpha_2)^{\frac12}(1+\alpha_1+\alpha_2)^{\frac12}}\right.$$
$$\left.\times\sin^{-1}\left(\frac{\alpha_1\alpha_2}{1+\alpha_1+\alpha_2+\alpha_1\alpha_2}\right)^{\frac12}\right],$$

$$\Theta_2^{\ 5}(12)=A\left[\frac{2+\alpha_1+\alpha_2}{3(1+\alpha_1+\alpha_2)(1+\alpha_1+\alpha_2+\alpha_1\alpha_2)}\right.$$
$$\left.+\frac{1}{3(\alpha_1\alpha_2)^{\frac12}(1+\alpha_1+\alpha_2)^{\frac12}}\sin^{-1}\left(\frac{\alpha_1\alpha_2}{1+\alpha_1+\alpha_2+\alpha_1\alpha_2}\right)^{\frac12}\right],$$

$$\Theta_3^{\ 1}(12)=\tfrac12 A\beta_1\left[\frac{1}{\alpha_1^{\frac12}}\sinh^{-1}\alpha_1^{\frac12}+\frac{1}{\alpha_2^{\frac12}}\sin^{-1}\left(\frac{\alpha_2}{1+\alpha_1+\alpha_2}\right)^{\frac12}\right.$$
$$\left.-\tfrac12\left(\frac{1+\alpha_2}{\alpha_1\alpha_2}\right)^{\frac12}\ln\kappa(12)\right],$$

$$\kappa(12)=\frac{[(1+\alpha_1)^{\frac12}(1+\alpha_2)^{\frac12}+(\alpha_1\alpha_2)^{\frac12}]^2}{1+\alpha_1+\alpha_2},$$

$$\Theta_3^{\ 3}(12)=\tfrac12 A\beta_1\left[\frac{\ln\kappa(12)}{2(\alpha_1\alpha_2)^{\frac12}(1+\alpha_2)^{\frac12}}\right],$$

$$\Theta_3^{\ 5}(12)=\tfrac12 A\beta_1\left[\frac{2+\alpha_1+\alpha_2}{3(1+\alpha_1+\alpha_2)(1+\alpha_2)(1+\alpha_1)^{\frac12}}\right.$$
$$\left.+\frac{\ln\kappa(12)}{6(\alpha_1\alpha_2)^{\frac12}(1+\alpha_2)^{\frac12}}\right],$$

$$\Theta_4^{\ 3}(12)=\tfrac18 A\beta_1\beta_2\left[\frac{1}{\alpha_1^{\frac12}}\sinh^{-1}\left(\frac{\alpha_1}{1+\alpha_2}\right)^{\frac12}\right.$$
$$\left.-\frac{1}{(\alpha_1\alpha_2)^{\frac12}}\sin^{-1}\left(\frac{\alpha_1\alpha_2}{1+\alpha_1+\alpha_2+\alpha_1\alpha_2}\right)^{\frac12}\right],$$

$$\Theta_{10}^{\ 3}(12)=\tfrac12 A\beta_1\left[-\tfrac13(1+\alpha_1)^{\frac12}+\frac{\alpha_1}{3\alpha_2^{\frac12}}\sin^{-1}\left(\frac{\alpha_2}{1+\alpha_1+\alpha_2}\right)^{\frac12}\right.$$
$$\left.+\frac{2\alpha_2}{3\alpha_1^{\frac12}}\sinh^{-1}\alpha_1^{\frac12}+\frac{(1+\alpha_2)^{\frac12}(1-2\alpha_2)}{6(\alpha_1\alpha_2)^{\frac12}}\ln\kappa(12)\right],$$

$$\Theta_{10}^{\ 5}(12)=\tfrac12 A\beta_1\left[\frac{(1+\alpha_1)^{\frac12}}{3(1+\alpha_1+\alpha_2)}-\frac{\ln\kappa(12)}{6(\alpha_1\alpha_2)^{\frac12}(1+\alpha_2)^{\frac12}}\right].$$

Fig 1

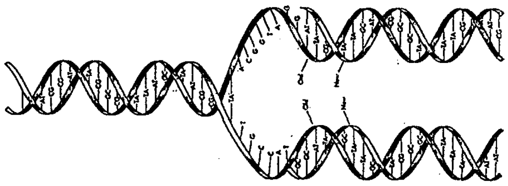


Fig 2

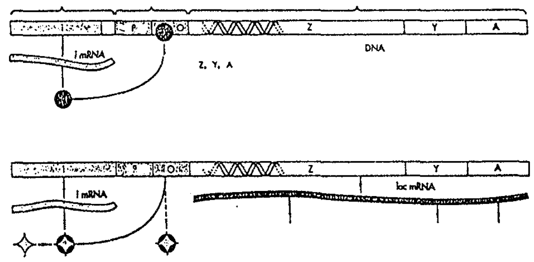


Fig 3

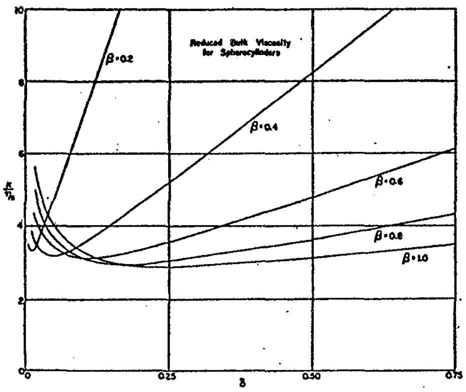


FIG. 3.

Fig 4

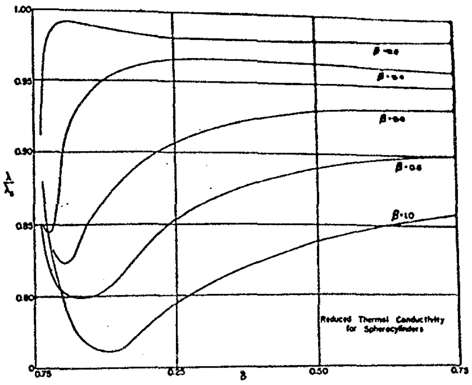


FIG. 4.

Fig 5

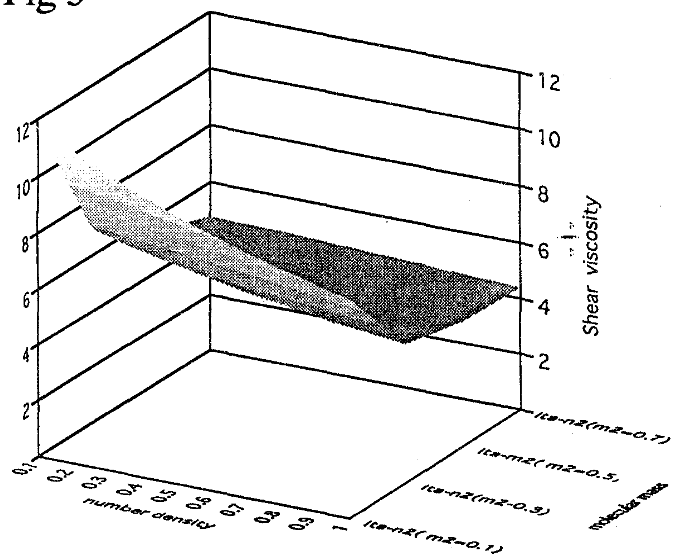
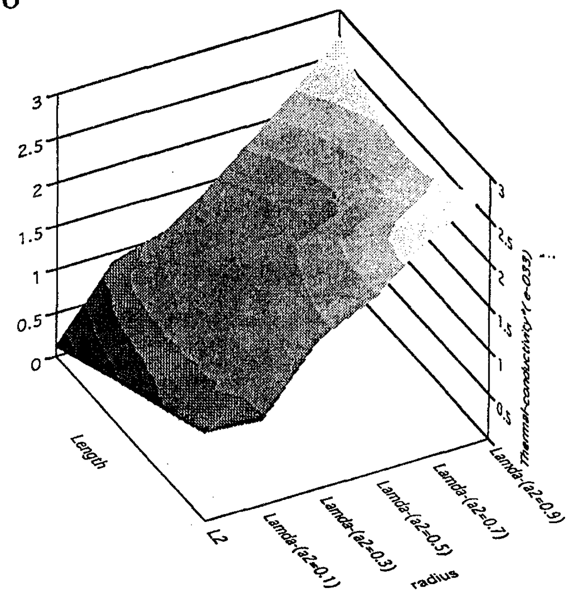


Fig 6



3. Results and Discussion.

Fig 1 shows double stranded DNA and Fig 2 shows diffusion of gene regulation protein particle to bind the operator region of the DNA. The lower part of Fig 2 shows the dissociation of the gene regulating particle. Fig 3 is the computed results by Curtis and Muckenfusss for the ratio between bulk viscosity κ to the shear viscosity η as a function of

$$\delta = \beta^2 (= L/(2a))^2/(2\alpha) = \Gamma/(m a^2)$$

where L is the length of cylindrical part of sphero cylindrical model, a is the radius of the spherical part. Γ is the moment of principle inertia. m is the mass. Fig 4 shows the ratio between the thermal conductivity of sphero cylindrical particle and rigid sphere one as a function of δ. In both of these figures, β was altered from 0.2 to 1.0.

Fig 5 shows three dimensional display of shear viscosity η as functions of number density and molecular mass. Fig 6 shows three dimensional display of thermal conductivity as functions of the length of the sphero cylindrical particle (denoted by length) and radius of the second particle (as the ratio to the first particle that changes from 0.9 to 0.1).

The preset investigation when extended will be available for evaluating the local physical potential field around the bio physical reaction field near the bases of genes,

6. References.

1. Curtiss , C,F and Muckenfuss,C. J. Chem. Physics. vol 26. pp 1619-1636. 1957.

2.Muckenfuss C and Curtiss CF. J. Chem. Physics. vol 29. pp 1257-1272. 1958.