Inverse Operator Technique for Treating Senftleben-Beenakker Effects without Using the Spherical Approximation

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The inverse operator technique used for the treatment of magnetic field influence on transport processes in polyatomic gases is extended to the case where the spherical approximation for the relaxation coefficient of $[W]^p\,[J]^q$ polarizations cannot be used. The general procedure is outlined and subsequently illustrated for the magnetic field influence on the heat conductivity.

1. Introduction

The inverse operator technique previously used by Kagan and Maksimov[1], Tip, Levi and McCourt[2], Coope and Snider[3] and Eggermont, Vestner and Knaap[4] is an effective and transparent method to treat transport properties in polyatomic gases under the influence of an external magnetic field[5]. In the papers mentioned it is assumed that a specified kind of rotational angular momentum polarization $\langle [W]^p\,[J]^q \rangle$ is responsible for the Senftleben-Beenakker effect [$\boldsymbol{W} = (m/2\,k_{\rm B}\,T)^{1/2}\,(\boldsymbol{c} - \langle \boldsymbol{c} \rangle)$ is the dimensionless peculiar velocity, $\boldsymbol{J}$ is the dimensionless operator for the rotational angular momentum, p and q are the ranks of the corresponding irreducible tensors $[W]^p$ and $[J]^q$ and the bracket $\langle \ldots \rangle$ means a nonequilibrium average]. From experiments[5] it is known that for almost all molecules the combination $p = 0$, $q = 2$ determines the field effect on the viscosity and $p = 1$, $q = 2$ the field effect on the heat conductivity. But for the field effect on viscosity of NH_3 there is also a strong $p = 2$, $q = 1$ contribution.

The Liouville operator $\mathcal{L} \equiv (1/n_0)\,\omega[\ ,\boldsymbol{h}\cdot\boldsymbol{J}]_-$ (n_0 is the number density, ω is the Larmor frequency and $\boldsymbol{h}$ is a unit vector in the direction of the magnetic field) which governs the free precessional motion of the molecular rotational angular momenta of linear diamagnetic non-polar molecules is diagonal with respect to a basis of expansion tensors written in spherical notation[5a], $[W]^p_m\,[J]^q_s$ (which may still be multiplied with polynomials in W^2 and J^2) with $-p \leqq m \leqq p$, $-s \leqq q \leqq s$ **:

$$n_0 \langle [W]^p_m [J]^q_s \mathcal{L} [W]^{p'}_{m'} [J]^{q'}_{s'} \rangle_0$$
$$= -\delta_{pp'}\,\delta_{qq'}\,\delta_{mm'}\,\delta_{ss'}\,s\,\omega\,[(2\,p+1)(2\,q+1)]^{-1} \cdot \langle [W]^p \odot [W]^p \rangle_0 \langle [J]^q \odot [J]^q \rangle_0 \,. \tag{1}$$

In Eq. (1), the bracket $\langle \ldots \rangle_0$ denotes an equilibrium average and the dot "$\odot$" denotes a contraction over all tensor indices. To simplify the calculations of the Senftleben-Beenakker effects, it is assumed in the papers mentioned above that matrix elements $\langle [W]^p_m [J]^q_s | R | [W]^p_{m'} [J]^q_{s'} \rangle_0$ of the linearized Waldmann-Snider collision operator[6, 7] are also proportional to $\delta_{mm'}\,\delta_{ss'}$. This is called the "spherical approximation" since it is valid for a purely spherical potential[8]. Thus the spherical approximation can be expected to work very well for molecules with small nonsphericity of their interaction, e. g. the hydrogen isotopic molecules, but it may be somewhat doubtful for all other molecules.

If the spherical approximation cannot be used, another basis set of expansion tensors is convenient, namely the totally irreducible $L^{\rm th}$ rank tensors

$$[[W]^p\,[J]^q]^L_M \equiv \sum_{ms} \sqrt{2\,L+1}\,(-1)^{p+q-M} \begin{pmatrix} p & q & L \\ m & s & -M \end{pmatrix} [W]^p_m [J]^q_s \,, \tag{2}$$

where $\left(\begin{smallmatrix} p & q & L \\ m & s & -M \end{smallmatrix}\right)$ is a $3\,j$-symbol. Because of rotational invariance, the collision operator is diagonal in L, M indices, i. e.

$$\langle [[W]^p\,[J]^q]^L_M\,R\,[[W]^{p'}\,[J]^{q'}]^{L'}_{M'} \rangle_0$$
$$= \delta_{LL'}\,\delta_{MM'}\,(2\,L+1)^{-1} \cdot \langle [[W]^p\,[J]^q]^L \odot R\,[[W]^{p'}\,[J]^{q'}]^L \rangle_0 \,. \tag{3}$$

But now the Liouville operator $\mathcal{L}$ is not diagonal with respect to L and, in general, it induces couplings between L-values which differ by 0, ±1. In

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** The z axis points in the direction of $\boldsymbol{h}$.

the following chapter it is shown how the inverse operator technique can be extended to this more general case. It should be mentioned, that the Senftleben-Beenakker effect of the heat conductivity without spherical approximation had already been treated by Tip[9] in 1967 with a different method.

2. Inverse Operator Technique

In Ref.[4] it has been shown that a tensorial transport coefficient in the dilute gas regime can be expressed as

$$\Lambda_{nn'} = \langle [Q]^l_n (R + i\,\mathcal{L})^{-1} [Q]^l_{n'} \rangle^*_0 , \tag{4}$$

with $[Q]^l_n$ being a spherical l^{th} rank tensor $(-l \leqq n, n' \leqq l)$ chosen according to the physical situation which is considered. For the viscosity tensor, e. g., one has $l = 2$ and $[Q]^2_n = \sqrt{2}\,[W]^2_n$ while for the heat conductivity tensor one has $l = 1$ and $[Q]^1_n = (2\,k_B{}^2\,T/m)^{1/2}\,[W]^1_n\,(W^2 - \frac{5}{2} + \varepsilon - \langle \varepsilon \rangle_0)$ (ε is the internal rotational energy divided by $k_B T$).

In the $1/R$ method[3, 4], the collision operator R is written as a sum $R = R_d + R_{nd}$ where R_{nd} exclusively couples tensors containing $[J]^q$ with $q \neq 0$ with tensors depending only on $\boldsymbol{W}$ and J^2, and where R_d accounts for all the other couplings. Defining $\tilde{R}_d$ as $R_d + i\,\mathcal{L}$, one expands now $(R + i\,\mathcal{L})^{-1}$ in powers of R_{nd} as follows:

$$(R + i\,\mathcal{L})^{-1} = \tilde{R}_d^{-1} - \tilde{R}_d^{-1} R_{nd}\,\tilde{R}_d^{-1} + \tilde{R}_d^{-1} R_{nd}\,\tilde{R}_d^{-1} R_{nd}\,\tilde{R}_d^{-1} + \dots \; . \tag{5}$$

One verifies easily that in $\Lambda_{nn'}$ the term independent of R_{nd} has no magnetic field dependence and that the term linear in R_{nd} vanishes. To look at the field dependence, only the contribution $\Lambda^{[2]}_{nn'}$ which is quadratic in R_{nd} has to be considered:

$$\Lambda^{[2]}_{nn'} = \langle [Q]^l_n\,\tilde{R}_d^{-1}\,R_{nd}\,\tilde{R}_d^{-1}\,R_{nd}\,\tilde{R}_d^{-1} [Q]^l_{n'} \rangle^*_0 . \tag{6}$$

Under the assumption that only one kind of angular momentum polarization $\Phi^{pq} \propto [W]^p\,[J]^q$ is important, one obtains

$$\begin{aligned}\Lambda^{[2]}_{nn'} = \sum_{\alpha\beta} \sum_{\substack{m\,m'\,m''\,m'''\\ s\,s'}} & \langle [Q]^l_n\,R_d^{-1}\,\Phi^{l(\alpha)}_m \rangle_0 \, \langle \Phi^{l(\alpha)}_m R_{nd}\,\Phi^{pq}_{m's} \rangle^*_0 \\ & \cdot \langle \Phi^{pq}_{m's}\,\tilde{R}_d^{-1}\,\Phi^{pq}_{m''s'} \rangle^*_0 \, \langle \Phi^{pq}_{m''s'}\,R_{nd}\,\Phi^{l(\beta)}_{m'''} \rangle^*_0 \\ & \cdot \langle \Phi^{l(\beta)}_{m'''}\,R_d^{-1} [Q]^l_{n'} \rangle_0 ,\end{aligned} \tag{7}$$

where α, β number different polynomials built up from W^2 and J^2. Eq. (7) is general and the essence now lies in the evaluation of $\langle \Phi^{pq}_{m's}\,\tilde{R}_d^{-1}\,\Phi^{pq}_{m''s'} \rangle_0$.

If one uses the spherical approximation, this evaluation is very easily done[4] and one obtains

$$\langle \Phi^{pq}_{m's}\,\tilde{R}_d^{-1}\,\Phi^{pq}_{m''s'} \rangle_0 \approx \delta_{m'm''}\,\delta_{ss'} \left(v_{\text{rel}}\,\mathfrak{S}\binom{pq}{pq}\,(1 - i\,s\,\omega\,\tau_{pq})\right)^{-1} , \tag{8}$$

where $v_{\text{rel}} \equiv (16\,k_B\,T/\pi\,m)^{1/2}$ is a thermal velocity and $\tau_{pq} \equiv [n_0\,v_{\text{rel}}\,\mathfrak{S}\binom{pq}{pq}]^{-1}$. Equation (8) can be considered to be also the definition of the cross section $\mathfrak{S}\binom{pq}{pq}$. Furthermore, due to the Wigner-Eckart Theorem, one can write[9a]

$$\begin{aligned}\langle \Phi^{l(\alpha)}_m R_{nd}\,\Phi^{pq}_{m's} \rangle_0 = {} & \sqrt{2\,q + 1}\,(-1)^{p+q+m} \\ & \cdot (-i)^{l-p-q} \begin{pmatrix} l & p & q \\ -m & m' & s \end{pmatrix} v_{\text{rel}}\,\mathfrak{S}\binom{\alpha}{pq}_l ,\end{aligned} \tag{9}$$

and one finally obtains for the field dependent part of the transport coefficient:

$$\begin{aligned}\Lambda^{[2]}_{nn'} = {} & \delta_{nn'}\,v_{\text{rel}} \frac{2\,q + 1}{(2\,l + 1)^2}\,\mathfrak{S}\binom{pq}{pq}^{-1} \\ & \cdot \sum_{\alpha\beta} \langle [Q]^l \odot R_d^{-1}\,\Phi^{l(\alpha)} \rangle_0 \, \langle \Phi^{l(\beta)} \odot R_d^{-1} [Q]^l \rangle_0 \\ & \cdot \mathfrak{S}\binom{\alpha}{pq}_l\,\mathfrak{S}\binom{pq}{\beta}_l \sum_{ms} \begin{pmatrix} l & p & q \\ -n & m & s \end{pmatrix}^2 (1 + i\,s\,\omega\,\tau_{pq})^{-1} .\end{aligned} \tag{10}$$

If one does not use the spherical approximation, one rather works with the coupling scheme

$$\Phi^{pq}_{ms} = \sum_{LM} \sqrt{2\,L + 1}\,(-1)^{p+q-M} \begin{pmatrix} p & q & L \\ m & s & -M \end{pmatrix} [\Phi^{pq}]^L_M . \tag{11}$$

Note that $|p - q| \leqq L, L' \leqq p + q$. With

$$\langle \Phi^{l(\alpha)}_m R_{nd} [\Phi^{pq}]^L_M \rangle_0 = (-i)^{l-p-q}\,v_{\text{rel}}\,\mathfrak{S}\binom{\alpha}{pq}_l\,\delta_{Ll}\,\delta_{Mm} \tag{12}$$

which may be considered as the equation defining the cross section $\overline{\mathfrak{S}}\binom{\alpha}{pq}_l$ one finds

$$\begin{aligned}\Lambda^{[2]}_{nn'} = {} & \delta_{nn'} \frac{v^2_{\text{rel}}}{(2\,l + 1)^2} \sum_{\alpha\beta} \langle [Q]^l \odot R_d^{-1}\,\Phi^{l(\alpha)} \rangle_0 \\ & \cdot \langle \Phi^{l(\beta)} \odot R_d^{-1} [Q]^l \rangle_0\,\overline{\mathfrak{S}}\binom{\alpha}{pq}_l\,\overline{\mathfrak{S}}\binom{pq}{\beta}_l\,\{\tilde{R}_d^{-1}\}^{*ll}_n ,\end{aligned} \tag{13}$$

where $\overline{\mathfrak{S}}\binom{\alpha}{pq}_l = [(2\,q + 1)/(2\,l + 1)]^{1/2}\,\mathfrak{S}\binom{\alpha}{pq}_l$ and where $\{\tilde{R}_d^{-1}\}^{ll}_n$ is the $l - l$-element of the matrix inverse to $\langle [\Phi^{pq}]^L_n\,\tilde{R}_d\,[\Phi^{pq}]^{L'}_n \rangle_0$. Thus the whole problem is reduced to the calculation of the matrix $\langle [\Phi^{pq}]^L_n\,\tilde{R}_d^{-1} [\Phi^{pq}]^{L'}_n \rangle_0$ and its inverse. Using Eqs. (11), (12) one finds immediately

$$\langle [\Phi^{pq}]^L_n (R_d + i\,\mathcal{L}) [\Phi^{pq}]^{L'}_n \rangle_0 = v_{\text{rel}}\,\overline{\mathfrak{S}}\binom{pq}{pq}_L [\delta^{LL'} - i\,\omega\,\tau_L(p\,q)\,F^{LL'}_n] , \tag{14}$$

where the $\overline{\mathfrak{S}}\binom{pq}{pq}_L$ are positive quantities defined analogously to the $\overline{\mathfrak{S}}\binom{\alpha}{pq}_L$ and where

$$\tau_L(p\,q) \equiv (n_0\,v_{\text{rel}}\,\overline{\mathfrak{S}}\binom{pq}{pq}_L)^{-1} . \tag{15}$$

The matrices $F_n^{LL'}(p\,q)$ are, with the help of Eq. (1), obtained as

$$F_n^{LL'}(p\,q) = [(2L+1)(2L'+1)]^{1/2} \cdot \sum_{mm'} \begin{pmatrix} p & q & L \\ m & m' & -n \end{pmatrix} m' \begin{pmatrix} p & q & L' \\ m & m' & -n \end{pmatrix} . \tag{16}$$

Observing the identity

$$m' = [(2q+1)\,q(q+1)]^{1/2}\,(-1)^{q+1-m'} \begin{pmatrix} q & 1 & q \\ m' & 0 & -m' \end{pmatrix}$$

and by using some Racah algebra, we can express the $F_n^{LL'}$ in terms of $6j$- and $3j$-symbols:

$$\begin{aligned} F_n^{LL'}(p\,q) &= (-1)^{p+q+L+L'} \\ &\cdot [(2L+1)(2L'+1)(2q+1)\,q(q+1)]^{1/2} \\ &\cdot (-1)^n \begin{pmatrix} L & L' & 1 \\ -n & n & 0 \end{pmatrix} \begin{Bmatrix} L & L' & 1 \\ q & q & p \end{Bmatrix} . \end{aligned} \tag{17}$$

Equation (17) shows that $L' = L,\ L \pm 1$ and that the following symmetries hold:

$$F_n^{LL'} = F_n^{L'L}\,; \quad F_{-n}^{LL'} = (-1)^{L+L'+1} F_n^{LL'} . \tag{18}$$

Equation (18) in particular implies $F_0^{LL} = 0$. Thus, for any p, q, the matrix $[\delta^{LL'} - i\,\omega\,\tau_L(p\,q)\,F_n^{LL'}]$ can easily be evaluated and, in order to get the field dependence of the transport coefficient $\Lambda_{nn}^{[2]}$, only one element of the inverse matrix has to be calculated. The scheme outlined in this chapter is general and can be applied to all polarizations of the $[W]^p\,[J]^q$ type. In the next section, as an example the Senftleben-Beenakker effect of the heat conductivity will be studied.

3. Example: Magnetic Field Influence on the Heat Conductivity

For the Senftleben-Beenakker effect of the heat conductivity usually the Kagan polarization

$$\Phi^{12} \propto \langle [W]^1\,[J]^2 \rangle$$

is taken as the decisive angular momentum polarization, i. e. $p = 1$, $q = 2$, $1 \leqq L,\ L' \leqq 3$. From Eq. (17) one calculates easily the $F_n^{LL'}(1,2)$ matrices for $n = 0,\ +1$:

$$F_0^{LL'}(1,2) \triangleq -\frac{1}{\sqrt{5}} \begin{pmatrix} 0 & \sqrt{3} & 0 \\ \sqrt{3} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix}, \tag{19}$$

$$F_1^{LL'}(1,2) \triangleq \begin{pmatrix} \dfrac{3}{2} & \dfrac{-3}{2\sqrt{5}} & 0 \\ \dfrac{-3}{2\sqrt{5}} & \dfrac{5}{6} & \dfrac{-4}{3\sqrt{5}} \\ 0 & \dfrac{-4}{3\sqrt{5}} & \dfrac{2}{3} \end{pmatrix} .$$

The $1-1$-element of $\{\tilde{R}_d^{-1}\}_0$ is then obtained as

$$\{R_d^{-1}\}_0^{11} = [v_{\text{rel}}\,\overline{\mathfrak{S}}\left(\begin{smallmatrix}12\\12\end{smallmatrix}\right)_1]^{-1} \frac{1 + \frac{2}{5}\,\omega^2\,\tau_2\,\tau_3}{1 + \frac{2}{5}\,\omega^2\,\tau_2\,\tau_3 + \frac{3}{5}\,\omega^2\,\tau_1\,\tau_2}, \tag{20}$$

where $\tau_{\text{L}} \equiv \tau_{\text{L}}(1,2)$.

The relative change of the heat conductivity parallel to the magnetic field, $\Delta\lambda^{\|}/\lambda = \Delta\lambda_{00}^{[2]}/\lambda$ is then, according to Eq. (13), given by $(\Lambda_{nn} \equiv \lambda_{nn})$

$$\frac{\Delta\lambda^{\|}}{\lambda} = -2\,\Psi_{12} \frac{\omega^2\,\tau_1\,\tau_2}{1 + \frac{2}{5}\,\omega^2\,\tau_2\,\tau_3 + \frac{3}{5}\,\omega^2\,\tau_1\,\tau_2} . \tag{21}$$

The quantity

$$\begin{aligned} \Psi_{12} = (v_{\text{rel}}/10)\,\langle \mathbf{Q} \cdot R_d^{-1}\,\mathbf{Q} \rangle_0^{-1} \sum_{\alpha\beta} \langle \mathbf{Q} \cdot R_d^{-1} \boldsymbol{\Phi}^{(\alpha)} \rangle_0 \\ \cdot \langle \boldsymbol{\Phi}^{(\beta)} \cdot R_d^{-1}\,\mathbf{Q} \rangle_0\,\overline{\mathfrak{S}}\left(\begin{smallmatrix}\alpha\\12\end{smallmatrix}\right)_1 \overline{\mathfrak{S}}\left(\begin{smallmatrix}12\\\beta\end{smallmatrix}\right)_1 / \overline{\mathfrak{S}}\left(\begin{smallmatrix}12\\12\end{smallmatrix}\right)_1 \end{aligned} \tag{22}$$

($\boldsymbol{\Phi}^{(\alpha)}$ being the normalized translational and rotational heat flux, respectively) determines the magnitude of the Senftleben-Beenakker effect. In spherical approximation, one has $\tau_1 = \tau_2 = \tau_3 \equiv \tau$ and the well-known result [10, 12]

$$\frac{\Delta\lambda^{\|}}{\lambda} = -2\,\Psi_{12} \frac{\omega^2\,\tau^2}{1 + \omega^2\,\tau^2} \tag{23}$$

is recovered. Similarly one finds for $n = \pm 1$:

$$\begin{aligned} \{\tilde{R}_d^{-1}\}_1^{11} &= \{\tilde{R}_d^{-1}\}_{-1}^{11*} = (v_{\text{rel}}\,\overline{\mathfrak{S}}\left(\begin{smallmatrix}12\\12\end{smallmatrix}\right)_1)^{-1} \\ &\cdot [1 - \tfrac{1}{5}\omega^2\,\tau_2\,\tau_3 - i\,\omega\,(\tfrac{5}{6}\,\tau_2 + \tfrac{2}{3}\,\tau_3)] \\ &\cdot [1 - \tfrac{4}{5}\,\omega^2\,\tau_1\,\tau_2 - \omega^2\,\tau_1\,\tau_3 - \tfrac{1}{5}\,\omega^2\,\tau_2\,\tau_3 \\ &\quad - i\,\omega\,(\tfrac{3}{2}\,\tau_1 + \tfrac{5}{6}\,\tau_2 + \tfrac{2}{3}\,\tau_3)]^{-1} . \end{aligned} \tag{24}$$

Thus the relative change of the heat conductivity perpendicular to the magnetic field, $\Delta\lambda^{\perp}/\lambda = \text{Re}\,\Delta[\lambda_{11}^{[2]}/\lambda]$ is given by

$$\begin{aligned} \frac{\Delta\lambda^{\perp}}{\lambda} &= \tfrac{10}{3}\,\Psi_{12}\,\omega^2\,\tau_1\,[(1 - \omega^2\,(\tfrac{4}{5}\,\tau_1\,\tau_2 + \tau_1\,\tau_3 + \tfrac{1}{5}\tau_2\,\tau_3)) \\ &\cdot (\tfrac{4}{5}\tau_2 + \tau_3) - (\tfrac{9}{4}\,\tau_1 + \tfrac{5}{4}\,\tau_2 + \tau_3)] \\ &\cdot [(1 - \omega^2\,(\tfrac{4}{5}\,\tau_1\,\tau_2 + \tau_1\,\tau_3 + \tfrac{1}{5}\tau_2\,\tau_3))^2 \\ &+ \omega^2\,(\tfrac{3}{2}\tau_1 + \tfrac{5}{6}\,\tau_2 + \tfrac{2}{3}\,\tau_3)^2]^{-1} . \end{aligned} \tag{25}$$

In spherical approximation Eq. (25) reduces to

$$\left(\frac{\Delta\lambda^{\perp}}{\lambda}\right) = -\Psi_{12} \left(\frac{\omega^2\,\tau^2}{1 + \omega^2\,\tau^2} + 2\,\frac{4\,\omega^2\,\tau^2}{1 + 4\,\omega^2\,\tau^2}\right) \tag{26}$$

in agreement with well-known results [10]. For the saturation value of the ratio $\Delta\lambda^{\perp}/\Delta\lambda^{\|}$ one infers from Eqs. (21), (25):

$$\left(\frac{\Delta\lambda^{\perp}}{\Delta\lambda^{\|}}\right)_{\text{sat}} = \frac{1}{3}\,\frac{(4\,\tau_2 + 5\,\tau_3)\,(2\,\tau_3 + 3\,\tau_1)}{4\,\tau_1\,\tau_2 + 5\,\tau_1\,\tau_3 + \tau_2\,\tau_3}, \tag{27}$$

which, in spherical approximation, yields the value of $\frac{3}{2}$.

Finally, the transverse coefficient $\lambda^{\text{tr}}/\lambda = -\text{Im}\,[\lambda_{11}^{[2]}/\lambda]$ is found as

$$\begin{aligned} \frac{\lambda^{\text{tr}}}{\lambda} &= -\tfrac{5}{9}\,\Psi_{12}\,\omega[(1 - \tfrac{1}{5}\,\omega^2\,\tau_2\,\tau_3)\,(9\,\tau_1 + 5\,\tau_2 + 4\,\tau_3) \\ &- (5\,\tau_2 + 4\,\tau_3)\,(1 - \omega^2\,(\tfrac{4}{5}\,\tau_1\,\tau_2 + \tau_1\,\tau_3 + \tfrac{1}{5}\,\tau_2\,\tau_3))] \\ &\cdot [(1 - \omega^2\,(\tfrac{4}{5}\,\tau_1\,\tau_2 + \tau_1\,\tau_3 + \tfrac{1}{5}\tau_2\,\tau_3))^2 \\ &+ \omega^2\,(\tfrac{3}{2}\tau_1 + \tfrac{5}{6}\,\tau_2 + \tfrac{2}{3}\,\tau_3)^2]^{-1} . \end{aligned} \tag{28}$$

Equation (28) reduces in spherical approximation to

$$\frac{\lambda^{\text{tr}}}{\lambda} = -\Psi_{12}\left[\frac{\omega\tau}{1+\omega^2\tau^2} + 2\,\frac{2\,\omega\tau}{1+4\,\omega^2\tau^2}\right]. \tag{29}$$

The saturation ratio, given by Eq. (27), may, in general, differ appreciably from the value $\frac{3}{2}$ for molecules with large nonsphericity. Concerning the field dependence of the parallel, perpendicular and transverse effects, respectively, the formulae are the same for the Senftleben-Beenakker effects of diffusion and thermal diffusion in mixtures of polyatomic gases with noble gases.

Finally, the relation between the more frequently used cross sections $\mathfrak{S}\binom{pq}{pq}_k$ of McCourt, Chen, Moraal and Snider [11] and those of the present paper is stated. The $\mathfrak{S}\binom{pq}{pq}_k$ are defined such that the velocity dependent tensors are coupled to each other and the same is done with the rotational angular momentum dependent ones. According to Ref. [11], both types of cross sections are connected by

$$\mathfrak{S}\binom{pq}{pq}_k = \sum_L (-1)^{p+q+L}(2L+1) \cdot (2k+1)\,\Omega(k\,p\,p)^{-1/2}\,\Omega(k\,q\,q)^{-1/2}\begin{Bmatrix} L & q & p \\ k & p & q\end{Bmatrix}\overline{\mathfrak{S}}\binom{pq}{pq}_L, \tag{30}$$

where $0 \leqq k \leqq \min(2p, 2q)$ and where

$$\Omega(k\,p\,p) \equiv \frac{(2p+k+1)!\,(2p-k)!\,k!\,k!}{(2k)!\,(2p)!\,(2p)!}\,\frac{3-(-1)^k}{2}. \tag{31}$$

In contradistinction to the $\overline{\mathfrak{S}}\binom{pq}{pq}_L$ which are always positive, the $\mathfrak{S}\binom{pq}{pq}_k$ have no definite sign for $k \neq 0$. For a purely spherical potential only $\mathfrak{S}\binom{pq}{pq}_0$ is nonzero.

In our special case $p = 1$, $q = 2$ one has $k = 0, 1, 2$ and from Eqs. (30), (31) one infers $[\mathfrak{S} \equiv \mathfrak{S}\binom{12}{12}]$:

$$\mathfrak{S}_0 = \tfrac{1}{30}\,(6\,\overline{\mathfrak{S}}_1 + 10\,\overline{\mathfrak{S}}_2 + 14\,\overline{\mathfrak{S}}_3), \tag{32 a}$$

$$\mathfrak{S}_1 = \tfrac{1}{30}\,(9\,\overline{\mathfrak{S}}_1 + 5\,\overline{\mathfrak{S}}_2 - 14\,\overline{\mathfrak{S}}_3), \tag{32 b}$$

$$\mathfrak{S}_2 = \tfrac{1}{30}\,(18\,\overline{\mathfrak{S}}_1 - 30\,\overline{\mathfrak{S}}_2 + 12\,\overline{\mathfrak{S}}_3). \tag{32 c}$$

After insertion of Eqs. (32 a – c) into Eqs. (21), (25), (28), one recovers the formulae first derived by Tip [9] and later used by Heemskerk [12].

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[9a] Note that in our short-hand notation the $\Phi^{l(\alpha)}$ correspond to the Φ^{lors} and the $\mathfrak{S}\binom{\alpha}{pq}_l$ correspond to the $\mathfrak{S}\binom{l\,o\,r\,s}{p\,q\,o\,o}$ of Ref. [4] (the collective index α stands for r, s, i. e. the Sonine- and WCUB polynomials).

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