On the Evaluation of Transport Collision Frequencies
I. The Integration of Empirical Data

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The computation of the transport collision frequencies is discussed, provided the transfer cross sections are given at least for a discrete set of relative kinetic energies. Numerical investigations show that the most satisfying results are achieved by the use of rational interpolation of the transfer cross sections.

Introduction

The connecting quantities between the mathematical formalism of the kinetic theory of gases, gas-mixtures and plasmas on one hand and the physical properties of the molecules on the other hand are the differential cross sections. They are averaged over the angle of deflection with certain weighting functions, which are polynomials of the cosine of this angle. This procedure yields the transfer collision cross sections [1], which in this paper we assume to be given by experiments or theoretical investigations. They are functions of the relative speed or — equivalently — of the relative kinetic energy of the colliding particles. Following the usual way of proceeding, the next step is the introduction of transfer collision frequencies, which still depend on the relative kinetic energy [2]. The series expansion of these functions in terms of generalized Laguerre (Sonine) polynomials yields the definition of the temperature dependent transport collision frequencies. They are integrals over the whole range of the energy and linear combinations of the Ω-integrals of Chapman and Cowling [3]. Their introduction enables to make use of their advantageous properties of convergence, depending on the molecular interaction.

In this paper we are concerned with the procedure leading from the transfer collision cross sections, given for a set of discrete energy values, to the transport collision frequencies for a given temperature. This procedure is decomposed in two parts,

a) the suitable representation of the energy-dependence of the transfer collision cross section and

b) the integration of the result, running from 0 to ∞. A discussion of the temperature-dependence of the transport collision frequencies will be given in Part II.

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1. Definitions

Our considerations are based on the transfer collision cross sections for isotropic interactions,

$$Q_{ij}{}^{(l)} = 2\pi \int_{-1}^{+1} \sigma_{ij}(\chi, g)\{1 - P_l(\cos\chi)\}\,\mathrm{d}\cos\chi\,, \quad (1.1)$$

depending on the relative speed g between the colliding particles of species i and j via the differential cross sections σ_{ij}, which are weighted with the Legendre-polynomials depending on the angle of deflection χ. We define "transfer collision frequencies"

$$\nu_{ij}{}^{(l)}(g) := n_j\, g\, Q_{ij}{}^{(l)}(g) \quad (1.2\text{a})$$

or

$$\nu_{ij}{}^{(l)}(\varepsilon) = n_j \sqrt{2/\mu_{ij}}\, \varepsilon^{1/2}\, Q_{ij}{}^{(l)}(\varepsilon) \quad (1.2\text{b})$$

respectively, where we used the relative kinetic energy

$$\varepsilon = \tfrac{1}{2}\mu_{ij}\, g^2 \quad (1.3)$$

with the reduced mass

$$\mu_{ij} = m_i\, m_j/(m_i + m_j) \quad (1.4)$$

and the particle density n_j.

The naturally occuring "combined temperature" T_{ij} [4] multiplied by the Boltzmann constant k_B,

$$\gamma := k_\mathrm{B}\, T_{ij} := \mu_{ij}\left(\frac{k_\mathrm{B}\, T_i}{m_i} + \frac{k_\mathrm{B}\, T_j}{m_j}\right), \quad (1.5)$$

T_i and T_j being the temperatures of the mixture components i and j, is used to introduce the normalized kinetic energy

$$\check{\varepsilon} := \varepsilon/\gamma\,. \quad (1.6)$$

Omitting the species indices i and j, we expand the transfer collision frequencies $\nu^{(l)}(\varepsilon)$, Eq. (1.2b), as

$$\nu^{(l)}(\varepsilon) =: \sum_{s=0}^{\infty} (-1)^s \nu^{(ls)}(\gamma) L_s^{(l+1/2)}(\check{\varepsilon}) \qquad (1.7)$$

with the generalized Laguerre (Sonine) polynomials [5]

$$L_s^{(l+1/2)}(\check{\varepsilon}) = \sum_{r=0}^{s} \frac{(-\check{\varepsilon})^r}{r!} \binom{s+l+1/2}{r+l+1/2}. \qquad (1.8)$$

The series expansion (1.7) acts as the definition of the transport collision frequencies $\nu^{(ls)}$, which yields

$$\nu^{(ls)}(\gamma) = \frac{(-1)^s s!}{\Gamma(s+l+3/2)} \cdot \int_0^{\infty} \check{\varepsilon}_l^{+1/2} e^{-\check{\varepsilon}} L_s^{(l+1/2)}(\check{\varepsilon}) \, \nu^{(l)}(\check{\varepsilon}\gamma) \, d\check{\varepsilon} \qquad (1.9)$$

because of the orthogonality of the Laguerre polynomials. The integral on the right-hand side of this equation is the subject of interest in the context of this paper. Note that the definition for the Ω-integrals of Chapman and Cowling [3] is closely related to Equation (1.9). The connection between the $\nu^{(ls)}$ and the $\Omega^{(l)}(r)$ is discussed in the appendix.

2. The Representation of the Transfer Collision Cross Sections

Suppose the transfer collison cross sections $Q^{(l)}(\varepsilon)$, Eq. (1.1), are given for a set of relative kinetic energies ε_k. Then the first problem, which arises, is the choice of a suitable function, which fits the $Q^{(l)}(\varepsilon_k)$. We compare three different methods of interpolation with an "exact" function, which — in the case of this paper — shall be given analytically in the form

$$Q_\alpha^{(l)}(\varepsilon) = \varepsilon^\alpha q_l \,. \qquad (2.1)$$

In the general case the "exact" function can be looked at for example as a function fitted by a spline procedure. Moreover we compare the two cases

a) $\varepsilon_k - \varepsilon_{k-1} =$ constant and

b) $\log \varepsilon_k - \log \varepsilon_{k-1} =$ constant in order to discuss the dependence of the results upon the spacing of the ε_k in the intervall under consideration.

The three different methods of interpolation are by

1) polynomials in ε,
2) polynomials in $\varepsilon^{1/2}$ and
3) rational functions or — more precisely — continued fractions [6].

There are three mean features to give a comparing discussion of these methods: The stability of the interpolating function in the range between given values of the argument, the dependence on the distribution of the set of ε_k and the asymptotic behaviour. With respect to all these points of view the rational interpolation has turned out to be the most suitable one. A particular advantage is the possibility to handle the asymptotic behaviour by choosing the degree of the numerator and denominator. Here we must add that this behaviour — in most cases — is usually not prescribed definitely. So the last method provides a possibility to compare different asymptotics. In the special example, which we have given in the next section, we varied the number of given argument values between 10 and 11, causing the polynomial in the numerator being of degree 4 or 5 respectively over a polynomial in the denominator of degree 4 in both cases. Hence the asymptotic behaviour for $\varepsilon \to \infty$ is constant or linearly increasing respectively.

Especially to fit the case of resonance peaks the rational interpolation is the only suitable one. Here we have to add as a last remark, that, in general, there are zeros of the denominator, yielding poles of the interpolating function. But, by experience it has turned out, that these are extremely sharp and can be eliminated by graphical considerations. The question of main importance, however, is the result of the integration over the energy range, cf. Eq. (1.9), due to the applied interpolating procedure. A discussion is given in the next section.

3. The Integrating Procedure

The special choice of our exact reference expression (2.1) enables to give the result of the integration (1.9) analytically: With

$$\nu_\alpha^{(l)}(\varepsilon) = n_j \sqrt{2/\mu}\, \varepsilon^{\alpha+1/2} q_l \qquad (3.1)$$

we obtain

$$\nu^{(ls)}(\gamma) = \frac{(-1)^s s!}{\Gamma(s+l+3/2)} n_j \sqrt{\frac{2}{\mu}}\, \gamma^{\alpha+1/2} q_l \cdot \int_0^{\infty} \check{\varepsilon}^{\alpha+l+1} e^{-\check{\varepsilon}} L_s^{(l+1/2)}(\check{\varepsilon}) \, d\check{\varepsilon} \,, \qquad (3.2)$$

which yields [7]

$$\nu^{(ls)}(\gamma) = \frac{(\alpha+1/2)!}{(\alpha-s+1/2)!} \cdot \frac{\Gamma(\alpha+l+2)}{\Gamma(l+s+3/2)} n_j q_l \sqrt{\frac{2}{\mu}} \gamma^{\alpha+1/2} . \tag{3.3}$$

Dividing Eq. (3.3) by $\nu^{(l0)}(\gamma)$ we introduce a normalized form, which is suitable for comparing discussions:

$$\check{\nu}^{(ls)} := \frac{\nu^{(ls)}(\gamma)}{\nu^{(l0)}(\gamma)} = \frac{\Gamma(l+3/2)}{\Gamma(l+s+3/2)} \frac{(\alpha+1/2)!}{(\alpha-s+1/2)!} . \tag{3.4}$$

In the following table we have listed these exact values together with the results of the integration after interpolating the transfer cross sections (2.1) for $\alpha = -1/3$, according to a r^{-6}-potential [8], and $l = 1$. The notation is in accordance to Sect. 2 from 1a) (polynomials in ε with a constant spacing of the set of ε_k) to 3b) (rational interpolation with logarithmically distributed ε_k). The cases 3a) and 3b) are subdivided by adding the index 10 or 11 resp., denoting the number of ε_k-values and thus the asymptotic behaviour (cf. Section 2).

This table clearly shows the effects, caused by the properties, which were discussed qualitatively in Section 2.

4. Concluding Remarks

In this paper we have compared different interpolating procedures with respect to their practical use for the evaluation of the transport collision frequencies $\nu^{(ls)}$ from a given set of values for the transfer collision cross sections $Q^{(l)}(\varepsilon)$. It has turned out that the rational interpolation by continued fractions has some advantageous properties as to the stability of the interpolating function and the possibility, to extend the given range of arguments as far as necessary to perform the integration from 0 to ∞ with a prescribed accuracy without further manipulations. Because of the necessarily existing lack of empirical data, we should keep in mind, however, that the integration and thereby some of the basic properties of the theory fail, if the result of the integration significantly depends upon the formal extrapolation.

In the context of this paper, the temperature-dependence of the transport collision frequencies has been ignored, in our special example it cancelled out because of the introduction of the normalized form (3.4). For practical use, however, it is necessary to express them as functions of the temperature. This question will be discussed in a subsequent Part II.

Appendix

The Relation Between the Ω-Integrals and the Transport Collision Frequencies

The Ω-integrals are defined as [3]

$$\Omega^{(l)}(r) = \frac{1}{2\sqrt{\pi}} \left(\frac{\mu}{2 k_B T}\right)^{r+3/2} \cdot \int_0^\infty \exp\left\{-\frac{\mu g^2}{2 k_B T}\right\} g^{2r+3} \Phi^{(l)}(g) \, dg , \tag{A.1}$$

where we omitted the particle species indices i and j. Here Chapman and Cowling used certain cross sections

$$\Phi^{(l)}(g) = 2\pi \int (1-\cos^l \chi) \, b \, db , \tag{A.2}$$

which in terms of the differential cross section

$$\sigma = \frac{1}{2} \frac{db^2}{d\cos\chi} \tag{A.3}$$

Table 1. Approximations of the transport collision frequencies for $\alpha = -1/3$; $l = 1$; $s = 0, 1, 2, 3$, normalized by the exact value $\nu^{(10)}(\gamma)$, Eq. (3.3), computed by means of several interpolating prodecures in comparison to the exact values $\check{\nu}^{(1s)}$.

	$s = 0$	$s = 1$	$s = 2$	$s = 3$
exact	1	$6.667 \cdot 10^{-2}$	$-1.587 \cdot 10^{-2}$	$6.467 \cdot 10^{-3}$
1a	0.8762	0.7444	-3.175	8.65
1b	$-6.568 \cdot 10^{4}$	$3.642 \cdot 10^{5}$	$-1.266 \cdot 10^{6}$	$2.971 \cdot 10^{6}$
2a	1.0006	$6.61 \cdot 10^{-2}$	$-1.56 \cdot 10^{-2}$	$5.69 \cdot 10^{-3}$
2b	0.8955	0.532	-1969	3.844
$3a_{10}$	1.00007	$6.660 \cdot 10^{-2}$	$-1.583 \cdot 10^{-2}$	$6.421 \cdot 10^{-3}$
$3a_{11}$	1.00003	$6.664 \cdot 10^{-2}$	$-1.586 \cdot 10^{-2}$	$6.445 \cdot 10^{-3}$
$3b_{10}$	0.999998	$6.6666 \cdot 10^{-2}$	$-1.588 \cdot 10^{-2}$	$6.459 \cdot 10^{-3}$
$3b_{11}$	0.999999	$6.6666 \cdot 10^{-2}$	$-1.588 \cdot 10^{-2}$	$6.463 \cdot 10^{-3}$

can be re-written as

$$\Phi^{(l)}(g) = 2\pi \int_{-1}^{+1} \sigma(1 - \cos^l \chi)\, \mathrm{d}\cos\chi\,. \tag{A.4}$$

If we substitute $\cos^l \chi$ by the Legendre polynomial $P_l(\cos\chi)$, we achieve our collision cross sections $Q^{(l)}$, Equation (1.1).

The Legendre polynomials can be represented as [9]

$$P_l(\cos\chi) = \frac{1}{2^l} \sum_{k=0}^{[l/2]} (-1)^k \binom{l}{k} \binom{2l-2k}{l} \cos^{l-2k}\chi \tag{A.5}$$

or in the simplified form

$$P_l(\cos\chi) = \sum_{k(2)}^{l} (-1)^{(l-k)/2} \frac{(l+k-1)!!}{k!(l-k)!!} \cos^k\chi\,, \tag{A.6}$$

where the sum has to be taken over all values of k with $0 \leqq l-k$ even. The inversion of this equation yields [10]

$$\cos^k\chi = \sum_{l(2)}^{k} (2l+1) \cdot \frac{k!}{(k+l+1)!!\,(k-l)!!} P_l(\cos\chi)\,. \tag{A.7}$$

We are now able to elaborate the relation between the quantities $\Phi^{(l)}$, Eq. (A.2), and the transfer collision cross sections $Q^{(l)}$, Equation (1.1). By means of Eq. (A.6) we have

$$Q^{(l)}(g) = 2\pi \int_{-1}^{+1} \sigma(\chi, g)\, \mathrm{d}\cos\chi - \sum_{k(2)}^{l} (-1)^{(l-k)/2} \frac{(l+k-1)!!}{k!(l-k)!!} \cdot 2\pi \int_{-1}^{+1} \sigma(\chi, g) \cos^k\chi\, \mathrm{d}\cos\chi\,, \tag{A.8}$$

which becomes

$$Q^{(l)}(g) = \sum_{k(2)}^{l} (-1)^{(l-k)/2} \frac{(l+k-1)!!}{k!(l-k)!!} \Phi^{(k)}(g) - 2\pi \int_{-1}^{+1} \sigma(\chi, g)\, \mathrm{d}\cos\chi \cdot \left\{ 1 - \sum_{k(2)}^{l} (-1)^{(l-k)/2} \frac{(l+k-1)!!}{k!(l-k)!!} \right\}. \tag{A.9}$$

The Legendre polynomials, however, are normalized to $P_l(1) = 1$, hence the term in curly brackets vanishes:

$$Q^{(l)}(g) = \sum_{k(2)}^{l} (-1)^{(l-k)/2} \frac{(l+k-1)!!}{k!(l-k)!!} \Phi^{(k)}(g)\,. \tag{A.10}$$

The inversion of this system of equations has been done already (cf. Equation (A.7)). We can immediately write down the according relation

$$\Phi^{(k)}(g) = \sum_{l(2)}^{k} (2l+1) \frac{k!}{(k+l+1)!!\,(k-l)!!} Q^{(l)}(g)\,. \tag{A.11}$$

Next we need the representation (1.8) for the generalized Laguerre polynomials. It can easily be shown that the inversion of this equation is given by (see also Eq. (3.3))

$$\check{\varepsilon}^k = \sum_{r=0}^{k} (-1)^r k! \binom{k+l+1/2}{r+l+1/2} L_r^{(l+1/2)}(\check{\varepsilon})\,. \tag{A.12}$$

This relation can be verified by inserting in Equation (1.8).

Using the normalized kinetic energy

$$\check{\varepsilon} := \mu g^2 / 2 k_\mathrm{B} T\,, \tag{A.13}$$

Equation (A.1) for the Ω-integrals can be written as

$$\Omega^{(l)}(r) = \frac{1}{4\sqrt{\pi}} \int_0^\infty e^{-\check{\varepsilon}} \check{\varepsilon}^{r+1/2} g\, \Phi^{(l)}(g)\, \mathrm{d}\check{\varepsilon}\,. \tag{A.14}$$

We insert the Eqs. (A.11) as well as (A.12) and obtain

$$\Omega^{(l)}(r) = \frac{1}{4n\sqrt{\pi}} \sum_{k=0}^{r-l} (-1)^k (r-l)! \binom{r+1/2}{k+l+1/2} \cdot \sum_{\lambda(2)}^{l} (2\lambda+1) \frac{l!}{(l+\lambda+1)!!\,(l-\lambda)!!} \cdot \int_0^\infty e^{-\check{\varepsilon}} \check{\varepsilon}^{l+1/2} \nu^{(l)}\, \mathrm{d}\check{\varepsilon} \tag{A.15}$$

with the restriction $r \geqq l$, where we used the definition (1.2a) for the transfer collision frequencies $\nu^{(l)}$. Equation (A.15), however, contains the integral of Eq. (1.9) for the transport collision frequencies. So we have after some simplifications

$$\Omega^{(l)}(r) = \frac{1}{4n\sqrt{\pi}} \sum_{s=0}^{r-l} (r-l)! \binom{r+1/2}{s+l+1/2} \cdot \sum_{\lambda(2)}^{l} (2\lambda+1) \frac{l!}{(l+\lambda+1)!!\,(l-\lambda)!!} \cdot \frac{\Gamma(s+\lambda+3/2)}{s!} \nu^{(\lambda s)}\,. \tag{A.16}$$

On the other hand we obtain from Eq. (1.9) by means of the Eqs. (1.8), (1.2a) and (A.13)

$$\nu^{(ls)} = 2n \frac{(-1)^s s!}{\Gamma(s+l+3/2)} \cdot \sum_{r=0}^{s} \frac{(-1)^r}{r!} \binom{s+l+1/2}{r+l+1/2} \int_0^\infty e^{-\check{\varepsilon}} \check{\varepsilon}^{r+l+3/2} Q^{(l)}\, \mathrm{d}g\,. \tag{A.17}$$

We insert Eq. (A.10), which yields

$$\nu^{(ls)} = 2n \frac{(-1)^s s!}{\Gamma(s+l+3/2)} \sum_{r=0}^{s} \frac{(-1)^r}{r!} \binom{s+l+1/2}{r+l+1/2} \cdot \sum_{\lambda(2)}^{l} (-1)^{(l-\lambda)/2} \frac{(l+\lambda-1)!!}{\lambda!(l-\lambda)!!} \cdot \int_0^\infty e^{-\check{\varepsilon}} \check{\varepsilon}^{s+l+3/2} \Phi^{(\lambda)} \, \mathrm{d}g \,. \tag{A.18}$$

Comparing with the definition (A.1) for the Ω-integrals, we obtain after some simplifications

$$\nu^{(ls)} = 4n\sqrt{\pi} \sum_{r=0}^{s} \frac{(-1)^{r+s}}{\Gamma(r+l+3/2)} \binom{s}{r} \cdot \sum_{\lambda(2)}^{l} (-1)^{(l-\lambda)/2} \frac{(l+\lambda-1)!!}{\lambda!(l-\lambda)!!} \Omega^{(\lambda)}(l+r) \,. \tag{A.19}$$

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