

# On the Evaluation of Transport Collision Frequencies

## II. An Approximating Method to Express the Temperature Dependence

Ulrich Weinert

Institute for Theoretical Physics, University of Düsseldorf

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The temperature dependence of the transport collision frequencies is discussed, provided they are given for one special reference temperature. An approximative procedure to express this dependence is elaborated using the definition of the transport collision frequencies as expansion coefficients.

### Introduction

The transport collision frequencies were introduced by Suchy and Rawer in the kinetic theory of gases, gas-mixtures and plasmas [1]. As pointed out already in Part I, they can be defined as coefficients of a generalized Laguerre (Sonine) polynomial-expansion of the transfer collision frequencies. These are closely related to the transfer collision cross sections, so the transport collision frequencies are comparable with the  $\Omega$ -integrals of Chapman and Cowling [2]. Advantageously, however, they are the coefficients of an orthogonal expansion with all its properties of convergence and optimality. As they can be calculated in closed form only in few cases, e.g. for inverse power potentials, their practical evaluation is based on numerical integrations, which take much time. Moreover, there is a dependence on a mean (“combined”) temperature, which means that all the numerical work must be done for each value of this parameter.

In this paper we shall discuss a method, which enables a fast approximate evaluation of the transport collision frequencies for a temperature  $T$ , if they are known for a reference temperature  $T_0$ . The general formalism will be given in Sect. 1 and after a discussion of the accuracy in Sect. 2 we add an example, which shows the essential features of the method. Some practical remarks will conclude the discussion.

### 1. General Formalism

Our starting point are the transfer collision cross sections for isotropic interaction [3],

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

Reprint requests to Dr. U. Weinert, Institute for Theoretical Physics of the University, Universitätsstr. 1, D-4000 Düsseldorf 1, West-Germany.

with the relative speed  $g$ , the angle of deflection  $\chi$  and the differential cross sections  $\sigma_{ij}(\chi, g)$  for a binary, elastic collision between particles of species  $i$  and  $j$ . We define the “transfer collision frequencies” [4]

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

with the particle density  $n_j$ , and express the relative speed  $g$  by means of the relative kinetic energy

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

with the reduced mass

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

So we obtain instead of Eq. (1.2):

$$\nu^{(l)}(\varepsilon) = n \sqrt{2/\mu} \varepsilon^{1/2} Q^{(l)}(\varepsilon), \quad (1.5)$$

where we have omitted the particle species indices  $i$  and  $j$ . We make use of the naturally occurring “combined temperature” [5] multiplied by the Boltzmann constant,

$$\gamma := k_B T := \mu \left( \frac{k_B T_i}{m_i} + \frac{k_B T_j}{m_j} \right), \quad (1.6)$$

and expand the transfer collision frequencies as

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

with the generalized Laguerre (Sonine) polynomials [6]

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

depending on the dimensionless variable

$$\tilde{\varepsilon} := \varepsilon/\gamma. \quad (1.9)$$

Equation (1.7) is the definition of the “transport collision frequencies”  $\nu^{(ls)}$  and yields



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$$\nu^{(ls)}(\gamma) = \frac{(-1)^s s!}{\Gamma(s+l+3/2)} \int_0^\infty \tilde{\epsilon}^{l+1/2} e^{-\tilde{\epsilon}} L_s^{(l+1/2)}(\tilde{\epsilon}) \nu^{(l)}(\tilde{\epsilon} \gamma) d\tilde{\epsilon} \quad (1.10)$$

because of the orthogonality of the Laguerre polynomials [7].

The temperature-dependence of the  $\nu^{(ls)}$  can be discussed using Eq. (1.7). For two different normalizing energies  $\gamma$  and  $\gamma_0$  we have

$$\sum_{s=0}^\infty (-1)^s \nu^{(ls)}(\gamma) L_s^{(l+1/2)}(\tilde{\epsilon}) = \sum_{s=0}^\infty (-1)^s \nu^{(ls)}(\gamma_0) L_s^{(l+1/2)}\left(\frac{\gamma_0}{\gamma} \tilde{\epsilon}\right). \quad (1.11)$$

We use the relation [8]

$$L_k^{(\alpha)}(\beta x) = \sum_{s=0}^k \beta^s (1-\beta)^{k-s} L_s^{(\alpha)}(x) \binom{k+\alpha}{s+\alpha} \quad (1.12)$$

and obtain

$$\sum_{s=0}^\infty (-1)^s \nu^{(ls)}(\gamma) L_s^{(l+1/2)}(\tilde{\epsilon}) = \sum_{k=0}^\infty (-1)^k \nu^{(lk)}(\gamma_0) \sum_{s=0}^k z^s (1-z)^{k-s} \binom{k+l+1/2}{s+l+1/2} L_s^{(l+1/2)}(\tilde{\epsilon}) \quad (1.13)$$

with

$$z = \gamma/\gamma_0. \quad (1.14)$$

Reordering the summations on the right-hand side of Eq. (1.13) we are able to compare coefficients with respect to the Laguerre polynomials, which yields

$$\nu^{(ls)}(\gamma) = z^s \sum_{k=s}^\infty \nu^{(lk)}(\gamma_0) (z-1)^{k-s} \binom{k+l+1/2}{s+l+1/2}. \quad (1.15)$$

This formula gives the temperature dependence of the  $\nu^{(ls)}$  if they are known for only one special value  $\gamma_0$ , the “reference temperature”. Evidently the utility of the formula depends on the convergence of the sum on the right-hand side. This problem is discussed in the next section.

## 2. Discussion of the accuracy

For practical purposes the sum over  $k$  in Eq. (1.15) has to be truncated at some value  $n \geq s$ , causing the error

$$F^{(ls)}(z; n, \gamma_0) = -z^s \sum_{k=n+1}^\infty \nu^{(lk)}(\gamma_0) (z-1)^{k-s} \binom{k+l+1/2}{s+l+1/2}. \quad (2.1)$$

To give an estimation of this expression we assume

$$|\nu^{(lk+1)}(\gamma_0)| \leq |\nu^{(lk)}(\gamma_0)| \quad \text{for all } k \geq n+1. \quad (2.2)$$

Then from Eq. (2.1) we obtain

$$|F^{(ls)}(z; n, \gamma_0)| \leq z^s |\nu^{(ln+1)}(\gamma_0)| \sum_{k=n+1}^\infty |z-1|^{k-s} \binom{k+l+1/2}{s+l+1/2}. \quad (2.3)$$

The sum over  $k$  can be rewritten as

$$\sum_{k=n+1-s}^\infty |z-1|^k \binom{k+s+l+1/2}{s+l+1/2} = \sum_{k=0}^\infty |z-1|^k \binom{k+s+l+1/2}{s+l+1/2} - \sum_{k=0}^{n-s} |z-1|^k \binom{k+s+l+1/2}{s+l+1/2}. \quad (2.4)$$

The first term on the right-hand side is a Taylor series expansion of the form

$$\sum_{k=0}^\infty x^k \binom{k+\beta}{\beta} = \frac{1}{(1-x)^{\beta+1}}. \quad (2.5)$$

With  $\beta = s+l+1/2$  and  $x = |z-1|$  we obtain

$$|F^{(ls)}(z; n, \gamma_0)| \leq |\nu^{(ln+1)}(\gamma_0)| f^{(ls)}(z; n) \quad (2.6)$$

Table 1.  $z^{-s} f^{(ls)}(z; n)$  for  $s + l = 1, 2, 3$  and  $n - s = 3, 9$  in the range  $0 < z \leq 1$ .

$z \setminus s + l$	$n - s = 3$			$n - s = 9$		
	1	2	3	1	2	3
0.1	$3.046 \cdot 10^2$	$3.141 \cdot 10^3$	$3.159 \cdot 10^3$	$2.568 \cdot 10^2$	$2.964 \cdot 10^3$	$3.105 \cdot 10^4$
0.2	$4.674 \cdot 10^1$	$2.633 \cdot 10^2$	$1.371 \cdot 10^3$	$2.477 \cdot 10^1$	$1.847 \cdot 10^2$	$1.141 \cdot 10^3$
0.3	$1.314 \cdot 10^1$	$5.536 \cdot 10^1$	$2.060 \cdot 10^2$	$3.598 \cdot 10^0$	$2.268 \cdot 10^1$	$1.137 \cdot 10^2$
0.4	$4.390 \cdot 10^0$	$1.565 \cdot 10^1$	$4.782 \cdot 10^1$	$5.217 \cdot 10^{-1}$	$3.020 \cdot 10^0$	$1.368 \cdot 10^1$
0.5	$1.493 \cdot 10^0$	$4.790 \cdot 10^0$	$1.293 \cdot 10^1$	$6.326 \cdot 10^{-2}$	$3.482 \cdot 10^{-1}$	$1.488 \cdot 10^0$
0.6	$4.661 \cdot 10^{-1}$	$1.393 \cdot 10^0$	$3.465 \cdot 10^0$	$5.421 \cdot 10^{-3}$	$2.886 \cdot 10^{-2}$	$1.189 \cdot 10^{-1}$
0.7	$1.183 \cdot 10^{-1}$	$3.361 \cdot 10^{-1}$	$7.904 \cdot 10^{-1}$	$2.535 \cdot 10^{-4}$	$1.319 \cdot 10^{-3}$	$5.303 \cdot 10^{-3}$
0.8	$1.943 \cdot 10^{-2}$	$5.316 \cdot 10^{-2}$	$1.201 \cdot 10^{-1}$	$3.756 \cdot 10^{-6}$	$1.922 \cdot 10^{-5}$	$7.590 \cdot 10^{-5}$
0.9	$1.036 \cdot 10^{-3}$	$2.756 \cdot 10^{-3}$	$6.041 \cdot 10^{-3}$	$3.120 \cdot 10^{-9}$	$1.609 \cdot 10^{-8}$	$6.296 \cdot 10^{-8}$
1	0	0	0	0	0	0

with the “form-factor”

$$f^{(ls)}(z; n) := z^s \left\{ \frac{1}{(1 - |1 - z|)^{s+l+3/2}} - \sum_{k=0}^{n-s} |1 - z|^k \binom{k + s + l + 1/2}{k} \right\}. \quad (2.7)$$

Evidently the range of validity for the procedure under consideration is limited by the two poles  $z_0 = 0$  and  $z_1 = 2$  of  $f^{(ls)}(z; n)$ . In the following tables we have listed the term in curly brackets, which is an even function of  $1 - z$ , for different values of  $n - s$  and  $s + l$ . It can be used to obtain an explicit impression of the maximum error, provided the  $v^{(ls)}$  are known for  $\gamma_0$  or  $z = 1$  respectively.

### 3. Examples

In this section we shall demonstrate the properties of our method by means of an example, which can be given explicitly: Let

$$Q^{(l)}(\varepsilon) = \varepsilon^\alpha q_l \quad (3.1)$$

according to a  $r^{-p}$  potential with  $p = -2/\alpha$  [9]. The transfer collision frequency (1.5) then becomes

$$v^{(l)}(\varepsilon) = n_j \sqrt{2/\mu} \varepsilon^{\alpha+1/2} q_l, \quad (3.2)$$

and the expansion (1.7) yields

$$\begin{aligned} q_l n_j \sqrt{2/\mu} \gamma^{\alpha+1/2} \tilde{z}^{\alpha+1/2} \\ = \sum_{s=0}^{\infty} (-1)^s v^{(ls)}(\gamma) L_s^{(l+1/2)}(\tilde{z}). \end{aligned} \quad (3.3)$$

We use the relation [10]

$$\begin{aligned} x^\beta = \sum_{s=0}^{\infty} (-1)^s \frac{\beta!}{(\beta-s)!} \\ \cdot \frac{\Gamma(\beta+l+3/2)}{\Gamma(l+s+3/2)} L_s^{(l+1/2)}(x) \end{aligned} \quad (3.4)$$

and comparing with Eq. (3.3) we obtain

$$\begin{aligned} v^{(ls)}(\gamma) &= \frac{(\alpha + 1/2)!}{(\alpha - s + 1/2)!} \\ &\cdot \frac{\Gamma(\alpha + l + 2)}{\Gamma(l + s + 3/2)} n_j q_l \sqrt{\frac{2}{\mu}} \gamma^{\alpha+1/2}. \end{aligned} \quad (3.5)$$

Dividing Eq. (3.5) by  $v^{(l0)}(\gamma_0)$  we obtain a normalized form of the  $v^{(ls)}(\gamma)$ ,

$$\begin{aligned} \tilde{v}^{(ls)}(z) &:= \frac{v^{(ls)}(\gamma)}{v^{(l0)}(\gamma_0)} \\ &= \frac{(\alpha + 1/2)!}{(\alpha - s + 1/2)!} \frac{\Gamma(l + 3/2)}{\Gamma(l + s + 3/2)} z^{\alpha+1/2}, \end{aligned} \quad (3.6)$$

which is useful for comparing discussions.

The approximate expression from Section 1, Eq. (1.15), in its normalized form reads

$$\begin{aligned} \tilde{v}_n^{(ls)}(z) \\ = z^s \sum_{k=s}^n \tilde{v}^{(lk)}(1) (z-1)^{k-s} \binom{k+l+1/2}{s+l+1/2}. \end{aligned} \quad (3.7)$$

We have taken  $\alpha = -1/3$  according to a  $r^{-6}$ -potential and plotted as an example the relative error

$$\Delta_n^{(ls)}(z) := \left| \frac{\tilde{v}_n^{(ls)}(z) - \tilde{v}^{(ls)}(z)}{\tilde{v}^{(ls)}(z)} \right| \quad (3.8)$$

for  $s = 0, 1, 2$  and  $n - s = 3, 9$  in the range  $0 \leq z \leq 2$ . Figure 1 shows the range of reasonable quality of the approximations.

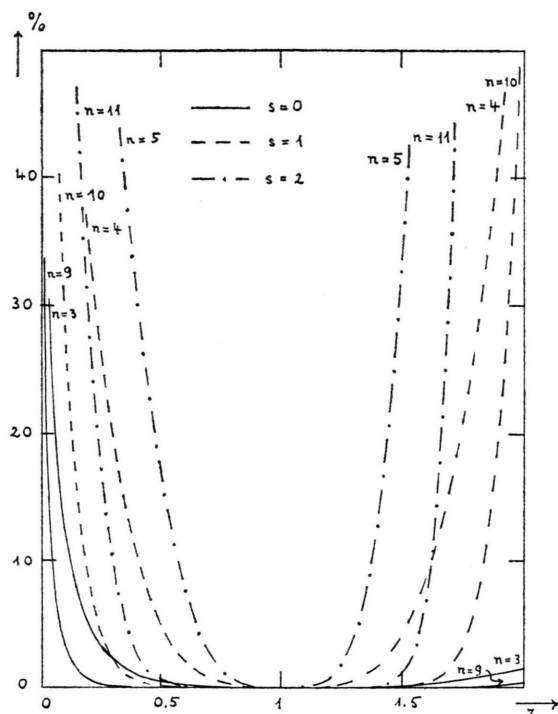


Fig. 1. Relative error  $\Delta_n^{(1s)}(z)$ , Eq. (3.8), for  $s=0, 1, 2$  and  $n-s=3, 9$ .

#### 4. Concluding Remarks

In the foregoing sections we have discussed a method to elaborate approximately the temperature dependence of the  $\nu^{(ls)}$  in a surrounding of a

reference temperature  $T_0$ , provided they are known for  $T_0$  (this question has been discussed in Part I). The range of validity upon the convergence of the  $\nu^{(ls)}$ , the number of them taken into account at  $T_0$  and the prescribed degree of accuracy.

An alternative way to obtain the temperature dependence of the  $\nu^{(ls)}$  is to perform the integrations numerically for a set of temperatures  $T_1, T_2, \dots, T_n, T_{n+1}$  and to interpolate the function  $\nu^{(ls)}(T)$  yielding a polynomial of degree  $n$ . To discuss our approximation method in contrast to this straightforward interpolation note that for  $s=0$  the same number of numerical integrations have to be done, but for  $s \geq 1$  the result of our method is of degree  $n$  in the temperature while only  $n-s+1$  integrations are needed, i.e.  $s$  integrations less than for the interpolating procedure.

There is, however, an interesting possibility to combine both methods: If the  $\nu^{(ls)}$  themselves are given as temperature dependent functions, even if only for  $s=0$ , they can be approximated by polynomials of the temperature. On the other hand we can reorganize the expression (1.15) with respect to powers of  $z$  and the whole set of  $\nu^{(ls)}$  at a suitable chosen value  $T_0$  can be obtained simply by comparing coefficients of equal powers. Then, taking  $T_0$  into account, the energy-dependent transfer collision frequencies  $\nu^{(l)}(\epsilon)$  can be evaluated via the expansion (1.7).

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