doi: 10.22564/rbgf.v12i2.1174

ON A NEW COMPUTATION OF THE COLLISIONAL TRANSFER RATES FOR MAXWELL MOLECULES INTERACTION

C.J. Zamlutti & I.S. Batista

A new computation of the collisional transfer rates for Maxwell molecules type interactions is presented. The relevance of the present computation is that an approximated analitical expression is proposed to substitute and invert the infinite series relating the apsidal angle to the impact parameter. This allow us to use more refined computer methods to compute the transfer integrals. A comparison with the old results is performed and conclusions are drawn as to the relevance of the discrepancies.

Key words: Collisional transfer rates; Maxwell molecules interactions.

SOBRE UM NOVO CÁLCULO DAS TAXAS DE TRANSFERÊNCIA COLISIONAIS PARA INTERAÇÕES DO TIPO MOLÉCULAS DE MAXWELL
Apresenta-se um novo cálculo de taxas de transferência colisionais para interações do tipo moléculas de Maxwell. Propõe-se uma expressão analítica aproximada para substituir e inverter a série infinita que relaciona o ângulo apsidal ao parâmetro de impacto. Isto permite o uso de métodos computacionais mais refinados para calcular as integrais de transferência. Faz-se a comparação com os resultados antigos e são feitos comentários acerca da relevância das discrepâncias encontradas entre os cálculos feitos neste trabalho e o anterior.

Palavras-chave: Taxas de transferência colisionais; Interações do tipo moléculas de Maxwell

Instituto Nacional de Pesquisas Espaciais - INPE
Av. dos Astronautas, 1758 - C.P. 515
12201-970 - São José dos Campos, SP, Brasil

INTRODUCTION

The collisional transfer rates can be expressed as:

$$S_j = 2\pi \int_0^\infty \left[1-(-1)^j \cos^j(2\theta)\right] s ds, \qquad (1)$$

(Burgers, 1969; Chapman & Cowling, 1970), where θ is the angle which the relative velocity of the colliding particles makes with the apse line and s is the impact parameter (see Chapman & Cowling, 1970)

To solve Eq. (1) it is necessary to know a relationship establishing the dependence of θ on *s*. This is possible provided that one knows the particular law governing the binary collision. Of special interest is the case of the inverse power law, for which the potential energy for the two interacting particles is given by:

$$U(x) = K/x^n \qquad (2)$$

where *K* is a constant and *x* is the radial distance between the particles. If we call $\underline{w}$ the relative velocity we finally get (Liboff, 1969):

$$\theta = s \int_{x_0}^\infty \left\{\left[1 - s^2/x^2\right] - 2U(x)/\left(\mu w^2\right)\right\}^{-1/} \qquad (3)$$

where x_0 satisfies:

$$1-s^2/x_0^2 = 2U(x_0)/(\mu w^2)$$

and μ stands for the reduced mass of the two colliding particles. Integration of Eq. (3) yields the desired relation between θ and s.

The case n = 4 merits special attention in upper atmosphere studies. Molecules that interact under this law are called Maxwell molecules (see Chapman & Cowling (1970) and references therein). For these molecules the transfer rates depends on w^{-1} and the final Boltzmann collision term results independent of the particular velocity distribution function governing the microscopic behavior of the gas particles. Ion-neutral interactions in the upper atmosphere can be properly described by this case (Schunk, 1975, 1977; Barakat & Schunk, 1982) and this plenty justifies a renewed interest on it.

In this work we undertake the computation of the collisional transfer rates for Maxwell molecules interactions using more advanced computational techniques than the earlier works reported by Burgers (1969) and Chapman & Cowling (1970).

COMPUTATIONAL PROCEDURES

The solution of Eq. (3) is presented in the appendix and according to Eq. (A-10) one can write:

$$\theta = f_1(b) f_2(b) = f(b), \qquad (4)$$

where b depends on s as expressed by Eq. (A-2), the function f_1 (b) is given by

$$f_1(b) = \frac{b\sqrt{2}}{\left[b^2 + \left(b^4+4\right)^{1/2}\right]^{1/2}} \qquad (5)$$

and f_2 (b) encloses the result of the elliptic integral as:

$$f_2(b) = (\pi/2)\left[\left[1-(1/2)^2 h + \left(\frac{1.3}{2.4}\right)^2 h^2 - \right.\right.$$

$$\left. -\left(\frac{1.3.5}{2.4.6}\right)^2 h^3 + \left(\frac{1.3.5.7}{2.4.6.8}\right)^2 h^4 - \ldots\right] \qquad (6)$$

with

$$h = \frac{\left(b^4+4\right)^{1/2} - b^2}{\left(b^4+4\right)^{1/2} + b^2} \qquad (7)$$

Since b has an infinite range in Eq. (1) it is better to express it as a function of θ to compute the transfer integrals. To do this we plotted in Fig. 1 the relation established by Eq. (4) and tried to invert it using simple functional relations. Our guideline to try a prospective analytical expression to invert and reproduce Eq. (4) was the limiting behavior of b $= f^{-1}(\theta)$ for $\theta \to 0$ and $\theta \to \pi/2$ (see Cercignani, 1988). The fitting methodology was the nonlinear least square fitting. Thus we arrived at the function:

$$b \cong \left(\frac{\pi/2-\theta}{\pi/2}\right)^{0.57} \tan\theta - \theta/10 \qquad (8)$$

that is also plotted in Fig. 1, for comparison.

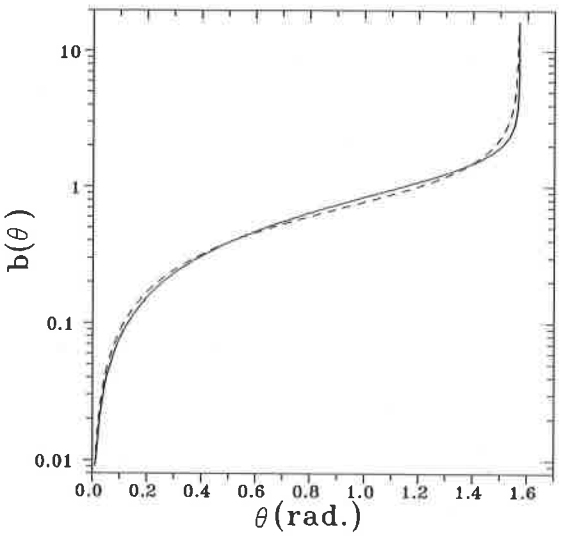

Figure 1 - The inverted function $b(\theta)$ (solid line) and its aproximation given by the analitic expression $\left(\frac{\pi/2-\theta}{\pi/2}\right)^{0.57}\tan\theta-\frac{\theta}{10}$ (dashed line).

Figura 1 - *Função invertida $b(\theta)$ (linha contínua) e sua aproximação dada pela expressão analítica* $\left(\frac{\pi/2-\theta}{\pi/2}\right)^{0.57}\tan\theta-\frac{\theta}{10}$ *(linha tracejada).*

Using Eqs. (1) and (8) together with the Romberg numerical integration method we get:

$$S_1 = 2\pi w^{-1}(2K/\mu)^{1/2}0.5712, \qquad (9)$$

$$S_2 = 2\pi w^{-1}(2K/\mu)^{1/2}0.6196. \qquad (10)$$

DISCUSSION

In order to compare the obtained results with those of earlier publications one must recall that the constant K of the present work is four times smaller than that of Chapman & Cowling (1970). Therefore, $K = K_{12}/4$, where K_{12} is the constant used in this last work. Replacing this value in Eqs. 9 and 10 one gets:

$$S_1 = 2\pi w^{-1}(K_{12}/\mu)^{1/2}0.4039, \qquad (11)$$

$$S_2 = 2\pi w^{-1}(K_{12}/\mu)^{1/2}0.4381. \qquad (12)$$

The results presented by Chapman & Cowling (1970) are:

$$S_1 = 2\pi w^{-1}(K_{12}/\mu)^{1/2}0.422, \qquad (13)$$

$$S_2 = 2\pi w^{-1}(K_{12}/\mu)^{1/2}0.436. \qquad (14)$$

The discrepancy between the present results and those published earlier is less than 5% and appears for S_1. As for S_2 the agreement is surprisingly good being of the order of 0.5%. Earlier computations (see references in Chapman & Cowling (1970)) were carried out before 1930 being difficult to retrieve. Thus they did not have the now available computer facilities to properly invert Eq. (4). Using Gaussian numerical integration methods to handle the infinite limit in Eq. (1) they were probably more subject to errors than the present computation. This suggests that the earlier value of S_1 could be over- estimated in 4%. Anyway, this discrepancy is not relevant. Much more important is the use of the correct value of K, since it depends on the actual form of U(x). This value is given by:

$$K = \alpha e^2 / 2 \qquad (15)$$

where α is the atomic polarizability of the neutral gas (Banks, 1966).

CONCLUSION

The collisional transfer rates for Maxwell molecules interactions were computed and the obtained results confirmed the earlier values published by Chapman & Cowling (1970). Attention was called, however, as to the importance of the actual form employed for the potential energy (see Eq. 2) to the final result. The form used in this work is consistent with that of Banks (1966) from which the constant K can be obtained for the most common ion neutral interactions in the upper atmosphere.

APPENDIX

A RELATION INVOLVING THE IMPACT PARAMETER AND THE APSE ANGLE

In this appendix we present the computation of the integral of Eq. (3) necessary to establish the formal relation between θ and s. To start with we define new variables as:

$$y = s/x, \qquad (A.1)$$

$$b = s[(\mu w^2)/(2K)]^{1/4} \qquad (A.2)$$

Replacement of variables in Eq. (3) yields:

$$\theta = \int_0^{\hat{y}} \frac{dy}{\left[1 - y^2 - (y/b)^n\right]^{1/2}} \qquad (A.3)$$

where $\hat{y}$ satisfies:

$$1 - \hat{y}^2 - (\hat{y}/b)^n = 0 \qquad (A.4)$$

We are interested in the particular case of n=4, for which the solution of Eq. (A.4) becomes:

$$\hat{y}^2_{1,2} = -\frac{1 \pm \left(1 + 4/b^4\right)^{1/2}}{2/b^4} \qquad (A.5)$$

and, in special, is the lower sign solution which has a physical sense. Hence:

$$\hat{y} = \hat{y}_2 = \pm\left[\frac{\left(b^8 + 4b^4\right)^{1/2} - b^4}{2}\right]^{1/2} \qquad (A.6)$$

To integrate Eq. (A.3) for the case n= 4 we write it as:

$$\theta = b^2 \int_0^{\hat{y}} \frac{dy}{\left[-\left(y^2 - \hat{y}_1^2\right)\left(y^2 - \hat{y}_1^2\right)\right]^{/}} \qquad (A.7)$$

which can be put in a more tractable form making the substitution $y = \hat{y} \sin u$.
One then gets:

$$\theta = b^2 \int_0^{\pi/2} \frac{du}{\left(\hat{y}^2 \sin^2 u - \hat{y}_1^2\right)^{1/2}} \qquad (A.8)$$

Now recalling that $\hat{y}^2 + \hat{y}_1{}^2 = -b^4$ we have:

$$\theta = b^2 \int_0^{\pi/2} \frac{du}{\left[\hat{y}^2\left(1 + \sin^2 u\right) + b^4\right]^{1/2}} \qquad (A.9)$$

If we call $a^2 = \hat{y}^2 + b^4$ and $k^2 = \hat{y}^2/a^2$ results:

$$\theta = \left(b^2/a\right)\int_0^{\pi/2} \frac{du}{\left(1 + k^2 \sin^2 u\right)^{1/2}} \qquad (A.10)$$

To solve it one uses the binomial expansion and get:

$$I = \int_0^{\pi/2} \left[1 - 0.5k^2\sin^2 u + 0.375k^4\sin^4 u - 0.3125k^6\sin^6 u + 0.2734k^8\sin^8 u - 0.2461k^{10}\sin^{10} u + 0.2256k^{12}\sin^{12} u - \ldots\right] du \qquad (A.11)$$

Note that $b \rightarrow 0 \Rightarrow k^2 \rightarrow 1$ and $b \rightarrow \infty \Rightarrow k^2 \rightarrow 0$. Hence the largest error in the computation of I occurs for $b \rightarrow 0$. However, in this case $(b^2/a) \rightarrow 0 \Rightarrow \theta \rightarrow 0$. The largest value of I occurs for $b \rightarrow \infty$, when $(b^2/a) \rightarrow 1$ and $k^2 \rightarrow 0$, in which case $I = \pi/2$ and then $\theta = \pi/2$. For values of b such that $0 < b < \infty$ the above integral of Eq. (A.11) converges rapidly since it can be expressed in the form:

$$I = (\pi/2)\left[1 - (1/2)^2 k^2 + \left(\frac{1.3}{2.4}\right)^2 k^4 - \left(\frac{1.3.5}{2.4.6}\right)^2 k^6 + \left(\frac{1.3.5.7}{2.4.6.8}\right)^2 k^8 - \ldots\right]. \qquad (A.12)$$

REFERENCES

Banks, P. -1966- Collision Frequencies and Energy Transfer: Ions. Planet Space Sci., **14:** 1105-1122.

Barakat, A.R. & Schunk, R.W. -1982- Transport Equations for Multicomponent Anisotropic Space Plasmas: A Review. Plasma Phys., **24:** 389-418.

Burgers, J.M. -1969- Flow Equations for Composite Gases. Academic Press, New York and London, 332 pp.

Cercignani, C. -1988- The Boltzmann Equation and its Applications. Springer-Verlag, New York, 455 pp.

Chapman, S. & Cowling, T.G. -1970- The Mathematical Theory of Non-Uniform Gases. Cambridge, 422 pp.

Liboff, R.L. -1969- Introduction to the Theory of Kinetic Equations. John Wiley, New York, 397 pp.

Schunk, R.W. -1975- Transport Equations for Aeronomy. Planet. Space Sci., **23:** 437-485.

Schunk, R.W. -1977- Mathematical Structure of Transport Equations for Multispecies Flows. Rev. Geophys. Space Phys., **15:** 429-445.

Submetido em: 15/03/94
Revisado pelo(s) autor(es) em: 18/10/94
Aceito em: 20/10/94