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1976 J. Phys. A: Math. Gen. 9 771

(http://iopscience.iop.org/0305-4470/9/5/012)

J. Phys. A: Math. Gen., Vol. 9, No. 5, 1976. Printed in Great Britain. © 1976

The Boltzmann equation for fast atoms

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Received 26 November 1975, in final form 28 January 1976

Abstract. A rigorous derivation of the linear equations which describe the relaxation of a gas mixture to equilibrium is given. These equations contain new representations of the collision kernel and enable a better understanding of the rate and manner of disturbances in a gas. By specializing to the case of stationary scattering centres, with a small perturbed fast group, we arrive at the general equations of radiation damage which yield the collision density of slowed down particles. The equation adjoint to this is shown to be closely related to the equations of radiation damage deduced by other authors. Our equations are obtained by a logical sequence of approximations based upon the non-linear Boltzmann equation for gas mixtures.

1. Introduction

The ubiquity of the Boltzmann transport equation is truly remarkable. This particle balance equation for the velocity distribution function describes the behaviour not only of gas atoms but also of charged particles, neutrons, photons and phonons. Early practical work on the transport equation, other than the pioneering advances of Boltzmann, Maxwell and Hilbert, may be associated with the names of Pidduck (1915), Chapman (1916, 1917) and Enskog (1917). The main purpose of these authors was to obtain solutions to the linearized transport equation for the calculation of intrinsic properties of gases such as viscosity, thermal conductivity and diffusion rates. Subsequent work extended the scope of the transport equation to cover new particles as they were discovered (Davison 1957, Chandrasekhar 1960, Jancel and Kahan 1966).

In recent years the Boltzmann equation has found further applications in the study of radiation damage (Sigmund 1972, Leibfried and Mika 1965, Dederichs *et al* 1966). In this important field of study, the main approach has been to regard the medium as a random collection of scatterers and to calculate the particle range and the number of atomic displacements, both of which can give a measure of damage. Also in this area falls the problem of surface sputtering, a topic of immense importance in assessing the viability of potential thermonuclear reactors. In this respect, the equations of damage have been formulated by basic balance considerations (Lindhard *et al* 1968) without direct reference to the Boltzmann equation. Such a derivation, whilst satisfactory, is unable to highlight the limitations of the method and can lead to misunderstandings when the effects of thermal motion are to be studied. Moreover, a consistent approximation procedure based upon well-established principles is intrinsically more satisfactory and less open to criticism.

It is the purpose of this paper to establish the equations for the slowing down of fast particles in a medium composed of an arbitrary number of different scattering species, directly from the Boltzmann equation. We must state at the outset that in order to do this in the context of radiation damage in solids or molecular liquids, it is necessary to assume binary collisions. Such an assumption is usually made in current damage theories and whilst it may be open to question in some situations we do not intend to offer any alternative here (Sigmund 1974). The other main assumption throughout this work is that there exists an energy (of the order of 25 eV) above which atoms recoil freely when struck as though they were the constituents of a gas. These recoil atoms in turn strike further atoms and so on, thereby producing a cascade process. Such a process is ideally described by the transport equation. We shall not consider the specific damage function, which determines the number of atomic displacements, since there are a variety of mechanisms postulated for this, none of which depend specifically on the Boltzmann equation.

In addition to a derivation of the basic damage equations we shall in the course of our work obtain a very general set of equations for the relaxation of a gas mixture governed by arbitrary scattering laws. The scattering kernels so obtained are generalizations of those obtained many years ago by other authors (Ferziger and Kaper 1972); we believe, however, that in the form presented here they are a novel contribution. The limit of these kernels for stationary scatterers is identical to those deduced by previous authors. Finally, we shall discuss the adjoint Boltzmann equation and its physical meaning.

2. General theory

2.1. The basic equation

The Boltzmann equation for a mixture of atoms undergoing binary collisions may be written as follows:

$$\left(\frac{\partial}{\partial t}+\boldsymbol{v}\cdot\nabla_{\boldsymbol{r}}+\boldsymbol{a}_i\cdot\nabla_{\boldsymbol{v}}\right)f_i(\boldsymbol{v},\boldsymbol{r},t)=\left(\frac{\partial f_i}{\partial t}\right)_{\text{coll}} \tag{1}$$

where $f_i(\boldsymbol{v}, \boldsymbol{r}, t)$ is the distribution function of atoms of type i and $\boldsymbol{a}_i$ is the acceleration on a particle due to external forces. The terms on the left-hand side of the equation denote drift out of a phase space element due to particle motion. The term on the right-hand side represents changes in the distribution function due to collisions. It is this term that must now be considered in some detail.

From the usual arguments (Williams 1971) we may write the collision terms as follows:

$$\begin{aligned}\left(\frac{\partial f_i}{\partial t}\right)_{\text{coll}}=\sum_j\int \mathrm{d}\boldsymbol{v}_1\int \mathrm{d}\boldsymbol{v}_1'\int \mathrm{d}\boldsymbol{v}'[W_{ij}(\boldsymbol{v}_1'\rightarrow\boldsymbol{v}_1;\boldsymbol{v}'\rightarrow\boldsymbol{v})f_i(\boldsymbol{v}')f_j(\boldsymbol{v}_1')\\ -W_{ij}(\boldsymbol{v}_i\rightarrow\boldsymbol{v}_1';\boldsymbol{v}\rightarrow\boldsymbol{v}')f_i(\boldsymbol{v})f_j(\boldsymbol{v}_1)]\end{aligned} \tag{2}$$

where $W_{ij}(\ldots)$ is the transition probability, defined below, for scattering of particles with velocities $(\boldsymbol{v}_1', \boldsymbol{v}')$ before collision to velocities $(\boldsymbol{v}_1, \boldsymbol{v})$ after collision. We have suppressed the independent variables $(\boldsymbol{r}, t)$ in the distribution functions.

In order to reduce equation (2) to a convenient form we shall write $f_i(\boldsymbol{v})$ as follows:

$$f_i(\boldsymbol{v})=n_if_{M_i}(\boldsymbol{v})+G_i(\boldsymbol{v}) \tag{3}$$

where n_i is the number of atoms in the equilibrium Maxwell–Boltzmann distribution $f_{M_i}(\boldsymbol{v})$ and $G_i(\boldsymbol{v})$ is the number of atoms disturbed from equilibrium. Inserting (3) into (2) and multiplying out, the quantity in square brackets becomes, in obvious notation,

$$\begin{aligned}\bar{W}_{ij}\{n_i n_j f_{M_i}(\boldsymbol{v}')f_{M_j}(\boldsymbol{v}_1') + n_j f_{M_j}(\boldsymbol{v}_1')G_i(\boldsymbol{v}') + n_i f_{M_i}(\boldsymbol{v}')G_j(\boldsymbol{v}_1') + G_i(\boldsymbol{v}')G_j(\boldsymbol{v}_1')\}\\ - \bar{W}_{ij}\{n_i n_j f_{M_i}(\boldsymbol{v})f_{M_j}(\boldsymbol{v}_1) + n_j f_{M_j}(\boldsymbol{v}_1)G_i(\boldsymbol{v}) + n_i f_{M_i}(\boldsymbol{v})G_j(\boldsymbol{v}_1)\\ + G_i(\boldsymbol{v})G_j(\boldsymbol{v}_1)\}. \qquad (4)\end{aligned}$$

Now using detailed balance, i.e. $\vec{W}_{ij} = \bar{W}_{ij}$, we note that the terms involving the equilibrium distributions $f_M(\boldsymbol{v})$ vanish. Moreover, we make the assumption that the density of perturbed atoms is so small that the chance of a perturbed atom colliding with another perturbed atom is negligibly small. Thus we may neglect the terms involving the products G_iG_j. The physical process therefore is one of perturbed atoms in collision with thermal atoms: note, however, that any struck thermal atom can enter the perturbed distribution and in turn cause further perturbations. We have therefore a cascade effect which is described accurately by the following collision rate:

$$\begin{aligned}\sum_j \int d\boldsymbol{v}_1 \int d\boldsymbol{v}_1' \int d\boldsymbol{v}'[\vec{W}_{ij}\{n_j f_{M_j}(\boldsymbol{v}_1')G_i(\boldsymbol{v}') + n_i f_{M_i}(\boldsymbol{v}')G_j(\boldsymbol{v}_1')\}\\ - \bar{W}_{ij}\{n_j f_{M_j}(\boldsymbol{v}_1)G_i(\boldsymbol{v}) + n_i f_{M_i}(\boldsymbol{v})G_j(\boldsymbol{v}_1)\}] = \left(\frac{\partial f_i}{\partial t}\right)_{\text{coll}}. \qquad (5)\end{aligned}$$

2.2. *The scattering kernel*

Any further progress depends upon an evaluation of the kernel appearing in equation (5). In specifying $\vec{W}_{ij}$ we follow the procedure discussed by Williams (1971) from which we can write

$$\begin{aligned}W_{ij}(\boldsymbol{v}_1' \to \boldsymbol{v}_1; \boldsymbol{v}' \to \boldsymbol{v})\\ = \sigma_{ij}(|\boldsymbol{v}_1' - \boldsymbol{v}'|; \cos^{-1}\{(\boldsymbol{v}_1' - \boldsymbol{v}') \cdot (\boldsymbol{v}_1 - \boldsymbol{v})/(\boldsymbol{v}_1' - \boldsymbol{v}')^2\}) \frac{2M_1}{M_2}(M_1 + M_2)^2\\ \times \delta_3(M_1\boldsymbol{v}' + M_2\boldsymbol{v}_1' - M_1\boldsymbol{v} - M_2\boldsymbol{v}_1)\delta(M_1v'^2 + M_2v_1'^2 - M_1v^2 - M_2v_1^2) \qquad (6)\end{aligned}$$

where the δ functions denote conservation of momentum and energy and $\sigma_{ij}(g, \theta_c)$ is the scattering cross section for particles with relative velocity $\boldsymbol{g}$ to be scattered through an angle θ_c in the centre-of-mass system.

Using equation (6) we may evaluate the averages over $\vec{W}_{ij}$ which arise in equation (5). Suppressing the subscripts i and j, we must calculate the following ($i = 1, j = 2$):

$$\int d\boldsymbol{v}_1 \int d\boldsymbol{v}_1' \int d\boldsymbol{v}' f_{M_2}(\boldsymbol{v}_1)G(\boldsymbol{v})\vec{W}_{ij}. \qquad (7)$$

Inserting the scattering kernel and performing the integration over $\boldsymbol{v}_1'$ with the properties of the delta function δ_3 noted, reduces the integral readily to one over $\boldsymbol{v}_1$ and $\boldsymbol{v}'$. Introducing a change of variables $\boldsymbol{g} = \boldsymbol{v}_1 - \boldsymbol{v}$ and $\boldsymbol{g}' = \boldsymbol{v}_1 + M_1\boldsymbol{v}/M_2 - (M_1 + M_2)\boldsymbol{v}'/M_2$ and noting that

$$d\boldsymbol{v}_1\, d\boldsymbol{v}' = \left(\frac{M_2}{M_1 + M_2}\right)^3 d\boldsymbol{g}\, d\boldsymbol{g}'$$

we can simplify our integral (7) into the following form:

$$2G(\boldsymbol{v}) \int d\boldsymbol{g} \int d\boldsymbol{g}' f_{M_2}(\boldsymbol{g}+\boldsymbol{v})\sigma(g'; \cos^{-1}\{\boldsymbol{g}'\,.\,\boldsymbol{g}/g'^2\})\delta(g^2-g'^2). \tag{8}$$

Defining polar coordinates such that $\boldsymbol{g}'\,.\,\boldsymbol{g} = gg'\cos\theta_c$ and $d\boldsymbol{g}' = g'^2\,dg'\sin\theta_c\,d\theta_c\,d\phi_c$ we find

$$G(\boldsymbol{v}) \int d\boldsymbol{g} f_{M_2}(\boldsymbol{g}+\boldsymbol{v}) g 2\pi \int_0^{\pi} \sin\theta_c\,d\theta_c \sigma(g, \theta_c) \tag{9}$$

which can be written

$$G(\boldsymbol{v}) \int d\boldsymbol{g} f_{M_2}(\boldsymbol{g}+\boldsymbol{v}) g\sigma(g) \equiv G(\boldsymbol{v}) v\bar{\sigma}(v) \tag{10}$$

where $\sigma(g)$ is the total cross section and $\bar{\sigma}(g)$ is defined by the average over f_{M_2} as indicated.

Now there are two important distributions to consider for $f_{M_2}(\boldsymbol{v})$. The first is the Maxwell–Boltzmann distribution when

$$f_{M_2}(\boldsymbol{v}) = \left(\frac{M_2}{2\pi kT}\right)^{3/2} \exp\left(-\frac{M_2 v^2}{2kT}\right) \tag{11}$$

and the second is $f_{M_2}(\boldsymbol{v}) = \delta(\boldsymbol{v})$, i.e. the limit of the Maxwellian as the scatterers become stationary. The latter distribution is a useful approximation when the perturbed particles have energies very much greater than kT.

In the case of the Maxwellian, equation (10) can be written

$$G(\boldsymbol{v}) \frac{4\pi kT}{M_2 v} \left(\frac{M_2}{2\pi kT}\right)^{3/2} \exp\left(-\frac{M_2 v^2}{2kT}\right) \int_0^{\infty} dg\, g^2 \sigma(g) \exp\left(-\frac{M_2 g^2}{2kT}\right) \sinh\left(\frac{M_2 v g}{kT}\right) \tag{12}$$

whereas for stationary scatterers it becomes

$$G(\boldsymbol{v}) v\sigma(v). \tag{13}$$

The next term to be obtained is

$$\int d\boldsymbol{v}_1 \int d\boldsymbol{v}_1' \int d\boldsymbol{v}' f_{M_2}(\boldsymbol{v}_1') G(\boldsymbol{v}') \vec{W}_{ij}. \tag{14}$$

Integrating out the δ_3 function as before we are left with an integral over $\boldsymbol{v}_1'$ and $\boldsymbol{v}'$. The integral over $\boldsymbol{v}'$ cannot be performed since $G(\boldsymbol{v}')$ is the dependent variable. However, writing equation (14) in the form

$$\int d\boldsymbol{v}' G(\boldsymbol{v}') \sigma_{\mathrm{I}}(\boldsymbol{v}' \to \boldsymbol{v}) \tag{15}$$

it is possible to obtain an expression for σ_{I}. This involves some careful integrating over the remaining delta function and a change of variable. Details are given in the appendix and the result can be written in the following concise manner:

$$\sigma_{\mathrm{I}}(\boldsymbol{v}' \to \boldsymbol{v}) = \frac{(M_1+M_2)^2}{M_2^2} \int d\boldsymbol{g}' f_{M_2}(\boldsymbol{g}'+\boldsymbol{v}') \sigma\left(g'; \cos^{-1}\left\{1 - \tfrac{1}{2}\left(\frac{M_1+M_2}{M_2}\right)^2 \frac{(\boldsymbol{v}'-\boldsymbol{v})^2}{g'^2}\right\}\right)$$
$$\times \delta\left(\frac{M_1+M_2}{2M_2}(\boldsymbol{v}'-\boldsymbol{v})^2 - \boldsymbol{g}'\,.\,(\boldsymbol{v}-\boldsymbol{v}')\right). \tag{16}$$

To proceed further, it is necessary to specify f_M. Thus in the case of the Maxwellian function, equation (16) may be cast into the following form (details in appendix):

$$\sigma_I(\boldsymbol{v}'\to\boldsymbol{v})=\frac{\pi}{8}\frac{(M_1+M_2)^4}{M_2^4}\left(\frac{M_2}{2\pi kT}\right)^{3/2}|\boldsymbol{v}'-\boldsymbol{v}|\exp\left\{-\frac{M_2v'^2}{2kT}-\frac{(M_1+M_2)^2}{8kTM_2}(\boldsymbol{v}'-\boldsymbol{v})^2 -\frac{M_1+M_2}{2kT}\boldsymbol{v}'\cdot(\boldsymbol{v}-\boldsymbol{v}')\right\}\int_0^{\pi}\frac{\sin\theta_c\,d\theta_c}{\sin^4\theta_c/2}\sigma\left(\frac{M_1+M_2}{2M_2}\frac{|\boldsymbol{v}'-\boldsymbol{v}|}{\sin\theta_c/2};\theta_c\right) \times\exp\left\{-\frac{(M_1+M_2)^2}{8kTM_2}(\boldsymbol{v}'-\boldsymbol{v})^2\cot^2\frac{\theta_c}{2}\right\}I_0\left(\frac{M_1+M_2}{2kT}|\boldsymbol{v}\times\boldsymbol{v}'|\cot\frac{\theta_c}{2}\right). \quad (17)$$

For stationary scatterers we can set $f_{M_2}(\boldsymbol{g}'+\boldsymbol{v}')=\delta(\boldsymbol{g}'+\boldsymbol{v}')$ in equation (16). σ_I then becomes

$$\sigma_I(\boldsymbol{v}'\to\boldsymbol{v})=\frac{(M_1+M_2)^2}{M_1M_2}\frac{\sigma(v',\theta_c)}{vv'}\delta\left(\mu_0-\frac{M_1+M_2}{2M_1}\frac{v}{v'}+\frac{M_2-M_1}{2M_1}\frac{v'}{v}\right) \quad (18)$$

where

$$\cos\theta_c\left(\frac{v}{v'}\right)=\frac{(M_1+M_2)^2}{2M_1M_2}\left(\frac{v}{v'}\right)^2-\frac{M_1^2+M_2^2}{2M_1M_2}$$

and μ_0 is the cosine of the angle between $\boldsymbol{v}$ and $\boldsymbol{v}'$.

The δ function in equation (18) implies the following restriction on v':

$$v\left|\frac{M_2+M_1}{M_2-M_1}\right|\geqslant v'\geqslant v.$$

The next term in equation (5) to be reduced is

$$\int d\boldsymbol{v}_1'\int d\boldsymbol{v}_1\int d\boldsymbol{v}'\,f_{M_1}(\boldsymbol{v}')G(\boldsymbol{v}_1')\vec{W}_{ij}. \quad (19)$$

Following the procedure outlined above and given in detail in the appendix, we obtain

$$\int d\boldsymbol{v}_1'\;G(\boldsymbol{v}_1')\sigma_{II}(\boldsymbol{v}_1'\to\boldsymbol{v}) \quad (20)$$

where

$$\sigma_{II}(\boldsymbol{v}_1'\to\boldsymbol{v})=\frac{(M_1+M_2)^2}{M_2^2}\int d\boldsymbol{g}'\,f_{M_1}(\boldsymbol{v}_1'-\boldsymbol{g}') \times\sigma\left(g';\cos^{-1}\left\{\frac{(M_1+M_2)^2}{2M_1M_2}\frac{(\boldsymbol{v}_1'-\boldsymbol{v})^2}{g'^2}-\frac{M_1^2+M_2^2}{2M_1M_2}\right\}\right) \times\delta\left(\frac{M_1}{M_2}\boldsymbol{g}'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})+\frac{M_2-M_1}{2M_2}g'^2-\frac{M_1+M_2}{2M_2}(\boldsymbol{v}_1'-\boldsymbol{v})^2\right). \quad (21)$$

When the Maxwellian $f_{M_1}(\boldsymbol{v})$ is used in equation (21), we find after some considerable effort

$$\sigma_{\mathrm{II}}(\boldsymbol{v}_1'\to\boldsymbol{v})=2\pi(M_1+M_2)^4\left(\frac{M_1}{2\pi kT}\right)^{3/2}|\boldsymbol{v}_1'-\boldsymbol{v}|\exp\left\{-\frac{M_1v_1'^2}{2kT}\right\}$$
$$\times\int_0^\pi\frac{\sin\theta_c\,d\theta_c}{(M_1^2+M_2^2-2M_1M_2\cos\theta_c)^2}\sigma\left(\frac{(M_1+M_2)|\boldsymbol{v}_1'-\boldsymbol{v}|}{(M_1^2+M_2^2-2M_1M_2\cos\theta_c)^{1/2}};\pi-\theta_c\right)$$
$$\times\exp\left\{-\frac{M_1}{2kT}\frac{(\boldsymbol{v}_1'-\boldsymbol{v})^2(M_1+M_2)^2}{M_1^2+M_2^2-2M_1M_2\cos\theta_c}\right.$$
$$\left.+\frac{M_1}{kT}\frac{(M_1+M_2)(M_1-M_2\cos\theta_c)}{M_1^2+M_2^2-2M_1M_2\cos\theta_c}\boldsymbol{v}_1'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})\right\}$$
$$\times I_0\left(\frac{M_1}{kT}|\boldsymbol{v}_1'\times\boldsymbol{v}|\frac{(M_1+M_2)M_2\sin\theta_c}{M_1^2+M_2^2-2M_1M_2\cos\theta_c}\right). \tag{22}$$

For stationary scatterers we get

$$\sigma_{\mathrm{II}}(\boldsymbol{v}_1'\to\boldsymbol{v})=\frac{(M_1+M_2)^2}{M_2^2}\frac{\sigma(v_1';\theta_c')}{vv_1'}\delta\left(\mu_0'-\frac{M_1+M_2}{2M_2}\left(\frac{v}{v_1'}\right)\right) \tag{23}$$

where

$$\cos\theta_c'\left(\frac{v}{v_1'}\right)=1-\frac{1}{2}\left(\frac{M_1+M_2}{M_2}\right)^2\left(\frac{v}{v_1'}\right)^2 \tag{24}$$

$$\equiv\cos\theta_c\left(1-\frac{M_1v^2}{M_2v_1'^2}\right)^{1/2} \tag{25}$$

This last relationship will prove to be of value in later work. μ_0' is the cosine of the angle between $\boldsymbol{v}$ and $\boldsymbol{v}_1'$, and v_1' is restricted in the following manner:

$$\infty>v_1'\geqslant\frac{M_1+M_2}{2M_2}v. \tag{26}$$

The final term to be considered is

$$\int d\boldsymbol{v}_1\int d\boldsymbol{v}_1'\int d\boldsymbol{v}'\,f_{M_1}(\boldsymbol{v})G(\boldsymbol{v}_1)\vec{W}_{ij} \tag{27}$$

the reduction of which follows that of equation (7). Hence we obtain

$$\int d\boldsymbol{v}_1G(\boldsymbol{v}_1)\sigma_{\mathrm{III}}(\boldsymbol{v}_1\to\boldsymbol{v}) \tag{28}$$

where

$$\sigma_{\mathrm{III}}(\boldsymbol{v}_1\to\boldsymbol{v})=f_{M_1}(\boldsymbol{v})|\boldsymbol{v}_1-\boldsymbol{v}|\sigma(|\boldsymbol{v}_1-\boldsymbol{v}|). \tag{29}$$

For the case of a Maxwellian–Boltzmann distribution

$$\sigma_{\mathrm{III}}(\boldsymbol{v}_1\to\boldsymbol{v})=\left(\frac{M_1}{2\pi kT}\right)^{3/2}\exp\left\{-\frac{M_1v^2}{2kT}\right\}|\boldsymbol{v}-\boldsymbol{v}_1|2\pi\int_0^\pi d\theta_c\sin\theta_c\sigma(|\boldsymbol{v}-\boldsymbol{v}_1|;\theta_c). \tag{30}$$

For stationary scatterers equation (28) reduces simply to

$$\delta(\boldsymbol{v})\int d\boldsymbol{v}_1 G(\boldsymbol{v}_1)v_1\sigma(v_1). \tag{31}$$

2.3. *Physical meaning of the scattering function*

The collision rate defined in equation (5) can now be written in a more concise fashion, namely:

$$\left(\frac{\partial f_i}{\partial t}\right)_{\text{coll}}=\sum_j\left\{n_j\int d\boldsymbol{v}'\, G_i(\boldsymbol{v}')\sigma_{\text{I}}^{(ij)}(\boldsymbol{v}'\to\boldsymbol{v})+n_i\int d\boldsymbol{v}_1'\, G_j(\boldsymbol{v}_1')\sigma_{\text{II}}^{(ij)}(\boldsymbol{v}_1'\to\boldsymbol{v})\right.$$
$$\left.-n_i\int d\boldsymbol{v}_1\, G_j(\boldsymbol{v}_1)\sigma_{\text{III}}^{(ij)}(\boldsymbol{v}_1\to\boldsymbol{v})-n_j v\overline{\sigma_{ij}}(v)G_i(\boldsymbol{v})\right\}. \tag{32}$$

Each of the cross sections $\sigma^{(ij)}$ has a definite physical meaning. Firstly, we consider the case when $i\neq j$, then $\sigma_{\text{I}}^{(ij)}$ is the cross section for a particle of mass M_i, velocity $\boldsymbol{v}'$ before collision to be scattered by a particle of mass M_j into unit velocity interval at $\boldsymbol{v}$. $\sigma_{\text{II}}^{(ij)}$ is the cross section for a particle of mass M_j velocity $\boldsymbol{v}_1'$ before collision to be scattered by a particle of mass M_i and for the particle M_i to be scattered into unit velocity interval at $\boldsymbol{v}$. $\sigma_{\text{III}}^{(ij)}$ is the cross section for a particle of mass M_j, velocity $\boldsymbol{v}_1$ after collision to be accompanied by a particle of mass M_i which is scattered into unit velocity interval at $\boldsymbol{v}$. Finally, $\overline{\sigma_{ij}}$ is the total cross section for scattering of particles M_i with particles M_j. We note that $\sigma_{\text{I}}^{(ij)}$ and $\sigma_{\text{II}}^{(ij)}$ contribute to the velocity interval $\boldsymbol{v}$ of particles M_i, whereas $\sigma_{\text{III}}^{(ij)}$ and $\overline{\sigma_{ij}}$ deplete that velocity interval. The cross sections for $i\neq j$ in equations (32) have not been given before. The case for $i=j$, i.e. a single species gas, has been given and our general results in equations (17), (22) and (30) reduce to that case (Ferziger and Kaper 1972).

3. Equation for the slowing down of fast atoms

3.1. *The velocity distribution*

A considerable amount of effort has gone into obtaining solutions of the Boltzmann equation in the case of atoms slightly perturbed from the equilibrium distribution. It has been shown for example that the relaxation of a uniform gas can be represented in the following form (Cercignani 1969):

$$G(\boldsymbol{v},t)=\sum_i g_i(\boldsymbol{v})\,e^{-\lambda_i t}+\int d\lambda g_\lambda(\boldsymbol{v})\,e^{-\lambda t}. \tag{33}$$

The λ_i denote discrete eigenvalues and the integral term a continuous spectrum. The cases of hard spheres and Maxwell molecules are fully understood (Williams 1971). Difficulties arise when the initial distribution is composed of atoms with energies very much greater than kT. In such a case the contribution of the continuous spectrum is paramount and the associated mathematical treatment is cumbersome even for the two models cited earlier. A much more direct method for studying the velocity distribution of 'fast' atoms is to allow the physical temperature to become zero and to use the 'slowing down' kernels given by equations (13), (18), (23) and (30). This type of approach is used extensively in neutron transport theory.

Following this procedure and denoting $G(\boldsymbol{v})$ by $G(v, \boldsymbol{\Omega})$, where $\boldsymbol{\Omega}$ is the unit vector in the direction of travel of the particle, we find the following set of equations:

$$\frac{\partial G_i(v, \boldsymbol{\Omega}, \boldsymbol{r}, t)}{\partial t} + v\boldsymbol{\Omega} \cdot \nabla_{\boldsymbol{r}} G_i(v, \boldsymbol{\Omega}, \boldsymbol{r}, t) + \boldsymbol{a}_i \cdot \nabla_{\boldsymbol{v}} G_i(v, \boldsymbol{\Omega}, \boldsymbol{r}, t)$$
$$= \sum_j \frac{(M_i+M_j)^2}{M_i M_j} n_j \int_v^{\min\{v|(M_i+M_j)/(M_i-M_j)|, v_{0i}\}} \frac{v'}{v} \, dv'$$
$$\times \int d\boldsymbol{\Omega}' \, G_i(v', \boldsymbol{\Omega}', \boldsymbol{r}, t) \sigma_{ij}\left(v'; \theta_c\left(\frac{v}{v'}\right)\right) \delta\left(\mu_0 - f_{ij}\left(\frac{v}{v'}\right)\right)$$
$$+ \sum_j \frac{(M_i+M_j)^2}{M_j^2} n_i \int_{[(M_i+M_j)/2M_j]v}^{v_{0i}} \frac{v_1'}{v} \, dv_1'$$
$$\times \int d\boldsymbol{\Omega}_1' \, G_j(v_1', \boldsymbol{\Omega}_1', \boldsymbol{r}, t) \sigma_{ij}\left(v_1'; \theta_c\left(\left(1 - \frac{M_i v^2}{M_j v_1'^2}\right)^{1/2}\right)\right) \delta\left(\mu_0' - h_{ij}\left(\frac{v}{v_1'}\right)\right)$$
$$- \sum_j n_j v \sigma_{ij}(v) G_i(v, \boldsymbol{\Omega}, \boldsymbol{r}, t) + Q_i(v, \boldsymbol{\Omega}, \boldsymbol{r}, t). \quad (34)$$

A few points in this equation require some explanation. For example, it should be noted that we have omitted the term involving $\sigma_{\rm III}^{(ij)}$. In view of the presence of the term $\delta(\boldsymbol{v})$, this omission is justified on the following grounds. It does not contribute to conservation of energy or momentum; moreover, it represents the contribution to $G(\boldsymbol{v})$ of the zero energy particles or, to put it otherwise, it is the reduction in the number of stationary scatterers due to those which have been scattered to higher energies. Since by definition this is a small number and cannot have any appreciable effect on the total scattering, it may be ignored. For $T \neq 0$ it must not be ignored.

Further points requiring elucidation are the quantities

$$f_{ij}\left(\frac{v}{v'}\right) = \frac{M_i+M_j}{2M_i}\frac{v}{v'} - \frac{M_j-M_i}{2M_i}\frac{v'}{v} \quad (35)$$

and

$$h_{ij}\left(\frac{v}{v_1'}\right) = \frac{M_i+M_j}{2M_j}\frac{v}{v_1'}. \quad (36)$$

Also $\mu_0 = \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}'$, $\mu_0' = \boldsymbol{\Omega} \cdot \boldsymbol{\Omega}_1'$ and v_{0i} is the speed of the fastest particle from the source.

Equation (34) is quite general and will describe the slowing down of particles prescribed by any scattering law $\sigma_{ij}(v; \theta_c)$.

3.2. The energy distribution

It is frequently more convenient to write the Boltzmann equation in terms of the energy variable $E = \frac{1}{2}Mv^2$. Thus we define $E = \frac{1}{2}M_i v^2$, $E' = \frac{1}{2}M_i v'^2$ and $E_1' = \frac{1}{2}M_j v_1'^2$; the particle density N can therefore be written

$$v^2 G_i(v, \boldsymbol{\Omega}) \, dv = N_i(E, \boldsymbol{\Omega}) \, dE \quad (37)$$

and the source

$$v^2 Q_i(v, \boldsymbol{\Omega}) \, dv = S_i(E, \boldsymbol{\Omega}) \, dE. \quad (38)$$

Thus with

$$\alpha_{ij} = \left(\frac{M_i - M_j}{M_i + M_j}\right)^2$$

and introducing the energy dependent flux $\phi(E) = vN(E)$ we can reduce equation (34) to the following form:

$$\begin{aligned}
&\left(\frac{1}{v}\frac{\partial}{\partial t} + \boldsymbol{\Omega}\,.\,\nabla_{\boldsymbol{r}}\right)\phi_i(E, \boldsymbol{\Omega}, \boldsymbol{r}, t) \\
&\quad = \sum_j \frac{2n_j}{1-\alpha_{ij}} \int_E^{\min(E/\alpha_{ij}, E_{0i})} \frac{\mathrm{d}E'}{E'} \int \mathrm{d}\boldsymbol{\Omega}'\, \phi_i(E', \boldsymbol{\Omega}', \boldsymbol{r}, t)\, \sigma_{ij}\left(\left(\frac{2E'}{M_i}\right)^{1/2}; \theta_c\left(\left(\frac{E}{E'}\right)^{1/2}\right)\right) \\
&\qquad \times \delta\left(\mu_0 - f_{ij}\left(\left(\frac{E}{E'}\right)^{1/2}\right)\right) + \sum_j \frac{2n_i}{1-\alpha_{ij}} \int_{E/(1-\alpha_{ij})}^{E_{0i}} \frac{\mathrm{d}E_1'}{E_1'} \int \mathrm{d}\boldsymbol{\Omega}_1'\, \phi_j(E_1', \boldsymbol{\Omega}_1', \boldsymbol{r}, t) \\
&\qquad \times \sigma_{ij}\left(\left(\frac{2E_1'}{M_j}\right)^{1/2}; \theta_c\left(\left(\frac{E_1'-E}{E_1'}\right)^{1/2}\right)\right) \delta\left(\mu_0' - h_{ij}\left(\left(\frac{M_jE}{M_iE_1'}\right)^{1/2}\right)\right) \\
&\qquad - \sum_j n_j \sigma_{ij}\left(\left(\frac{2E}{M_i}\right)^{1/2}\right) \phi_i(E, \boldsymbol{\Omega}, \boldsymbol{r}, t) + S_i(E, \boldsymbol{\Omega}, \boldsymbol{r}, t)
\end{aligned} \tag{39}$$

where for simplicity we have omitted the force term on the left-hand side. The equation will be recognized as being similar to the equation for neutron slowing down. The difference arises from the second integral term on the right-hand side which accounts for the recoil of the scattered particles. In neutron transport theory this may be neglected, whereas in many other problems involving particle cascades it may not. If the time and space dependence of equation (39) is omitted and the equation is integrated over the angular variable, it reduces to the infinite medium, steady state equations of Kostin (1965, 1966) and Kostin and Felder (1966). The equations (39) have not appeared in the literature before.

3.3. *The adjoint equation*

An important conclusion of our work may be obtained by considering the equation partially adjoint to equation (39) with respect to energy: thus if we define $\psi(E, \boldsymbol{\Omega}, \boldsymbol{r}, t)$ as the partial adjoint, it becomes the solution of

$$\begin{aligned}
&\left(\frac{1}{v}\frac{\partial}{\partial t} + \boldsymbol{\Omega}\,.\,\nabla_{\boldsymbol{r}}\right)\psi_i(E, \boldsymbol{\Omega}, \boldsymbol{r}, t) \\
&\quad = \sum_j \frac{2n_j}{1-\alpha_{ij}} \int_{\alpha_{ij}E}^{E} \frac{\mathrm{d}E'}{E} \int \mathrm{d}\boldsymbol{\Omega}'\, \psi_i(E', \boldsymbol{\Omega}', \boldsymbol{r}, t) \sigma_{ij}\left(\left(\frac{2E}{M_i}\right)^{1/2}; \theta_c\left(\left(\frac{E'}{E}\right)^{1/2}\right)\right) \\
&\qquad \times \delta\left(\mu_0 - f_{ij}\left(\left(\frac{E'}{E}\right)^{1/2}\right)\right) \\
&\qquad + \sum_j \frac{2n_j}{1-\alpha_{ij}} \int_0^{(1-\alpha_{ij})E} \frac{\mathrm{d}E_1'}{E} \int \mathrm{d}\boldsymbol{\Omega}_1'\ \psi_j(E_1', \boldsymbol{\Omega}_1', \boldsymbol{r}, t) \\
&\qquad \times \sigma_{ij}\left(\left(\frac{2E}{M_i}\right)^{1/2}; \theta_c\left(\left(\frac{E-E_1'}{E}\right)^{1/2}\right)\right) \delta\left(\mu_0' - h_{ij}\left(\left(\frac{M_iE_1'}{M_jE}\right)^{1/2}\right)\right) \\
&\qquad - \sum_j n_j \sigma_{ij}\left(\left(\frac{2E}{M_i}\right)^{1/2}\right) \psi_i(E, \boldsymbol{\Omega}, \boldsymbol{r}, t) + S_i^{\dagger}(E, \boldsymbol{\Omega}, \boldsymbol{r}, t).
\end{aligned} \tag{40}$$

Setting $E' = E - E'_1$ in the first integral term on the right-hand side of equation (40) that term becomes

$$\sum_j \frac{2n_j}{1-\alpha_{ij}} \int_0^{(1-\alpha_{ij})E} \frac{\mathrm{d}E'_1}{E} \int \mathrm{d}\boldsymbol{\Omega}'\, \psi_i(E-E'_1, \boldsymbol{\Omega}, \boldsymbol{r}, t)\sigma_{ij}\left(\left(\frac{2E}{M_i}\right)^{1/2}; \theta_c\left(\left(\frac{E-E'_1}{E}\right)^{1/2}\right)\right)$$
$$\times \delta\left(\mu_0 - f_{ij}\left(\left(\frac{E-E'_1}{E}\right)^{1/2}\right)\right). \tag{41}$$

Defining $T = E'_1$, we have then changed our Boltzmann equation to the 'backward' form deduced by Sigmund and Lindhard *et al.* To complete the picture the adjoint source must be defined as

$$S_i^\dagger(E, \boldsymbol{\Omega}, \boldsymbol{r}, t) = \frac{1}{4\pi}\delta(\boldsymbol{r}-\boldsymbol{r}_0)\delta(E-E_{0i})\delta(t) \tag{42}$$

then, from the definition of the adjoint (or importance) function (Lewins 1965),

$$\psi(E, \boldsymbol{\Omega}, \boldsymbol{r}_0, 0 \to E_{0i}, \boldsymbol{r}, t)\, \mathrm{d}E_{0i}\, \mathrm{d}\boldsymbol{r} \tag{43}$$

is the mean number of atoms averaged over direction with energy in the range $(E_{0i}, E_{0i} + \mathrm{d}E_{0i})$ in the volume element $\mathrm{d}\boldsymbol{r}$ at time t due to a primary atom of energy E, direction $\boldsymbol{\Omega}$ at $\boldsymbol{r}_0$ at time zero. It should be noted that in the backward formulation, it is the initial energies and directions that are the independent variables.

4. Discussion

In the introduction we have outlined the large range of problems in which the Boltzmann equation can be employed. The derivation that followed of the equations of radiation damage reinforce that remark and also illustrate the role played by the adjoint equation or backward formulation. As we have noted, the backward equations can be derived from direct physical arguments. However, it does not seem possible to obtain them in that form directly from the non-linear Boltzmann equation. The most rigorous formulation in that respect would be to start from the backward form of the Smoluchowski equations, which are inherently linear and do not therefore enable the limitations of the perturbation theory to be assessed (Lindhard and Nielsen 1971). The present method is an advance since it enables errors to be assessed by solving the non-linear equations which arise from overlapping cascades. Whilst the equations derived here are similar to those deduced by earlier workers, the associated scattering kernels in their most general form have not appeared before and therefore open the way to a better understanding of time and space relaxation in gas mixtures.

We have not discussed any applications of the damage equations since this aspect and the related one of time and space variation will be presented in a companion paper.

Appendix. Derivation of the scattering kernel

In order to demonstrate the general technique used to calculate the scattering kernels we shall consider only σ_{II}; the calculations of σ_I and σ_{III} are similar.

The explicit form of equation (20) in the text may be written thus

$$\int d\boldsymbol{v}_1 \int d\boldsymbol{v}_1' \int d\boldsymbol{v}' f_{M_1}(\boldsymbol{v}') G(\boldsymbol{v}_1') \frac{2M_1}{M_2}(M_1+M_2)^2$$
$$\times \delta_3(M_1\boldsymbol{v}'+M_2\boldsymbol{v}_1'-M_1\boldsymbol{v}-M_2\boldsymbol{v}_1)\ \delta(M_1v'^2+M_2v_1'^2-M_1v^2-M_2v_1^2)$$
$$\times\sigma\left(|\boldsymbol{v}_1'-\boldsymbol{v}'|;\cos^{-1}\left\{\frac{(\boldsymbol{v}_1'-\boldsymbol{v}')\cdot(\boldsymbol{v}_1-\boldsymbol{v})}{(\boldsymbol{v}_1'-\boldsymbol{v}')^2}\right\}\right). \tag{A.1}$$

Integrating over $\boldsymbol{v}_1$ using the property of the delta function δ_3, we find

$$\int d\boldsymbol{v}_1' \int d\boldsymbol{v}' f_{M_1}(\boldsymbol{v}') G(\boldsymbol{v}_1') \frac{2M_1}{M_2^2}(M_1+M_2)^2$$
$$\times\sigma\left(|\boldsymbol{v}_1'-\boldsymbol{v}'|;\cos^{-1}\left\{\frac{(\boldsymbol{v}_1'-\boldsymbol{v}')\cdot[\boldsymbol{v}_1'+(M_1/M_2)(\boldsymbol{v}'-\boldsymbol{v})-\boldsymbol{v}]}{(\boldsymbol{v}_1'-\boldsymbol{v}')^2}\right\}\right)$$
$$\times\delta(M_1v'^2+M_2v_1'^2-M_1v^2-M_2\{\boldsymbol{v}_1'+(M_1/M_2)(\boldsymbol{v}'-\boldsymbol{v})\}^2). \tag{A.2}$$

Now setting $\boldsymbol{g}'=\boldsymbol{v}_1'-\boldsymbol{v}'$ and noting that

$$\frac{M_1}{M_2}\boldsymbol{g}'\cdot\left(\frac{M_1+M_2}{M_1}(\boldsymbol{v}_1'-\boldsymbol{v})-\boldsymbol{g}'\right)\equiv\frac{(M_1+M_2)^2}{2M_1M_2}(\boldsymbol{v}_1'-\boldsymbol{v})^2-\frac{M_1^2+M_2^2}{2M_1M_2}g'^2$$

we obtain equations (20) and (21) of the text.

For stationary scatterers we can set

$$f_{M_1}(\boldsymbol{v}_1'-\boldsymbol{g}')=\delta(\boldsymbol{v}_1'-\boldsymbol{g}')$$

from which equation (A.2) reduces to

$$\frac{(M_1+M_2)^2}{M_2^2}\int d\boldsymbol{v}_1'\ G(\boldsymbol{v}_1')\sigma\left(v_1';\cos^{-1}\left\{1-\frac{(M_1+M_2)^2}{2M_2^2}\left(\frac{v}{v_1'}\right)^2\right\}\right)$$
$$\times\delta\left(\boldsymbol{v}\cdot\boldsymbol{v}_1'-\frac{M_1+M_2}{2M_2}v^2\right) \tag{A.3}$$

where the delta function relationship has been used to simplify the argument of the $\cos^{-1}\{\ldots\}$ term. Since $\cos\theta_c$ is given by

$$\cos\theta_c\left(\frac{v}{v'}\right)=\frac{(M_1+M_2)^2}{2M_1M_2}\left(\frac{v}{v'}\right)^2-\frac{M_1^2+M_2^2}{2M_1M_2}$$

it is clear that

$$1-\frac{(M_1+M_2)^2}{2M_2^2}\left(\frac{v}{v_1'}\right)^2=\cos\theta_c\left(\left(1-\frac{M_1v^2}{M_2v_1'^2}\right)^{1/2}\right). \tag{A.4}$$

In addition, the delta function written as

$$\frac{1}{vv_1'}\delta\left(\mu_0'\frac{M_1+M_2}{2M_2}\frac{v}{v_1'}\right) \tag{A.5}$$

clearly restricts v_1' to the bounds indicated by equation (26).

The reduction of equation (A.2), when f_{M_1} is the Maxwell–Boltzmann function, is more complicated. Inserting the form for f_{M_1} leads to

$$\sigma_{\rm II}(\boldsymbol{v}_1'\rightarrow\boldsymbol{v})=\frac{(M_1+M_2)^2}{M_2^2}\left(\frac{M_1}{2\pi kT}\right)^{3/2}\exp\left(-\frac{M_1v_1'^2}{2kT}\right)\int g'^2\,{\rm d}g'\,\sigma(g';\ldots)\exp\left(-\frac{M_1g'^2}{2kT}\right)$$
$$\times\int_0^{2\pi}{\rm d}\phi'\int_{-1}^{1}{\rm d}\mu'\exp\left(\frac{M_1}{kT}v_1'g'\mu_0\right)$$
$$\times\delta\left(\frac{M_1}{M_2}g'|\boldsymbol{v}_1'-\boldsymbol{v}|\mu'+\frac{M_2-M_1}{2M_2}g'^2-\frac{M_1+M_2}{2M_2}(\boldsymbol{v}_1'-\boldsymbol{v})^2\right)\tag{A.6}$$

where $\mu_0=\boldsymbol{v}_1'\cdot\boldsymbol{g}'/v_1'g'$ and $g'|\boldsymbol{v}_1'-\boldsymbol{v}|\mu'=\boldsymbol{g}'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})$. Using the relationship between μ_0, μ' and μ, where $v_1'|\boldsymbol{v}_1'-\boldsymbol{v}|\mu=\boldsymbol{v}_1'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})$, namely:

$$\mu_0=\mu\mu'+(1-\mu^2)^{1/2}(1-\mu'^2)^{1/2}\cos(\phi'-\phi)$$

and integrating over ϕ', we obtain

$$\sigma_{\rm II}(\boldsymbol{v}_1'\rightarrow\boldsymbol{v})=\frac{(M_1+M_2)^2}{M_2^2}\left(\frac{M_1}{2\pi kT}\right)^{3/2}2\pi\frac{M_2}{M_1}\frac{\exp(-M_1v_1'^2/2kT}{|\boldsymbol{v}_1'-\boldsymbol{v}|}$$
$$\times\int_{|\boldsymbol{v}_1'-\boldsymbol{v}|}^{|(M_2+M_1)/(M_2-M_1)||\boldsymbol{v}_1'-\boldsymbol{v}|}g'\,{\rm d}g'\sigma(g';\ldots)\exp\left\{-\frac{M_1g'^2}{2kT}+\frac{M_1}{kT}\frac{\boldsymbol{v}_1'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})}{(\boldsymbol{v}_1'-\boldsymbol{v})^2}\right.$$
$$\left.\times\left[\frac{M_1+M_2}{2M_1}(\boldsymbol{v}_1'-\boldsymbol{v})^2-\frac{M_2-M_1}{2M_1}g'^2\right]\right\}I_0\left(\frac{M_1}{kT}v_1'\left(1-\frac{\{\boldsymbol{v}_1'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})\}^2}{v_1'^2(\boldsymbol{v}_1'-\boldsymbol{v})^2}\right)^{1/2}\right.$$
$$\left.\times\left(g'^2-\left\{\frac{M_1+M_2}{2M_1}|\boldsymbol{v}_1'-\boldsymbol{v}|-\frac{M_2-M_1}{2M_1}\frac{g'^2}{|\boldsymbol{v}_1'-\boldsymbol{v}|}\right\}^2\right)^{1/2}\right).\tag{A.7}$$

The limits on g' are given by the physical roots of the equation defined by the delta function in equation (A.6).

Setting $g'^2=t^2(\boldsymbol{v}_1-\boldsymbol{v})^2$ and simplifying, equation (A.7) becomes

$$\sigma_{\rm II}(\boldsymbol{v}_1'\rightarrow\boldsymbol{v})=\frac{(M_1+M_2)^2}{M_2^2}\left(\frac{M_1}{2\pi kT}\right)^{3/2}2\pi\frac{M_2}{M_1}|\boldsymbol{v}_1'-\boldsymbol{v}|\exp\left(-\frac{M_1v_1'^2}{2kT}\right)$$
$$\times\int_1^{|(M_2+M_1)/(M_2-M_1)|}t\,{\rm d}t\,\sigma\left(|\boldsymbol{v}_1'-\boldsymbol{v}|t;\cos^{-1}\left\{\frac{(M_1+M_2)^2}{2M_1M_2}\frac{1}{t^2}-\frac{M_1^2+M_2^2}{2M_1M_2}\right\}\right)$$
$$\times\exp\left\{-\frac{M_1}{2kT}(\boldsymbol{v}_1'-\boldsymbol{v})^2t^2-\frac{M_1}{2kT}\frac{M_2-M_1}{M_1}\boldsymbol{v}_1'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})t^2\right.$$
$$\left.+\frac{M_1}{2kT}\frac{M_1+M_2}{M_1}\boldsymbol{v}_1'\cdot(\boldsymbol{v}_1'-\boldsymbol{v})\right\}$$
$$\times I_0\left(\frac{M_1}{kT}|\boldsymbol{v}_1'\times\boldsymbol{v}|\left(t^2-\left\{\frac{M_1+M_2}{2M_1}-\frac{M_2-M_1}{2M_1}t^2\right\}^2\right)^{1/2}\right).\tag{A.8}$$

Now set

$$\frac{(M_1+M_2)^2}{2M_1M_2}\frac{1}{t^2}-\frac{M_1^2+M_2^2}{2M_1M_2}=-\cos\theta_c\tag{A.9}$$

and eliminate t in favour of θ_c. We then arrive at equation (22) in the text.

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