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Boltzmann equation for inelastic scattering

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Abstract. We develop a formalism for introduction of inelastic collision processes in the Boltzmann equation. This is equivalent to including participant species with internal degrees of freedom. We consider a two-species mixture, where one of the particles has two allowed internal energy states. We analyse the resulting evolution equations and find exact solutions for interaction models associated with electron and neutron transport.

1. Introduction

The usual formulation of the Boltzmann equation considers particles without internal degrees of freedom, consequently the scattering kernel must conserve the kinetic energy. The possibility of internal structure in the colliding species has been introduced for the derivation of transport properties of polyatomic gases. In this case, molecules in unequal quantum states are treated as different species, and this results in a coupled set of equations equivalent to that of a mixture of monoatomic gases [1]. However, there are physical situations where point particles interact with composite systems. This is the problem of transport of neutrons and electrons in gases. In this case many *ad hoc* equations have been proposed to account for the inelastic contributions [2]. Inelastic scattering contributions, due to the nuclear interaction, are important for high-energy neutrons leaving the collided nucleus in an excited state, whereas for low-energy neutrons they are mainly given by kinetic-energy transfer in the form of atomic or molecular excitation in gas media, or phonon production in solid materials [3]. On the other hand, inelastic processes are important for electron transport even at low energies, such as in swarm propagation in gases [4], or slowing down of electrons beams in solids [5]. In the present paper we present a formal derivation of the Boltzmann equation with inelastic processes, and we obtain solutions for simple models, which simulate neutron or electron transport.

2. Boltzmann equation for inelastic collisions

We consider an inelastic reaction between a point particle A, with mass m_1, and another, B, with one possible excited state B^*, and mass m_2:

$$A + B \leftrightarrow A + B^* . \tag{1}$$

For simplicity we will not introduce the already known treatment of the elastic channels and we will consider a single excited state. We call $\Delta E \geqslant 0$ the difference of internal energy between the state B^* and B, and denote:

$$M = m_1 + m_2 \qquad \mu_i = m_i/M \qquad \epsilon^2 = 2\Delta E/\mu_1 \cdot \mu_2 \cdot M \qquad g = |v - \omega|$$
$$\hat{\Omega} = \frac{1}{g}(v - \omega) \qquad g_+ = (g^2 + \epsilon^2)^{1/2} \qquad g_- = (g^2 - \epsilon^2)^{1/2} \qquad \cos\chi = \hat{\Omega} \cdot \hat{\Omega}'. \tag{2}$$

The cross sections for the direct $I_{ij}(g, \chi)$ and reverse I_{ji} reactions satisfy

$$I_{ij} = I_{ji} \tag{3}$$

(here azimuthal dependence could be included). The microreversibility conditions can be written [6]

$$gI_{12}(g, \chi) = U(g - \epsilon)\frac{g_-^2}{g}I_{13}(g_-, \chi) \qquad gI_{13}(g, \chi) = \frac{g_+^2}{g}I_{12}(g_+, \chi) \tag{4}$$

where U is the step function. Considering states B and B^* as different species and labelling species A, B and B^* by the indices 1, 2 and 3, the kinetic equations for the reactions indicated by (1) take the form

$$\frac{\partial f_i}{\partial t} + v \cdot \nabla_r f_i = J_i[f_1, f_2, f_3] \tag{5}$$

where the inelastic collision terms can be written

$$\begin{aligned}
J_1[f_1, f_2, f_3] = &\int \mathrm{d}\omega\, \mathrm{d}\hat{\Omega}'\, gI_{13}(g, \chi) \\
&\times \left[f_1(\mu_1 v + \mu_2\omega + \mu_2 g_+\hat{\Omega}') f_2(\mu_1 v + \mu_2\omega - \mu_1 g_+\hat{\Omega}') - f_1(v) f_3(\omega) \right] \\
&+ \int \mathrm{d}\omega\, \mathrm{d}\hat{\Omega}'\, U(g - \epsilon) gI_{12}(g, \chi) \\
&\times \left[f_1(\mu_1 v + \mu_2\omega + \mu_2 g_-\hat{\Omega}') f_3(\mu_1 v + \mu_2\omega - \mu_1 g_-\hat{\Omega}') - f_1(v) f_2(\omega) \right] \\
J_2[f_1, f_2, f_3] = &\int \mathrm{d}\omega\, \mathrm{d}\hat{\Omega}'\, U(g - \epsilon) gI_{12}(g, \chi) \\
&\times \left[f_3(\mu_2 v + \mu_1\omega + \mu_1 g_-\hat{\Omega}') f_1(\mu_2 v + \mu_1\omega - \mu_2 g_-\hat{\Omega}') - f_2(v) f_1(\omega) \right] \\
J_3[f_1, f_2, f_3] = &\int \mathrm{d}\omega\, \mathrm{d}\hat{\Omega}'\, gI_{13}(g, \chi) \\
&\times \left[f_2(\mu_2 v + \mu_1\omega + \mu_1 g_+\hat{\Omega}') f_1(\mu_2 v + \mu_1\omega - \mu_2 g_+\hat{\Omega}') - f_3(v) f_1(\omega) \right].
\end{aligned} \tag{6}$$

From here on we leave implicit the space and time variables. Typically the density of electrons or neutrons propagating in gases is much smaller than the gas density and the probability of neutron–neutron or electron–electron scattering is negligible, so that nonlinear terms are not required in the transport equation. The elastic channels and sources can be introduced in (5) adding the usual terms [7]. A loss term:

$$J_3^D[f_3] = -\lambda f_3(v) \tag{7}$$

and a gain term:

$$J_2^D[f_3] = \int \mathrm{d}\omega\, \Lambda(v, \omega) f_3(\omega) \qquad \int \Lambda(w, \omega)\, \mathrm{d}v = \beta \leqslant \lambda \tag{8}$$

could be added to (6) in the case that species B^* is allowed to decay by an external mechanism, e.g. natural emission of photons or β emission. When B^* is a highly excited state it can produce delayed neutrons in the nuclear case or Auger electrons in atoms. These effects could be taken into account by additional terms in (5).

3. General properties of inelastic scattering terms

From the relation

$$g'\,\mathrm{d}v\,\mathrm{d}\omega\,\mathrm{d}\hat{\Omega}' = g\,\mathrm{d}v'\,\mathrm{d}\omega'\,\mathrm{d}\hat{\Omega} \tag{9}$$

expressing the Jacobian of the transformation from the pre-collisional to the post-collisional velocities, we can show that

$$\begin{aligned}
\int \mathrm{d}v\,\varphi_1(v)J_1(v) &= \int \mathrm{d}v\,\mathrm{d}\omega\,\mathrm{d}\hat{\Omega}'\big\{U(g-\epsilon)gI_{12}(g,\chi)f_2(v)f_1(\omega)\\
&\quad\times\big[\varphi_1(\mu_2 v+\mu_1\omega-\mu_2 g_-\hat{\Omega}')-\varphi_1(\omega)\big]\\
&\quad+gI_{13}(g,\chi)f_3(v)f_1(\omega)\big[\varphi_1(\mu_2 v+\mu_1\omega-\mu_2 g_+\hat{\Omega}')-\varphi_1(\omega)\big]\big\}\\
\int \mathrm{d}v\,\varphi_2(v)J_2(v) &= \int \mathrm{d}v\,\mathrm{d}\omega\,\mathrm{d}\hat{\Omega}' f_1(\omega)\big\{gI_{13}(g,\chi)f_3(v)\varphi_2(\mu_2 v+\mu_1\omega+\mu_1 g_+\hat{\Omega}')\\
&\quad-U(g-\epsilon)gI_{12}(g,\chi)f_2(v)\varphi_2(v)\big\}\\
\int \mathrm{d}v\,\varphi_3(v)J_3(v) &= \int \mathrm{d}v\,\mathrm{d}\omega\,\mathrm{d}\hat{\Omega}' f_1(\omega)\\
&\quad\times\big\{U(g-\epsilon)gI_{12}(g,\chi)f_2(v)\varphi_3(\mu_2 v+\mu_1\omega+\mu_1 g_-\hat{\Omega}')\\
&\quad-gI_{13}(g,\chi)f_3(v)\varphi_3(v)\big\}
\end{aligned}$$

and

$$\begin{aligned}
\sum_{i=1}^{3}\int \mathrm{d}v\,\varphi_i(v)J_i(v) &= \int \mathrm{d}v\,\mathrm{d}\omega\,\mathrm{d}\hat{\Omega}' f_1(\omega)\\
&\quad\times\Big\{gI_{13}(g,\chi)f_3(v)\Big[\varphi_1(\mu_2 v+\mu_1\omega-\mu_2 g_+\hat{\Omega}-\varphi_1(\omega)\\
&\quad+\varphi_2(\mu_2 v+\mu_1\omega+\mu_1 g_+\hat{\Omega}')-\varphi_3(v)\Big]\\
&\quad+U(g-\epsilon)gI_{12}(g,\chi)f_2(v)\Big[\varphi_1(\mu_2 v+\mu_1\omega-\mu_2 g_-\hat{\Omega}')-\varphi_1(\omega)\\
&\quad+\varphi_3(\mu_2 v+\mu_1\omega+\mu_1 g_-\hat{\Omega}')-\varphi_2(v)\Big]\Big\}.
\end{aligned}\tag{10}$$

By using these relations we obtain the Boltzmann inequality,

$$\begin{aligned}
\sum_{i=1}^{3}\int \ln f_i(v)J_i(v)\,\mathrm{d}v &= -\int \mathrm{d}v\,\mathrm{d}\omega\,\mathrm{d}\hat{\Omega}' gI_{13}(g,\chi)\\
&\quad\times\ln\Big[f_2(\mu_2 v+\mu_1\omega+\mu_1 g_+\hat{\Omega}')f_1(\mu_2 v+\mu_1\omega-\mu_2 g_+\hat{\Omega}')/f_3(v)f_1(\omega)\Big]\\
&\quad\times\Big[f_2(\mu_2 v+\mu_1\omega+\mu_1 g_+\hat{\Omega}')f_1(\mu_2 v+\mu_1\omega-\mu_2 g_+\hat{\Omega}')-f_3(v)f_1(\omega)\Big]\\
&\leqslant 0
\end{aligned}\tag{11}$$

which determines a kind of Liapunov functional controlling the time evolution of the system, and the conservation laws,

$$\sum_{i=1}^{3}\int \varphi_i^{(k)}(v)J_i[f_1,f_2,f_3]\,\mathrm{d}v = 0 \qquad k=0,1,2 \tag{12}$$

where

$$\begin{aligned}
&\varphi_i^{(0)}(v) = m_1 && \varphi_i^{(1)}(v) = m_i v && i=1,2,3\\
&\varphi_1^{(2)}(v) = m_1 v^2/2 && \varphi_2^{(2)}(v) = m_2 v^2/2 && \varphi_3^{(2)}(v) = m_3 v^2/2+\Delta E\,.
\end{aligned}$$

Defining

$$\rho_i = m_i \int f_i(v)\,\mathrm{d}v \qquad \rho_i u_i = m_i \int f_i(v) v\,\mathrm{d}v \tag{13}$$

we integrate (5) to obtain the mass-density conservation equations:

$$\begin{aligned}
&\partial\rho_1/\partial t + \nabla\cdot(\rho_1 u_1) = 0\\
&\partial\rho_2/\partial t + \nabla\cdot(\rho_2 u_2) = m_2 \int J_2(v)\,\mathrm{d}v + \beta\rho_3\\
&\partial\rho_3/\partial t + \nabla\cdot(\rho_3 u_3) = -m_2 \int J_2(v)\,\mathrm{d}v - \lambda\rho_3
\end{aligned}\tag{14}$$

where we have introduced for species B^* the alternative decay channel described above. The momentum-conservation equations, for the space homogeneous case, read

$$\begin{aligned}
&\partial(\rho_1 u_1)/\partial t = m_1 \int v J_1(v)\,\mathrm{d}v\\
&\partial(\rho_2 u_2)/\partial t = m_2 \int v J_2(v)\,\mathrm{d}v + m_2 \int v\,\mathrm{d}v \int \Lambda(\omega, v) f_3(\omega)\,\mathrm{d}\omega\\
&\partial(\rho_3 u_3)/\partial t = m_2 \int v J_3(v)\,\mathrm{d}v - \lambda\rho_3 u_3\,.
\end{aligned}\tag{15}$$

In the energy case we define a kinetic energy, associated with each species:

$$K_i = \frac{m_i}{2} \int v^2 f_i\,\mathrm{d}v \qquad \text{and} \qquad K = \sum_{i=1}^{3} K_i \tag{16}$$

and obtain, again in the space-homogeneous case,

$$\begin{aligned}
&\partial K_1/\partial t = \frac{m_1}{2} \int v^2 J_1(v)\,\mathrm{d}v\\
&\partial K_2/\partial t = \frac{m_2}{2} \int v^2 J_2(v)\,\mathrm{d}v + \frac{m_2}{2} \int v^2\,\mathrm{d}v \int \Lambda(\omega, v) f_3(\omega)\,\mathrm{d}\omega\\
&\partial K_3/\partial t = \frac{m_2}{2} \int v^2 J_3(v)\,\mathrm{d}v - \lambda K_3\,.
\end{aligned}\tag{17}$$

From equation (12) with $k = 2$,

$$\partial K/\partial t = -\Delta E \int J_3(v)\,\mathrm{d}v - \lambda K_3 + \frac{m_2}{2} \int f_3(v)\,\mathrm{d}v \int \omega^2 \Lambda(v, \omega)\,\mathrm{d}\omega\,. \tag{18}$$

This equation accounts for the transformation of kinetic into internal energy, and can be written as

$$\frac{\partial}{\partial t}\left(K + \frac{\Delta E}{m_2}\rho_3\right) = -\lambda\left(K_3 + \frac{\Delta E}{m_3}\rho_3\right) + \frac{m_2}{2} \int f_3(v)\,\mathrm{d}v \int \omega^2 \Lambda(v, \omega)\,\mathrm{d}\omega\,.$$

When decay is not allowed the right-hand side is zero and we obtain the total energy conservation equation.

4. Explicit solutions for simple test cases

If the energy of the transported particles is larger than a few electron volts the thermal motion of the target may be neglected and it can be considered at rest in the laboratory system. Furthermore, inelastic atomic and nuclear reactions involve an energy transfer larger than the thermal-motion kinetic energy. This case can be modelled assuming that species 2 is a background, at rest, with distribution function $f_2(\boldsymbol{r}, \boldsymbol{v}, t) = n_2(\boldsymbol{r}, t)\delta(\boldsymbol{v})$, i.e. a Maxwellian equilibrium at low temperature. In the physical cases we have in mind, the mass of the electron and neutron are smaller than that of the atoms and molecules in the medium, and we can assume $\mu_1 = 0$. Compatibility between the respective evolution equations for f_2 and f_3 requires that $f_3 = n_3\delta(\boldsymbol{v})$ too, and $n_3(\boldsymbol{r}, t)$ must be related to $n_2(\boldsymbol{r}, t)$. The equation for the light particles reads

$$\begin{aligned}\partial f_1/\partial t + \boldsymbol{v}\cdot\nabla_{\boldsymbol{r}} f_1 = {} & \frac{n_2}{v}\int v_+^2 I_{12}(v_+, \hat{\Omega}\cdot\hat{\Omega}') f_1(v_+\hat{\Omega}')\,\mathrm{d}\hat{\Omega}' \\ & - f_1(\boldsymbol{v})\frac{1}{v}\int\left[n_3 v_+^2 I_{12}(v_+, \hat{\Omega}\cdot\hat{\Omega}') + n_2 U(v-\epsilon)v^2 I_{12}(v, \hat{\Omega}\cdot\hat{\Omega}')\right]\mathrm{d}\hat{\Omega} \\ & + \frac{n_3}{v}\int U(v-\epsilon)v^2 I_{12}(v, \hat{\Omega}\cdot\hat{\Omega}') f_1(v_-\hat{\Omega}')\,\mathrm{d}\hat{\Omega}' \end{aligned} \tag{19}$$

where $v_+ = (v^2+\epsilon^2)^{1/2}$ and $v_- = (v^2-\epsilon^2)^{1/2}$. Futhermore, the transport of light particles will not noticeably change an initial spatially homogeneous medium and n_2 and n_3 can be considered as constants. Radiation damage could change the local structure of a solid background, but without changing densities.

Equation (19) has a simple form when we consider a very hard particle interaction model [8]:

$$v^2 I_{12}(v, \hat{\Omega}\cdot\hat{\Omega}') = \sigma(\hat{\Omega}\cdot\hat{\Omega}') \tag{20}$$

resulting in

$$\begin{aligned}\partial f_1/\partial t + \boldsymbol{v}\cdot\nabla_{\boldsymbol{r}} f_1 = {} & \frac{n_2}{v}\int \sigma(\hat{\Omega}\cdot\hat{\Omega}') f_1(v+\hat{\Omega}')\,\mathrm{d}\hat{\Omega}' - \frac{\sigma_\mathrm{t}}{v}[n_3 + n_2 U(v-\epsilon)] f_1(\boldsymbol{v}) \\ & + \frac{n_3}{v}U(v-\epsilon)\int \sigma(\hat{\Omega}\cdot\hat{\Omega}') f_1(v_-\hat{\Omega}')\,\mathrm{d}\hat{\Omega}' . \end{aligned} \tag{21}$$

We will first consider electron propagation in a medium. The cross section for inelastic electron–atom scattering is strongly peaked in the forward direction [9], and assuming $\sigma(\hat{\Omega}\cdot\hat{\Omega}') = \sigma_t\delta(\hat{\Omega}\cdot\hat{\Omega}')$, where $\sigma_\mathrm{t} = \int\sigma(\hat{\Omega}\cdot\hat{\Omega}')\,\mathrm{d}\hat{\Omega}'$, we obtain

$$\begin{aligned}\frac{\partial f_1}{\partial t} + v\hat{\Omega}\cdot\nabla_r f_1 = {} & \frac{n_2\sigma_\mathrm{t}}{v} f_1(v_+\hat{\Omega}) - \frac{\sigma_\mathrm{t}}{v}[n_3 + n_2U(v-\epsilon)] f_1(v\hat{\Omega}) \\ & + \frac{n_3\sigma_\mathrm{t}}{v}U(v-\epsilon) f_1(v_-\hat{\Omega}) . \end{aligned} \tag{22}$$

The angle $\hat{\Omega}$ only remains as a parameter, since the motion direction of the particles in the initial (or boundary) conditions is not changed by the assumed inelastic cross section. This is the usual situation in electron-beam propagation where the angular dispersion of the beam is mainly produced by elastic collisions [10]. We define a variable ρ measuring the distance along a motion ray, such that

$$\hat{\Omega}\cdot\nabla_r = \partial/\partial\rho \tag{23}$$

and

$$\begin{aligned} & \xi = v^2/\epsilon^2 \qquad \phi(\xi, s, \tau) = f_1(\boldsymbol{v}, \boldsymbol{r}, t) \\ & s = \sigma_\mathrm{t} n_2\rho/\epsilon^2 \qquad \tau = \sigma_\mathrm{t} n_2 t/\epsilon \qquad \alpha = n_3/n_2 . \end{aligned} \tag{24}$$

It follows that

$$\xi^{1/2}\frac{\partial\phi}{\partial\tau} + \xi\frac{\partial\phi}{\partial s} = \phi(\xi+1, s, \tau) - [\alpha + U(\xi-1)]\phi(\xi, s, \tau) + U(\xi-1)\alpha\phi(\xi-1, s, \tau) . \tag{25}$$

This equation can be solved exactly in both the cases of isotropic space-independent and stationary distribution. Writing $\theta = \tau/\xi^{1/2}$ in the first case and $\theta = s/\xi$ in the second, the solution is

$$\phi(\xi, \theta) = \sum_{k=-\infty}^{\infty} \phi(\xi + k, 0) \sum_{n=|k|}^{\infty} \frac{\theta^n}{n!} a_{n,k} \tag{26}$$

with

$$a_{nk} = (-1)^{n-k} \sum_{j=|k|}^{n} \alpha^{j-k} \binom{n}{j} \binom{n}{j-k} \qquad \text{for} \quad \xi > 1 \tag{27}$$

or

$$a_{nk} = (-1)^{n-k} \binom{n}{k} \alpha^{n-k} U(k) \qquad \text{for} \quad \xi < 1 \, . \tag{28}$$

The solution is expressed in terms of the initial or boundary conditions given by $\phi(\xi + k, 0)$. This condition is implicitly understood to be zero for $\xi + k < 0$, imposing an additional lower bound for the k summation in (27). Positive (negative) k-values account for contributions to the ξ–energy from energy loss (gain) collisions. For $\xi < 1$, energy-gain collisions do not contribute. The case when species 3 is not background, but is either non-participating or has negligible total density, is described by the above equations with $\alpha = 0$.

The next examples are relevant to neutron transport. When neutrons move in a medium the dominant collisions will occur with the atomic nucleus and the interaction potential is short-ranged. In this case the scattering amplitude is dominated by s-waves and the cross section is independent of the scattering angle. For the VHP interaction model [8] we can put

$$\sigma(\hat{\Omega} \cdot \hat{\Omega}') = \sigma_t / 4\pi \tag{29}$$

in (21), and get

$$\partial f_1/\partial t + v \cdot \nabla_r f_1 = \frac{n_2}{v} \frac{\sigma_t}{4\pi} \int f_1(v_+ \hat{\Omega}') \, d\hat{\Omega}' - \frac{\sigma_t}{v} [n_3 + n_2 U(v - \epsilon)] f_1(v\hat{\Omega})$$
$$+ \frac{n_3}{v} U(v - \epsilon) \frac{\sigma_t}{4\pi} \int f_1(v_- \hat{\Omega}') \, d\hat{\Omega}' \, . \tag{30}$$

Now we define ξ as above, and

$$\begin{aligned} &\tau = n_2 \sigma_t t/\epsilon \qquad \rho = n_2 \sigma_t r/\epsilon^2 \\ &\psi(\xi) = \psi(\rho, \xi, \hat{\Omega}, \tau) = f(r, v, t) \\ &\hat{\psi}(\xi, \tau) = \frac{1}{4\pi} \int f_1(r, v\hat{\Omega}', t) \, d\hat{\Omega}' \, . \end{aligned} \tag{31}$$

then

$$\xi^{1/2} \frac{\partial \psi}{\partial \tau} + \xi \hat{\Omega} \cdot \nabla_\rho \psi = \hat{\psi}(\xi + 1, \tau) - [\alpha + U(\xi - 1)] \psi(\xi, \tau) + \alpha U(\xi - 1) \hat{\psi}(\xi - 1, \tau) \, . \tag{32}$$

Now $\hat{\Omega}$ does not play the role of a parameter any more, but in the space-homogeneous case an analytical solution can be obtained:

$$\psi(\xi, \hat{\Omega}, \tau) = e^{-[\alpha + U(\xi-1)]\tau/\xi^{1/2}} \psi(\xi, \hat{\Omega}, 0)$$
$$+ \xi^{-1/2} \int e^{[\alpha + U(\xi - 1)](\tau' - \tau)/\xi^{1/2}} \left[\hat{\psi}(\xi + 1, \tau') + \alpha U(\xi - 1) \hat{\psi}(\xi - 1, \tau') \right] d\tau' \, . \tag{33}$$

The function $\hat{\psi}$ is determined by an equation obtained by angular integration of (32):

$$\xi^{1/2}\frac{\partial\hat{\psi}(\xi,\tau)}{\partial\tau} = \hat{\psi}(\xi+1,\tau) - [\alpha + U(\xi-1)]\hat{\psi}(\xi,\tau) + \alpha U(\xi-1)\hat{\psi}(\xi-1,\tau) \tag{34}$$

which has a solution similar to that given by (26)–(28). Substituting this solution in (33), we obtain an explicit expression for the distribution. We observe that velocity anisotropy is only due to the initial condition.

Now we will study the case in which the particle's interaction is given by a Maxwellian model:

$$vI_{12}(v, \hat{\Omega}\cdot\hat{\Omega}') = \alpha(\hat{\Omega}\cdot\hat{\Omega}')\,. \tag{35}$$

This has an energy dependence softer than the VHP model formerly considered. We introduce the same hypothesis as before, about a background at rest and obtain from (19):

$$\begin{aligned}\frac{\partial f_1}{\partial t} + \boldsymbol{v}\cdot\nabla_r f_1 = \frac{n_2}{v}\int v_+\alpha(\hat{\Omega}\cdot\hat{\Omega}')f_1(v_+\hat{\Omega}')\,\mathrm{d}\hat{\Omega}' \\ -f_1(v)\alpha_t\left[n_3\frac{v_+}{v} + n_2U(v-\epsilon)\right] + n_3U(v-\epsilon)\int\alpha(\hat{\Omega}\cdot\hat{\Omega}')f_1(v_-\hat{\Omega}')\,\mathrm{d}\hat{\Omega}'\end{aligned} \tag{36}$$

where

$$\alpha_t = \int\alpha(\hat{\Omega}\cdot\hat{\Omega}')\,\mathrm{d}\hat{\Omega}'\,. \tag{37}$$

Denoting

$$f(r, v\hat{\Omega}, t) = vf_1(r, v\hat{\Omega}, t) \tag{38}$$

we have

$$\begin{aligned}\frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\nabla_x f = n_2\int\alpha(\hat{\Omega}\cdot\hat{\Omega}')f(v_+\hat{\Omega}')\,\mathrm{d}\hat{\Omega}' - f(v\hat{\Omega})\alpha_t\left[n_3\frac{v_+}{v} + n_2U(v-\epsilon)\right] \\ +\frac{n_3v}{v_-}U(v-\epsilon)\int\alpha(\hat{\Omega}\cdot\hat{\Omega}')f(v\hat{\Omega}')\,\mathrm{d}\hat{\Omega}'\,.\end{aligned} \tag{39}$$

For high velocities, $v_+/v \approx v/v_- \approx 1$ and this equation reduces to (21), and can be solved for similar cases and with the same procedures.

When no external excitation source acts on the system, the atoms (or nuclei) constituting the background can only be excited by collisions with the test particles. Then, the species 3 will be much more rarified than species 2 and we can assume $n_2/n_3 \approx 0$. In this case the right-hand side of (38) contains only two terms and, for neutron transport with isotropic cross section, we obtain

$$\frac{\partial f}{\partial t} + \boldsymbol{v}\cdot\nabla_r f = n_2\alpha_t\int f(v_+\hat{\Omega}')\,\mathrm{d}\hat{\Omega}' - n_2U(v-\epsilon)\alpha_t f(v\hat{\Omega})\,. \tag{40}$$

The solution of the space-homogeneous case follows as before. Instead we will consider a stationary neutron flux in a plane slab bounded by parallel plates r_1 = constant. In such a mono-dimensional problem the distribution depends only on r_1, $\eta = \cos(\hat{e}_1, \hat{\Omega})$ and speed v. We define ξ as before and

$$x = \alpha_t n_2 r\eta/\epsilon \qquad \phi(x,\xi,\eta) = f(r, v\hat{\Omega}) \qquad \hat{\phi}(x,\xi) = 2\pi\int_{-1}^{1}\phi(x,\xi,\eta)\,\mathrm{d}\eta\,. \tag{41}$$

The function $\hat{\phi}$ is the total number of particles with dimensionless velocity ξ per unit volume around x. For $0 < x < L$ (L is the dimensionless thickness of the slab) we have

$$\xi^{1/2}\eta\frac{\partial\phi(x,\xi,\eta)}{\partial x} + U(\xi-1)\phi(x,\xi,\eta) = \hat{\phi}(x,\xi+1) \tag{42}$$

with the boundary conditions

$$\begin{aligned} &\phi(0,\xi,\eta) = \phi_i(\xi,\eta) && \text{for} \quad \eta > 0 \\ &\phi(L,\xi,\eta) = 0 && \text{for} \quad \eta < 0 \end{aligned} \tag{43}$$

which prescribes the incoming fluxes impinging on the two sides of the medium (in particular, no incident flux from the right). Then:

$$\begin{aligned} \phi(x,\xi,\eta) &= \phi_i(\xi,\eta)\mathrm{e}^{-(-U(\xi-1)/\xi^{1/2}\eta)x} + \frac{1}{\xi^{1/2}\eta}\int_0^L \mathrm{e}^{-(U(\xi-1)/\xi^{1/2}\eta)(x-x')}\hat{\phi}(x',\xi+1)\,\mathrm{d}x' \\ &\qquad \text{for} \quad \eta > 0 \\ \phi(x,\xi,\eta) &= -\frac{1}{\xi^{1/2}\eta}\int_x^L \mathrm{e}^{-(U(\xi-1)/\xi^{1/2}\eta)(x-x')}\hat{\phi}(x',\xi+1)\,\mathrm{d}x' \qquad \text{for} \quad \eta < 0\,. \end{aligned} \tag{44}$$

The meaning of this solution is clear: for $\eta > 0$ the first term gives the attenuation of the incident flux and the second gives the contribution from the dispersion in the medium. Meanwhile only the isotropic scattering brings particles to the negative values of η. The solution becomes explicit once $\hat{\phi}$ has been determined, but, as is well known, integration of (42) over η does not yield a self-consistent equation for $\hat{\phi}$. An integral equation for $\hat{\phi}$ can be derived from (44) itself:

$$\hat{\phi}(x,\xi) = 2\pi\int_0^1 \phi_i(\xi,\eta)\mathrm{e}^{-(x/\eta\xi^{1/2})}\,\mathrm{d}\eta + \frac{1}{2\xi^{1/2}}\int_0^L E_1\left(\frac{|x-x'|}{\xi^{1/2}}\right)\hat{\phi}(x',\xi+1)\,\mathrm{d}x' \tag{45}$$

where

$$E_1(x) = \int_0^1 \frac{\mathrm{e}^{-x/y}}{y}\,\mathrm{d}y \tag{46}$$

denotes an exponential integral function. This equation does not seem to have a straightforward solution. However, let us suppose that the initial condition is monochromatic, i.e. $\phi(\xi,\eta) = \chi(\eta)\delta(\xi-\xi_0)$. During the transport process the inelastic collisions will only populate discrete energies $\xi = \xi_0 - k$, down to $k = [\xi_0]$, where $[\xi_0]$ denotes the largest integer not greater than ξ_0. The corresponding $\hat{\phi}$ can be calculated recurrently:

$$\hat{\phi}(x,\xi_0-k) = \frac{1}{2(\xi_0-k)^{1/2}}\int_0^L E_1\left(\frac{|x-x'|}{(\xi_0-k)^{1/2}}\right)\hat{\phi}(x',\xi_0-k+1)\,\mathrm{d}x' \tag{47}$$

($k \geqslant 1$), starting from

$$\hat{\phi}(x,\xi_0) = 2\pi\int_0^1 \chi(\eta)\mathrm{e}^{-x/\eta\xi_0^{1/2}}\,\mathrm{d}\eta\,. \tag{48}$$

From (44) it is possible to derive the space dependence of the distributions.

5. Conclusions

We have generalized the formulation of the Boltzmann equation to a system of particles which transfers energy to one internal degree of freedom. For formal simplicity we allowed for only two internal discrete states, one ground and one excited level, separated by a fixed energy step. However there is no difficulty in extending the formalism to a multilevel system, or even to continuous spectra.

In the equations derived we have not included the already known terms for the elastic channels. These could be added simply to the present equations.

We searched for exact solutions for simple cases, related to the transport of electrons and neutrons. This is achieved by suitable hypothesis on mass ratios and cross sections for the considered particles. This allows us to find some of these solutions for the space-homogeneous and the stationary cases.

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