RELAXATION OF A GAS DESCRIBED BY BOLTZMANN KINETIC EQUATION

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We consider a problem of a classical gas relaxing towards Maxwellian distribution function in the case when the initial nonequilibrium distribution function depends only on the modulus of velocity. The quintuple Boltzmann collision integral is reduced to a double integral with the subsequent possibility of application of numerical methods to the solution of the problem. Simplification of the collision integral is also carried out for the case of a mixture of gases.

Numerical results are presented in graphical form, showing the behavior of the distribution function with time.

Let us consider a homogeneous quiescent gas composed of molecules, which we assume to be perfectly rigid smooth spheres of diameter σ and mass m.

The state of such a gas can be described in terms of its distribution function $f(t, u, v, w)$ which is a function of time t and components u, v and w of velocity of the molecules. In this case the Boltzmann equation for f will be

$$\frac{\partial f}{\partial t} = \frac{\sigma^2}{2}\int_{-\infty}^{+\infty}\int\int\int_0^{2\pi}\int_0^{\pi}[f(t, u_1', v_1', w_1')f(t, u', v', w') - \\ - f(t, u, v, w)f(t, u_1, v_1, w_1)]\,|q|\sin\theta\, d\theta\, d\varphi\, du_1\, dv_1\, dw_1 \qquad (1)$$

$$u' = u + lq, \qquad v' = v + mq, \; w' = w + nq, \qquad u_1' = u_1 - lq$$

$$v_1' = v_1 - mq, \qquad w_1' = w_1 - nq, \qquad q = l(u_1 - u) + m(v_1 - v) + n(w_1 - w)$$

$$l = \cos\theta, \qquad m = \sin\theta\cos\varphi, \qquad n = \sin\theta\sin\varphi$$

and we shall now state the Cauchy's problem for it. When $t = 0$, we have a given initial distribution function $f = f(t = 0, (u^2 + v^2 + w^2)^{1/2})$ depending only on the modulus of velocity and different from the Maxwellian distribution function.

It is necessary to find a distribution function satisfying (1) when $t > 0$ and coinciding with the initial function when $t = 0$.

We shall seek a solution of this problem in the form

$$f = f(t, \sqrt{u^2 + v^2 + w^2})$$

Inserting it into (1) and adopting spherical coordinates given in the velocity space by

$$u = V\cos\psi, \qquad v = V\sin\psi_1\cos\chi, \qquad w = V\sin\psi\sin\chi$$

$$u_1 = V_1\cos\psi_1, \qquad v_1 = V_1\sin\psi_1\cos\chi_1, \qquad w_1 = V_1\sin\psi_1\sin\chi_1$$

we obtain

$$\frac{\partial f(t, V)}{\partial t} = \frac{\sigma^2}{2}\int_0^{\infty}\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi}\int_0^{\pi}[f(t, \sqrt{p_1})f(t, \sqrt{p}) -$$

$$-f(t, V) f(t, V_1)] \mid q \mid V_1^2 \sin\theta \sin\psi_1 \, d\theta \, d\varphi \, d\psi_1 \, d\chi_1 \, dV_1 \tag{2}$$

$$p_1 = V_1^2 - 2V_1 (\cos\psi_1 \cos\theta + \sin\psi_1 \cos\chi_1 \sin\theta \cos\varphi + \sin\psi_1 \sin\chi_1 \sin\theta \sin\varphi) q + q^2$$

$$p = V^2 + 2V (\cos\psi \cos\theta + \sin\psi \cos\chi \sin\theta \cos\varphi + \sin\psi \sin\chi \sin\theta \sin\varphi) q + q^2$$

$$q = V_1 (\cos\psi_1 \cos\theta + \sin\psi_1 \cos\chi_1 \sin\theta \cos\varphi + \sin\psi_1 \sin\chi_1 \sin\theta \sin\varphi) - V (\cos\psi \cos\theta + \sin\psi \cos\chi \sin\theta \cos\varphi + \sin\psi \sin\chi \sin\theta \sin\varphi)$$

To simplify the collision term further, we shall have to use the following identity, valid for any single-valued integrable function F

$$\int_0^{2\pi} \int_0^{\pi} F(\cos\alpha_1 \cos\alpha + \sin\alpha_1 \cos\beta_1 \sin\alpha \cos\beta + \sin\alpha_1 \sin\beta_1 \sin\alpha \sin\beta, \alpha, \beta) \sin\alpha_1 \, d\alpha_1 \, d\beta_1 = 2\pi \int_0^{\pi} F(\cos\alpha_1, \alpha, \beta) \sin\alpha_1 d\alpha_1 \tag{3}$$

To confirm its validity, we shall write its left-hand side in the form

$$\iint_{\Sigma} F[\cos(\mathbf{n}, \mathbf{n}_1), \alpha, \beta] \, d\Sigma \tag{4}$$

where Σ is a unit radius sphere, integration being carried out over its surface; $\mathbf{n}$ is a fixed unit vector with origin at the center of the sphere and with direction cosines given by ($\cos\alpha$, $\sin\alpha\cos\beta$, $\sin\alpha\sin\beta$); $\mathbf{n}_1$ is a unit vector variable under integration, with the origin at the center of the sphere. It supports an elementary surface $d\Sigma$ and its direction cosines are ($\cos\alpha_1$, $\sin\alpha_1\cos\beta_1$, $\sin\alpha_1\sin\beta_1$).

We see from (4) that the value of the integral is coordinate independent. We can therefore direct the coordinate axis from which α_1 is counted, along the fixed vector $\mathbf{n}$, and this yields the integral (4) in the form of the right-hand side of (3).

Let us now consider separately the integrals in ψ_1 and χ_1 appearing in the collision term of (2). We can simplify it using the identity (3) in which ψ_1 and χ_1 replace α_1 and β_1. Repeating it for the integrals in θ and φ, we obtain the Boltzmann equation in the form

$$\frac{\partial f}{\partial t} = 2\pi^2\sigma^2 \int_0^{\infty} \int_0^{\pi} \int_0^{\pi} [f(t, \sqrt{p_1}) f(t, \sqrt{p}) - f(t, V) f(t, V_1)] \mid q \mid V_1^2 \sin\theta \sin\psi_1 d\theta \, d\psi_1 \, dV_1$$

$$p_1 = V_1^2 \sin^2\psi_1 + V^2 \cos^2\theta, \quad p = V^2 \sin^2\theta + V_1^2 \cos^2\psi_1, \quad q = V_1 \cos\psi_1 - V\cos\theta \tag{5}$$

Integration in the second part of the collision integral can be performed with respect to θ and ψ_1 and the resulting expression is

$$-2\pi^2\sigma^2 f(t, V) \int_0^{\infty} f(t, x) \frac{(V+x)^3 - |V-x|^3}{3V} \cdot x \, dx$$

Here the integration variable V_1 is denoted by x.

We shall now introduce new variables of integration into the first part of the collision integral, putting

$$x = \sqrt{V^2 \sin^2\theta + V_1^2 \cos^2\psi_1}, \quad y = \sqrt{V_1^2 \sin^2\psi_1 + V^2 \cos^2\theta}, \quad q = V_1 \cos\psi_1 - V\cos\theta$$

This substitution makes integration with respect to q possible, thus converting a triple integral into a double integral. The Boltzmann equation (5) in its final form is

$$\frac{\partial f(t, V)}{\partial t} = 2\pi^2\sigma^2 \int_0^V \int_{\sqrt{V^2 - x^2}}^{V} f(t, x) f(t, y) \frac{4\sqrt{x^2 + y^2 - V^2}}{V} xy \, dy \, dx + 2\pi^2\sigma^2 \left(\int_V^{\infty} f(t, x) 2x \, dx\right)^2 + 2\pi^2\sigma^2 \int_0^V f(t, x) \frac{4x^2}{V} dx \int_V^{\infty} f(t, x) 2x \, dx - 2\pi^2\sigma^2 f(t, V) \int_0^{\infty} f(t, x) \frac{(V+x)^3 - |V-x|^3}{3V} x \, dx \tag{6}$$

Thus, Cauchy's problem posed for the Boltzmann equation under the assumption that the initial distribution function is a function of the velocity modulus only, has becomed a Cauchy's problem for (6).

Recently, the problem of temperature relaxation in two-temperature mixtures of classical gases [1] received some attention.

Assuming that initial distribution functions of any gas depend only on the velocity modulus, we can also carry out a similar simplification of the collision integral in this case. Suppose that the mixture of gases consists of two types of molecules which we shall assume to be perfectly rigid, smooth spheres of respective diameters σ_1 and σ_2 and masses m_1 and m_2.

We shall also assume, for definiteness, that $m_1 \leqslant m_2$. Respective distribution functions will be $f(t, \mathbf{c}_1)$ and $F(t, \mathbf{c}_2)$ where $\mathbf{c}_1$ and $\mathbf{c}_2$ are velocities of respective molecules. The system of Boltzmann equations [2] will then be given by

$$\frac{\partial f(t, \mathbf{c}_1)}{\partial t} = I_{11}[f(t, \mathbf{c}_1)] + \left(\frac{\sigma_1+\sigma_2}{2}\right)^2 \frac{1}{2} \int\int\int_{-\infty}^{+\infty} \int_0^{2\pi}\int_0^{\pi} [f(t, \mathbf{c}_1') F(t, \mathbf{c}_2') - $$
$$- f(t, \mathbf{c}_1) F(t, \mathbf{c}_2)] \, |(\mathbf{g}_{21}\cdot\mathbf{k})| \sin\theta \, d\theta \, d\varphi \, d\mathbf{c}_2 \tag{7}$$
$$\frac{\partial F(t, \mathbf{c}_2)}{\partial t} = I_{22}[F(t, \mathbf{c}_2)] + \left(\frac{\sigma_1+\sigma_2}{2}\right)^2 \frac{1}{2} \int\int\int_{-\infty}^{+\infty} \int_0^{2\pi}\int_0^{\pi} [f(t, \mathbf{c}_1') F(t, \mathbf{c}_2') - $$
$$- F(t, \mathbf{c}_2) f(t, \mathbf{c}_1)] \, |(\mathbf{g}_{21}\cdot\mathbf{k})| \sin\theta \, d\theta \, d\varphi \, d\mathbf{c}_1$$
$$\mathbf{c}_2' = \mathbf{c}_2 - \frac{2m_1}{m_1+m_2}\mathbf{k}(\mathbf{g}_{21}\cdot\mathbf{k}), \qquad \mathbf{c}_1' = \mathbf{c}_1 + \frac{2m_2}{m_1+m_2}\mathbf{k}(\mathbf{g}_{21}\cdot\mathbf{k})$$
$$\mathbf{g}_{21} = \mathbf{c}_2 - \mathbf{c}_1, \qquad \mathbf{k} = (\cos\theta, \sin\theta\cos\varphi, \sin\theta\sin\varphi)$$

where I_{11} and I_{22} have the form of the right-hand side of (1) in which we replace σ with σ_1 and σ_2 and $f(t, \mathbf{c})$ with $f(t, \mathbf{c}_1)$ and $F(t, \mathbf{c}_2)$.

We shall seek a solution of (7) in the form $f = f(t, |\mathbf{c}_1|)$ and $F(t, |\mathbf{c}_2|)$. Inserting these functions into (7) and performing transformations analogous to those made for Eq. (1), we arrive at the following system:

$$\partial f(t, V) / \partial t = I_{11}(f, f) + I_{12}(f, F), \qquad \partial F(t, V)/\partial t = I_{21}(F, f) + I_{22}(F, F)$$

Here V denotes both the variable $|\mathbf{c}_1|$ in f and $|\mathbf{c}_2|$ in F. Expression $I_{11}(f, f)$ denotes the right-hand side of (6) in which σ is replaced with σ_1. $I_{22}(F, F)$ denotes the right-hand side of (6) with σ replaced with σ_2 and f replaced with F

$$I_{12}(f, F) = \left(\frac{\sigma_1+\sigma_2}{2}\right)^2 \frac{2\pi^2}{2V}\left(\frac{m_1+m_2}{2m_2}\right)^2 \left\{\int_0^{\infty}\int_{y_1}^{y_2} f(t, x) F(t, y)\left[(x+V) - \right.\right.$$
$$\left. - \frac{m_2}{m_1}\left| y - \left(y^2 + \frac{m_1}{m_2}(x^2 - V^2)\right)^{1/2}\right|\right] 4xy \, dy \, dx + \int_0^{\infty}\int_{y_2}^{\infty} f(t, x) F(t, y)(x + V - |x - V|) \times$$
$$\times 4xy \, dy \, dx + \int_{x_1}^{V}\int_{y_0}^{y_1} f(t, x) F(t, y) \frac{m_2}{m_1} 2\left(y^2 + \frac{m_1}{m_2}(x^2 - V^2)\right)^{1/2} 4xy \, dy \, dx +$$
$$\left. + \int_V^{x_2}\int_0^{y_1} f(t, x) F(t, y) \, 2\frac{m_2}{m_1} y \, 4xy \, dy \, dx\right\} - \left(\frac{\sigma_1+\sigma_2}{2}\right)^2 2\pi^2 f(t, V)\int_0^{\infty} F(t, y)\frac{(V+y)^3 - |V-y|^3}{3V} y dy$$

$$I_{21}(F, f) = \left(\frac{\sigma_1+\sigma_2}{2}\right)^2 \frac{2\pi^2}{2V}\left(\frac{m_1+m^2}{2m_1}\right)^2 \left\{\int_0^{\infty}\int_{y_1 m_2/m_1}^{y_2 m_2/m_1} f(t, y) F(t, x) \times \right.$$
$$\times \left[\frac{m_1}{m_2}\left(y + \left(y^2 + \frac{m_2}{m_1}(x^2 - V^2)\right)^{1/2}\right) - |V - x|\right] 4xy \, dy \, dx + \int_0^{\infty}\int_{y_2 m_2/m_1}^{\infty} f(t, y) F(t, x) \times$$
$$\times (V + x - |V - x|) \, 4xy \, dy \, dx + \int_{x_1}^{V}\int_{y_0 m_2/m_1}^{y_1 m_2/m_1} f(t, y) F(t, x) \, 2\frac{m_1}{m_2}\left(y^2 + \frac{m_2}{m_1}(x^2 - V^2)\right)^{1/2} \times$$

$$\times 4xy\,dy\,dx + \int_{V}^{x_2}\int_{0}^{y_1 m_2/m_1} f(t,y)\,F(t,x)\,2\frac{m_1}{m_2}\,y4xy\,dy\,dx\Big\} -$$

$$-\left(\frac{\sigma_1+\sigma_2}{2}\right)^2 2\pi^2 F(t,V)\int_0^{\infty} f(t,y)\,\frac{(V+y)^3-|V-y|^3}{3V}\,y\,dy$$

where

$$x_1 = \frac{m_2-m_1}{m_2+m_1}V, \qquad x_2 = \frac{m_2+m_1}{m_2-m_1}V, \qquad y_0 = \left[\frac{m_1}{m_2}(V^2-x^2)\right]^{1/2}$$

$$y_1 = {}^1/_2\,|(V-x)+(V+x)\,m_1/m_2|, \qquad y_2 = {}^1/_2\,|(V+x)+m_1(V-x)/m_2|$$

Only double integrals are present in the above system and this reduces appreciably the amount of computation necessary when a computer is used to obtain a solution.

Next we shall investigate a numerical method of solution of Cauchy's problem for Eq. (6). L

Let us introduce the dimensionless distribution function f' which is to be determined and dimensionless variables t' and V', all defined by

$$t = \frac{\sqrt{m}}{4n\sigma^2\sqrt{\pi kT}}\,t', \qquad V = \sqrt{\frac{3kT}{m}}\,V', \qquad f = \frac{4\sqrt{2}}{9}\,n\left(\frac{m}{2\pi kT}\right)^{3/2} f'$$

where n and T are the density and termperature of the gas.

The factor preceding t' is equal to the mean time elapsing between two consecutive collosions of a molecule, while the RMS velocity is taken as a characteristic velocity.

Eq. (6) can be transformed into dimensionless variables by supplementing all magnitudes with a prime and omitting the factor $2\pi^2\sigma^2$ in its right-hand side. The initial distribution function shall correspond to the following problem. Let us suppose that at $t = 0$ we have a homogeneous quiescent gas. One half of its molecules exhibits Maxwellian distribution with the temperature $T_1 = T/2$, while the other half exhibits a Maxwellian distribution with temperature $T_2 = 3T/2$ where T is the temperature of the whole gas.

Let n be the gas density. Then the initial distribution function is

$$f_0 = \frac{n}{2}\left(\frac{m}{2\pi kT_1}\right)^{3/2}\exp\frac{-mV^2}{2kT_1} + \frac{n}{2}\left(\frac{m}{2\pi kT_2}\right)^{3/2}\exp\frac{-mV^2}{2kT_2}$$

which in dimensionless form becomes

$$f_0' = (9/4)\exp(-3V'^2) + (\sqrt{3}/4)\quad\exp(-V'^2) \tag{8}$$

As $t' \to \infty$, the solution tends to the Maxwellian distribution function, which in its dimensionless form can be written as

$$f' = ({}^9/_4\sqrt{2})\ \exp\ (-3V'^2/2) \tag{9}$$

Now denoting the right-hand side of (6), in its dimensionless form by $I(f', f')$, we can write it as

$$\partial f'/\partial t' = I\ (f', f')$$

The first time interval allowing the departure from the initial distribution function $f_0'(V')$ was obtained from the Euler's method $f'(\Delta t', V') = f_0'(V') + I(f_0', f_0')\,\Delta t'$ where $\Delta t'$ denotes the interval of time. Further steps were computed using a modified Euler's formula

$$f'(t_{k+1}', V') = f'(t_{k-1}', V') + I\,[f'(t_k', V'), f'(t_k', V')]\,2\Delta t', \qquad k \geqslant 1$$

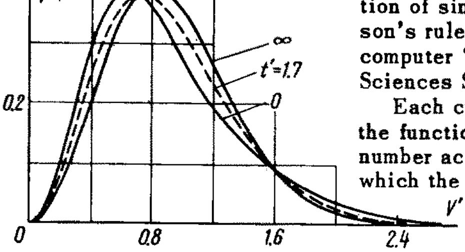

Fig. 1

Double integrals were calculated by repeated integration of single integrals, which were computed using Simpson's rule. Figs. 1 and 2 show the results obtained on the computer "Strela" at the Computer Center of the Acad. of Sciences SSSR.

Each curve of Fig. 1 shows the relationship between the function $V'^2 f'(t', V')$ and the velocity modulus. The number accompanying each curve denotes the instant to which the function corresponds. Function (8) was used as an initial distribution function. Fig. 2 shows the plots of $f'(t', V')$ corresponding to the following instants: $t' = 0$, 0.5, 1.0, 3.5. The curve labelled $t' = \infty$ corresponds to function (9).

We see that at $t' = 3.5$, the solution resembles a Maxwellian distribution function. However, as it approaches the equilibrium value, $\partial f'/\partial t'$ decreases and the limiting process of attaining Maxwellian distribution becomes very slow. To overcome this difficulty, we must use the asymptotic of the distribution function as $t' \to \infty$. We can, e.g. use the asymptotic of a linearized Boltzmann equation given in [3]. An approximate modelling equation is often used [4] to describe the motion of a rarefied gas. The latter, written in dimensionless variables used in Boltzmann equation, has the form

$$\partial f' / \partial t' = (4/5)\,[(9/4\sqrt{2})\ \exp\ (-3V'^2/2) - f']$$

Its initial Cauchy's problem has the following solution (10)

$$f' = f_0'(V')\exp(-4t'/5) + [1 - \exp(-4t'/5)](9/4\sqrt{2})\exp(-3V'^2/2)$$

where $f_0'(V')$ is the initial distribution function. Fig. 3 gives a comparison of solution of a modelling equation with that of Boltzmann equation by showing the plots of $V'^2 f'(t', V')$ at the instant $t' = 1$. The distribution function marked $t' = 0$ on Fig. 2 was taken as an initial function. The graph shows that at higher values of V', the solution of the modelling equation exceeds the value of the distribution function several times.

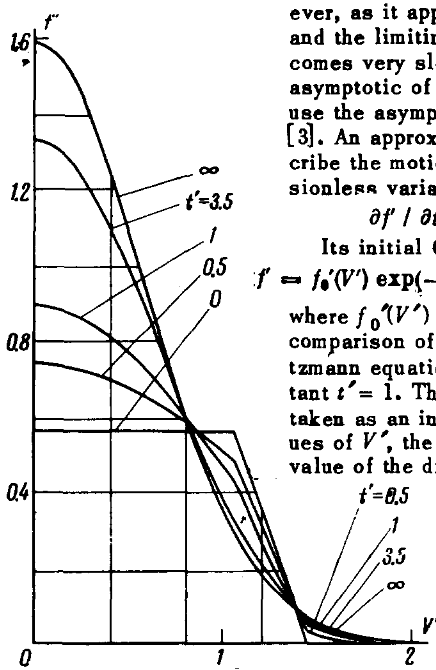

Fig. 2

This leads to an excess in the value of moments of order higher than that of the density and temperature, computed according to the distribution function (10).

Another characteristic feature of solution (10) is that the distribution function is time independent at the points V_k' at which the initial distribution function $f_0'(V')$ is equal to the Maxwellian distribution function $(9/4(2)^{1/2})\exp(-3V'^2/2)$.

In the case of the Boltzmann equation, computations show that the distribution function, which is its solution, changes its value with time.

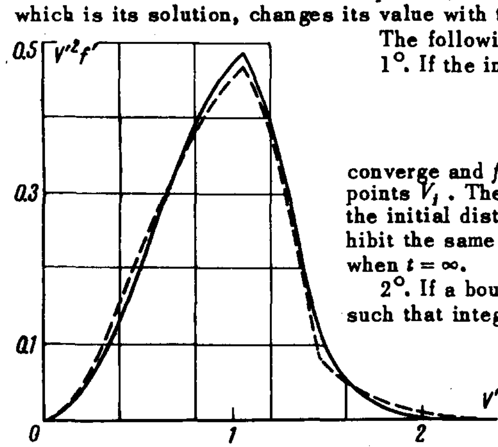

Fig. 3

The following two assertions are useful for computations.

1°. If the initial distribution function $f_0(V)$ is bounded,

$$\int_0^\infty V^2 f_0(V)\,dV, \qquad \int_0^\infty V^4 f_0(V)\,dV$$

converge and $f_0(V)$ has finite discontinuities at isolated points V_j. The solutions of the Boltzmann equation where the initial distribution function is also $f_0(V)$, will also exhibit the same discontinuities and they will disappear only when $t = \infty$.

2°. If a bounded and continuous initial function $f_0(V)$ is such that integrals

$$\int_0^\infty V^2 f_0(V)\,dV \qquad \int_0^\infty V^4 f_0(V)\,dV$$

converge and a derivative $\partial f_0(V)/\partial V$ exists which may undergo finite discontinuities at isolated points, then the derivative of the distribution function $\partial f(t, V)/\partial V$ will also exhibit discontinuities at these points and they will only disappear when $t = \infty$.

To prove the first assertion we shall write Eq. (6) with initial conditions at $t = 0$ taken into account, in an integral form

$$f(t, V) = f_0(V)\exp\left[-\int_0^t L(\tau, V)\,d\tau\right] + \int_0^t G(\tau, V)\exp\left[-\int_\tau^t L(s, V)\,ds\right]d\tau \qquad (11)$$

where

$$L(t, V) = 2\pi^2\sigma^2 \int_0^\infty f(t, x) \frac{(V + x)^3 - |V - x|^3}{3V} x dx$$

$$G(t, V) = 2\pi^2\sigma^2 \int_0^V \int_{\sqrt{V^2 - x^2}}^V f(t, x) f(t, y) \sqrt{x^2 + y^2 - V^2} \frac{4xy}{V} dy\, dx +$$

$$+ 2\pi^2\sigma^2 \int_0^V f(t, x) \frac{4x^2}{V} dx \int_V^\infty f(t, x) 2x dx + 2\pi^2\sigma^2 \left(\int_V^\infty f(t, x) 2x dx \right)^2$$

In [5] it was shown that under the above assertions there exists such a constant M, that the inequality $f(t, V) < M$ is valid for the solution of the Boltzmann equation at any t and V. Since an indefinite integral of a bounded function is a continuous function, then

$$\exp\left[- \int_0^t L(\tau, V) d\tau \right], \qquad \int_0^t G(\tau, V) \exp\left[- \int_\tau^t L(s, V) ds \right] d\tau$$

will be continuous in t and V.

Consequently, the existence of discontinuities in $f_0(V)$ implies the existence of discontinuities at the same points V_i in $f(t, V)$.

The integral representation (11) shows that its first term tends to zero with increasing time. Indeed, from the H-Theorem it follows that f tends to the Maxwellian distribution function as $t \to \infty$, therefore $L(t, V) \to L(\infty, V)$ as $t \to \infty$, where $L(\infty, V)$ is larger than some positive value at any V. Hence

$$\int_0^t L(\tau, V) d\tau \to +\infty \quad \text{as} \quad t \to \infty$$

from which it follows that the first term of (11) vanishes.

Proof of the second assertion is as follows. Under the assumption made in 2°, the Carleman Theorem III ([5], part 1, Ch. 2, par. 1) stating that $f(t, V)$ is a bounded, uniform and continuous function of V, is valid.

Differentiating (11) with respect to V and following the argument used in the proof of 1° together with the continuity of $f(t, V)$ in V, we arrive at the conclusion that $\partial f/\partial V$ will have discontinuities at the same points as $\partial f_0/\partial V$, and that these discontinuities will, again, disappear as $t \to \infty$.

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