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Formation of Maxwellian Tails*

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Using two models, we study the relaxation to a Maxwell distribution in the context of classical kinetic theory. For the first model, an exact solution of the nonlinear Boltzmann equation is derived. For the second model, an asymptotic solution exhibits the remarkable feature of a transient tail population sometimes much larger than the equilibrium Maxwell distribution. This phenomenon may be of importance for calculating rates of fast chemical reactions and for controlled thermonuclear fusion.

In this Letter, we report some preliminary results on the relaxation of nonequilibrium distribution functions to Maxwellian form.[1] Our interest is centered on behavior in the high-energy tail of the velocity distribution. Modification of the tail away from a Maxwell distribution can significantly change calculated values of certain gas-phase reaction rates, at given kinetic temperature, e.g., in pulsed devices for hydrogen fusion. Depletion of the Maxwellian tail has also been suggested[2,3] as an explanation for the discrepancy between observed and predicted fluxes of solar neutrinos.

We study two models, both classical and nonrelativistic. The system of interest here is an infinite, spatially homogeneous and isotropic gas with one species of molecule. It is assumed that only binary elastic scattering need be taken into account, so that the Boltzmann equation applies. In general, the elastic differential cross section σ is a function of relative velocity g and of scattering angle χ in the center-of-mass system. For the first model, we assume that σ is proportional to g^{-1}; in the second model σ is proportional to g^{-3}. For definiteness, we assume in this Letter that the scattering is isotropic; i.e., σ is independent of χ. Actually, introduction of an arbitrary angular distribution leads to only slight complication.

For the first model, we have found an exact solution of "shock transition" type for the *nonlinear* Boltzmann equation. This solution permits an analysis of the relaxation process for *all* velocities including, in particular, formation of the Maxwellian tail. Furthermore, guided by the form of solution for the first model, we find an asymptotic solution for the second model. This asymptotic solution exhibits the remarkable feature that the far tail population is for some time significantly larger (up to a factor 6) than the equilibrium Maxwell distribution.

Maxwell[1] established that the low-order moments of the distribution function effectively relax to their equilibrium values in just a few mean collision times. This corresponds to the property that the low-energy part of the distribution attains Maxwellian form in such a time interval. Although implicit in Maxwell's classic paper, this result appears first to have been stated explicitly by Jeans.[4] Nonlinear relaxation has also been discussed by Kac.[5] The effects discussed here are not related to those of Widom.[6]

The state of the gas at time t is described by a distribution function $nf(v, t)$, where n is the constant number density, $\vec{v}$ is a velocity variable, and $v = |\vec{v}|$. Conservation of mass and energy imply that

$$\int f(v,t)\,d^3v = 1\,,$$
$$\int v^2 f(v,t)\,d^3v = 3kT/m \equiv 3\beta^2\,, \tag{1}$$

where T is the constant kinetic temperature, m is the molecular mass, and k is Boltzmann's constant. Also, as $t\to\infty$, $f(v,t)$ tends to the Maxwell function

$$f(v,\infty) \equiv \frac{\exp(-v^2/2\beta^2)}{(2\pi\beta^2)^{3/2}}\,. \tag{2}$$

For our first model, we choose the differential cross section σ for elastic scattering to be

$$\sigma(g,\chi) = \kappa/g\,, \tag{3}$$

where κ is independent of both g and χ. It is now convenient to introduce the dimensionless time variable

$$\tau = 4\pi n\kappa t \tag{4}$$

which measures time in units of mean collision time. With the cross section (3) the Boltzmann equation can then be written (using standard notation) in the form

$$\frac{\partial f(v,\tau)}{\partial\tau} = -f(v,\tau) + \frac{1}{4\pi}\int d^3w \int_0^\pi d\chi\,\sin\chi \int_0^{2\pi} d\epsilon\, f(v',\tau) f(w',\tau)\,, \tag{5}$$

with

$$v'^2 = \tfrac{1}{2}(v^2+w^2) + \tfrac{1}{2}(v^2-w^2)\cos\chi + |\vec{v}\times\vec{w}|\sin\chi\cos\epsilon \tag{6}$$

and

$$w'^2 = \tfrac{1}{2}(v^2+w^2) - \tfrac{1}{2}(v^2-w^2)\cos\chi - |\vec{v}\times\vec{w}|\sin\chi\cos\epsilon\,. \tag{7}$$

Normalized moments $M_k(\tau)$ of f are defined by the equation

$$M_k \equiv \frac{\sqrt{\pi}}{2(2\beta^2)^k\,\Gamma(k+\frac{3}{2})}\int v^{2k} f(v,\tau)\,d^3v\,, \qquad k = 0,1,2,\dots\,. \tag{8}$$

It follows from Eqs. (1) and (2) that

$$M_0(\tau) \equiv 1\,,\quad M_1(\tau) \equiv 1\,, \tag{9}$$

and

$$M_k(\infty) = 1\,,\quad k = 0,1,2,\dots\,. \tag{10}$$

Multiplication of Eq. (5) by v^{2k} and integration over $\vec{v}$ space leads, after some manipulation, to the infinite sequence of moment equations

$$\frac{dM_k}{d\tau} + M_k = \frac{1}{k+1}\sum_{m=0}^{k} M_m M_{k-m}\,, \qquad k = 0,1,2,\dots\,. \tag{11}$$

Since we do not truncate this infinite sequence of equations, no information is lost in taking moments. In other words, (11) is equivalent to (5).

The form of these equations suggests that we introduce the generating function for the normalized moments

$$G(\xi,\tau) \equiv \sum_{k=0} \xi^k M_k(\tau)\,. \tag{12}$$

Then $G(\xi,\tau)$ satisfies the partial differential equation

$$\frac{\partial}{\partial\xi}\left(\xi\frac{\partial G}{\partial\tau} + \xi G\right) = G^2(\xi,\tau)\,. \tag{13}$$

Under the transformation

$$x = (1-\xi)/\xi\,,\quad y(x,\tau) = \xi G(\xi,\tau)\,, \tag{14}$$

Eq. (13) reduces to the form

$$\frac{\partial^2 y}{\partial x\,\partial\tau} + \frac{\partial y}{\partial x} + y^2 = 0\,. \tag{15}$$

The structure of Eq. (15) suggests that we seek a similarity solution of the form

$$y = x^{-1} z(\eta)\,,\quad \eta = \ln x + c\tau\,, \tag{16}$$

where c is a constant still to be determined. It then follows that $Z \equiv z'$, regarded as a function of z, satisfies the first order equation

$$cZ\,dZ/dz + (1-c)Z - z(1-z) = 0. \tag{17}$$

Boundary conditions corresponding to Eqs. (9) and (10) determine that

$$c = \tfrac{1}{6} \tag{18}$$

and therefore the explicit solution of Eq. (17),

$$Z(z) = 2(1-z)[1-(1-z)^{1/2}]\,. \tag{19}$$

It is easily shown that this solution corresponds to the distribution function

$$f(v,\tau)=\frac{\exp(-v^2/2K\beta^2)}{2(2\pi K\beta^2)^{3/2}}\left(\frac{(5K-3)}{K}+\frac{(1-K)}{K^2}\frac{v^2}{\beta^2}\right), \tag{20}$$

where

$$K=1-e^{-\tau/6}. \tag{21}$$

As a distribution function, f must be nonnegative. Therefore $K \geqslant \frac{5}{3}$, or

$$\tau \geqslant \tau_0 \equiv 6\ln\tfrac{5}{2} \sim 5.498. \tag{22}$$

The second model is characterized by the differential cross section

$$\sigma(g,\chi)=\kappa\beta^2/g^3, \tag{23}$$

where κ is again independent of g and χ. We have not been able to find any nontrivial exact solution for this case. However, an asymptotic solution for $v\to\infty$ is readily obtained.

For large v, we introduce the approximation of setting $w=0$ in Eqs. (23), (6), and (7). The Boltzmann equation reduces to the form

$$\frac{v^2}{\beta^2}\frac{\partial f(v,\tau)}{\partial\tau}=-f(v,\tau)+\tfrac{1}{2}\int_{-1}^{+1} f\left(v\left(\frac{1+\mu}{2}\right)^{1/2},\tau\right) f\left(v\left(\frac{1-\mu}{2}\right)^{1/2},\tau\right)d\mu. \tag{24}$$

This nonlinear equation admits an explicit solution of the form

$$f(v,\tau)=f(v,\infty)e^{-\zeta}(1-\tfrac{22}{3}\zeta+\tfrac{44}{3}\zeta^2), \tag{25}$$

where

$$\zeta=(45/22\tau)v^2/\beta^2. \tag{26}$$

More precisely, Eq. (25) is an asymptotic solution of the Boltzmann equation with the cross section (23), in the limit of large v and large τ, such that the variable ζ is fixed.

In Fig. 1, we plot the ratio $F(\zeta)=f(v,\tau)/f(v,\infty)$ given by the explicit formula (25) as a function of ζ. We note the rather large peak around $\zeta=2$, with maximum value of 6.1922 for F. There is also a deep valley near $\zeta=0.25$, with a minimum value of 0.064 808. The presence of the peak implies that, under certain conditions, *transient chemical or nuclear reaction rates may attain values substantially larger than would be expected from the Maxwell distribution.*

As mentioned earlier, both models can be generalized to permit arbitrary dependence of the cross section σ on scattering angle χ. For the first model, the only modification thereby introduced is a change of the time scale. For the second model there are, in addition, changes in the shape of the curve for $F(\zeta)$. However, there is always a peak and a valley, with the peak value of F at least 3.1516 for any angular distribution.

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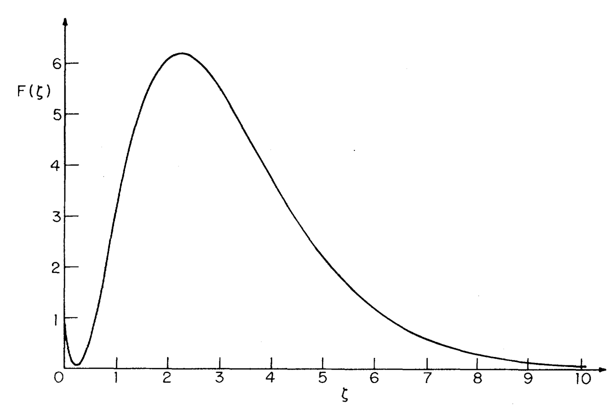

FIG. 1. Invariant shape of transient tail distribution for the second model.

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