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Solution of the BGK Model Kinetic Equation for Very Hard Particle Interaction

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We study the Bhatnagar–Gross–Krook model kinetic equation with a velocity-dependent collision frequency. We derive the conditions that must be verified in order to keep the main physical properties of the Boltzmann equation, i.e., H-theorem and conservation laws. The particular case of the so-called VHP interaction is considered, and the resulting kinetic equation is solved for a homogeneous and isotropic gas. Overpopulation phenomena are observed and analyzed for some kinds of initial conditions. The results are compared, where possible, with the exact solution of the Boltzmann equation.

KEY WORDS: Boltzmann equation; BGK model kinetic equation; VHP interaction; Tjon effect.

1. INTRODUCTION

In the last few years a great effort has been devoted to the search for particular solutions of the Boltzmann equation.[1] Because of the mathematical complexity, studies have been restricted to very simple physical situations, and simplified collision models have been considered. Nevertheless, the results have turned out to be very interesting. For instance, an overpopulation phenomenon at high energies (the so-called Tjon effect) has been discovered.[1]

Most of the solutions of the Boltzmann equation we are aware of refer to a spatially homogeneous and isotropic system. Usually, the particles are assumed to interact via a Maxwell potential, although some stochastic interactions have also been proposed and analyzed.[1–3]

In this paper we will be concerned with the Bhatnagar–Gross–Krook (BGK) model kinetic equation,[4] where the Boltzmann collision term is

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approximated by an exponential relaxation towards a reference state. In spite of its apparent simplicity, this equation has only been studied with some detail for cases where the collision frequency does not depend on the velocity. Then, the usual local equilibrium is taken as the reference state. However, if the collision frequency is velocity dependent, the above choice is not adequate if one wants to keep the conservation of mass, momentum, and kinetic energy. Following a discussion by Cercignani,[4] we propose here a BGK equation where the reference distribution function is assumed to be a Gaussian function of the velocity. The parameters appearing in this function are expressed as functionals of the actual distribution function of the system. This is done by requiring the conservation laws to be verified. For the case of velocity-independent collision frequency, we recover the standard equation. One of the advantages of the model is that it allows the study of the evolution of homogeneous and isotropic systems, for which the local equilibrium distribution coincides with the total equilibrium one. So, the BGK equation with a velocity-independent collision frequency becomes trivial in this case.

The paper is organized as follows. In Section 2 we construct our model and derive the consistency equations for the parameters appearing in the reference distribution function. We also discuss the formal relation between the Boltzmann equation and the BGK model. The results are particularized for Maxwell molecules and for the VHP interaction.[5]

In Section 3, the general theory is applied to a homogeneous and isotropic gas. For the VHP interaction, the reference distribution function is determined by the second energy moment. The time evolution of the moments is analyzed in Section 4. It is shown that the nth energy moment can be expressed as a non-Markovian functional of the second moment plus a term depending on the entire initial distribution. As a consequence, we get a well-defined equation for the second moment.

For Maxwell molecules, Hauge[6] proposed a general criterion determining whether the Boltzmann equation presents the Tjon effect. The relevant quantity appears to be the initial second energy moment. We discuss the validity of this criterion in our model in Section 5, where several kinds of initial conditions are considered. Our conclusion is that for situations where the initial second moment plays the main role in the evolution of the system, Hauge's criterion applies. These situations are characterized by a monotone relaxation of the second moment. In other cases, higher-order initial moments must be considered.

Finally, in Section 6, we present some numerical results corresponding to the VHP interaction for two and three dimensions with different initial conditions. It is seen that the overpopulation effect shows up for cases where it is predicted by the second moment criterion. For the two-dimensional case,

the results are compared with the analytic solution of the VHP interaction Boltzmann equation.[1,5]

2. DESCRIPTION OF THE MODEL

We start with the Boltzmann equation governing the evolution of the one-particle distribution function $f(\mathbf{r}, \mathbf{v}; t)$ of a dilute gas. In standard notation, it reads

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f(\mathbf{r}, \mathbf{v}; t) = \int d\mathbf{v}_1 \int d\hat{\mathbf{n}}\, gI(g, \chi)[f(\mathbf{r}, \mathbf{v}'; t) f(\mathbf{r}, \mathbf{v}_1'; t) - f(\mathbf{r}, \mathbf{v}; t) f(\mathbf{r}, \mathbf{v}_1; t)] \tag{2.1}$$

where $g = |\mathbf{v} - \mathbf{v}_1|$, $I(g, \chi)$ is the differential cross section of the collision $(\mathbf{v}, \mathbf{v}_1) \to (\mathbf{v}', \mathbf{v}_1')$, χ is the scattering angle, and $d\hat{\mathbf{n}}$ is the solid angle element. Equation (2.1) can be formally written as

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f(\mathbf{r}, \mathbf{v}; t) = -\zeta(\mathbf{r}, \mathbf{v}; t)[f(\mathbf{r}, \mathbf{v}; t) - f_R(\mathbf{r}, \mathbf{v}; t)] \tag{2.2}$$

with

$$\zeta(\mathbf{r}, \mathbf{v}; t) = \int d\mathbf{v}_1 \int d\hat{\mathbf{n}}\, gI(g, \chi) f(\mathbf{r}, \mathbf{v}_1; t) \tag{2.3}$$

and

$$f_R(\mathbf{r}, \mathbf{v}; t) = [\zeta(\mathbf{r}, \mathbf{v}; t)]^{-1} \int d\mathbf{v}_1 \int d\hat{\mathbf{n}}\, gI(g, \chi) f(\mathbf{r}, \mathbf{v}'; t) f(\mathbf{r}, \mathbf{v}_1'; t) \tag{2.4}$$

Equation (2.2) can be understood as a relaxation time equation, where the effect of collisions is given by the relaxation of $f(\mathbf{r}, \mathbf{v}; t)$ towards the "reference" distribution function $f_R(\mathbf{r}, \mathbf{v}; t)$. In fact, $\zeta(\mathbf{r}, \mathbf{v}; t)$ is the collision frequency for molecules of velocity $\mathbf{v}$.

As is well known, the Boltzmann equation describes very satisfactorily the time evolution of a simple dilute gas. From a physical point of view, the two main properties of the Boltzmann equation are the following:

(i) The collision term conserves the mass, the momentum and the energy. Using the form (2.2), we express this as

$$\int d\mathbf{v}\, A^{\alpha}(\mathbf{v})\, \zeta(\mathbf{r}, \mathbf{v}; t)[f(\mathbf{r}, \mathbf{v}; t) - f_R(\mathbf{r}, \mathbf{v}; t)] = 0 \tag{2.5}$$

where

$$\{A^{\alpha}(\mathbf{v})\} = \{1, \mathbf{v}, v^2\} \tag{2.6}$$

(ii) The Boltzmann equation leads to the H-theorem, showing the irreversible evolution of the system towards equilibrium:

$$\int d\mathbf{v} \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f(\mathbf{r}, \mathbf{v}; t) \log f(\mathbf{r}, \mathbf{v}; t) \leqslant 0 \tag{2.7}$$

The equality in (2.7) is verified by a solution of the Boltzmann equation only if the system is at equilibrium,[7] i.e., if the distribution function is

$$f^{\text{eq}}(v) = n \left(\frac{m}{2\pi k_B T}\right)^{d/2} \exp\left(-\frac{mv^2}{2k_B T}\right) \tag{2.8}$$

Here, n is the number density, T is the temperature, k_B is the Boltzmann constant, m is the mass of a particle, and d is the dimension of the system.

The formal solution of the Boltzmann equation (2.2) can be written as

$$\begin{aligned} f(\mathbf{r}, \mathbf{v}; t) = {} & e^{-t\mathbf{v}\cdot\nabla} U(\mathbf{r}, \mathbf{v}; t) f(\mathbf{r}, \mathbf{v}; 0) \\ & + \int_0^t ds\, e^{-t\mathbf{v}\cdot\nabla} U(\mathbf{r}, \mathbf{v}; t)\, U^{-1}(\mathbf{r}, \mathbf{v}; s) \\ & \times e^{s\mathbf{v}\cdot\nabla_r} \zeta(\mathbf{r}, \mathbf{v}; s) f_R(\mathbf{r}, \mathbf{v}; s) \end{aligned} \tag{2.9}$$

where we have introduced the quantity

$$U(\mathbf{r}, \mathbf{v}; t) = \exp\left[-\int_0^t ds\, \zeta(\mathbf{r} + s\mathbf{v}, \mathbf{v}; s)\right] \tag{2.10}$$

Nevertheless, getting from (2.9) an explicit solution is a very hard task, due to the complex structure of the collision kernel. And this refers to analytic as well as numerical calculations. Only very simplified models have been solved up to now.[1] For interaction potentials of the form

$$\varphi(r) \sim r^{-\varepsilon} \tag{2.11}$$

the collision rate factorizes in the form

$$gI(g, \chi) = g^{1-2(d-1)/\varepsilon} \alpha_{\varepsilon}(\chi) \tag{2.12}$$

So, for these potentials, the collision frequency (2.3) is given by

$$\zeta(\mathbf{r}, \mathbf{v}; t) = C_{\varepsilon} \int d\mathbf{v}_1\, g^{1-2(d-1)/\varepsilon} f(\mathbf{r}, \mathbf{v}_1; t) \tag{2.13}$$

Here, C_ε is a constant resulting from the integration over the angular variables. The simplest case corresponds to the so-called Maxwell molecules, for which $\varepsilon = 2(d-1)$. Then, the collision rate does not depend on g and

$$\zeta_M(\mathbf{r}, \mathbf{v}; t) = \zeta_M(\mathbf{r}, t) = C_M n(\mathbf{r}, t) \tag{2.14}$$

i.e., the collision frequency is velocity independent and it is proportional to the local density of particles $n(\mathbf{r}, t)$ defined as

$$n(\mathbf{r}, t) = \int d\mathbf{v}\, f(\mathbf{r}, \mathbf{v}; t) \tag{2.15}$$

Bobylev,[8] and also Krook and Wu,[9] found an exact, although particular, solution of the Boltzmann equation for Maxwell molecules. They considered a homogeneous gas with an isotropic velocity distribution, assuming a very special initial condition. Later on, the general solution for arbitrary initial conditions was obtained in terms of Laguerre series.[10]

One of the most interesting interaction potentials is the hard sphere potential, which can be obtained from (2.11) in the limit $\varepsilon \to \infty$. Although it has been extensively used in kinetic theory, no one has up to now succeeded in finding an exact solution of the Boltzmann equation for this potential. The reason is that it leads to a collision rate proportional to g, and then the integral defining the collision frequency in Eq. (2.13) becomes very intricate. Ernst[5] realized that there is a case where $\zeta(\mathbf{r}, \mathbf{v}; t)$ can be expressed in a simple way, namely, when

$$gI(g, \chi) = g^2 \alpha(\chi) \tag{2.16}$$

That means that the collision rate grows with g even faster than for hard sphere interaction, and so Eq. (2.16) does not correspond to any physical potential. Following Ernst, we will refer to this model as the very hard particle (VHP) model. The collision frequency for this model is

$$\zeta_{\text{VHP}}(\mathbf{r}, \mathbf{v}; t) = C_{\text{VHP}} n(\mathbf{r}, t) \left\{ d \frac{k_B T(\mathbf{r}, t)}{m} + [\mathbf{v} - \mathbf{u}(\mathbf{r}, t)]^2 \right\} \tag{2.17}$$

where we have introduced the local temperature $T(\mathbf{r}, t)$ and the local velocity $\mathbf{u}(\mathbf{r}, t)$ defined by

$$n(\mathbf{r}, t)\, \mathbf{u}(\mathbf{r}, t) = \int d\mathbf{v}\, \mathbf{v} f(\mathbf{r}, \mathbf{v}; t) \tag{2.18}$$

$$\frac{d}{2} n(\mathbf{r}, t)\, k_B T(\mathbf{r}, t) = \int d\mathbf{v}\, \frac{m}{2} [\mathbf{v} - \mathbf{u}(\mathbf{r}, t)]^2 f(\mathbf{r}, \mathbf{v}; t) \tag{2.19}$$

Again, C_{VHP} is a constant depending on the form of the function $\alpha(\chi)$ in Eq. (2.16).

The Boltzmann equation for the VHP model has been solved for a two-dimensional gas, in the case of homogeneity in space and isotropy in velocities.[5]

Of course, the chance of exactly solving the Boltzmann equation for a given model is directly related to the simplicity of the collision frequency. The Maxwell and the VHP models correspond to the two simplest choices. It is easily seen that any other collision rate may lead to a much more complicated equation.

The above difficulties have prompted and stimulated the search for simplified versions of the Boltzmann equation. They are usually referred to as model kinetic equations. Perhaps one of the best known is the Bhatnagar–Gross–Krook (BGK) model.[4] The idea is to substitute the functions $f_R(\mathbf{r}, \mathbf{v}; t)$ and $\zeta(\mathbf{r}, \mathbf{v}; t)$ appearing in Eq. (2.2) by simpler functionals of the distribution $f(\mathbf{r}, \mathbf{v}; t)$. The usual choice for f_R is the local equilibrium form; i.e., one takes

$$f_R(\mathbf{r}, \mathbf{v}; t) = f_l(\mathbf{r}, \mathbf{v}; t)$$
$$= n(\mathbf{r}, t) \left[\frac{m}{2\pi k_B T(\mathbf{r}, t)}\right]^{d/2} \exp\left\{-\frac{m[\mathbf{v} - \mathbf{u}(\mathbf{r}, t)]^2}{2k_B T(\mathbf{r}, t)}\right\} \tag{2.20}$$

where $n(\mathbf{r}, t)$, $\mathbf{u}(\mathbf{r}, t)$, and $T(\mathbf{r}, t)$ are defined by Eqs. (2.15), (2.18), and (2.19), respectively. The distribution (2.20) satisfies the conditions

$$\int d\mathbf{v}\, A^{\alpha}(\mathbf{v}) f(\mathbf{r}, \mathbf{v}; t) = \int d\mathbf{v}\, A^{\alpha}(\mathbf{v}) f_l(\mathbf{r}, \mathbf{v}; t) \tag{2.21}$$

where the A^{α}'s are defined in Eq. (2.6). Also, different approximations for the collision frequency are used, depending on the problem at hand. However, if ζ depends on the velocity, Eqs. (2.5) and (2.21) cannot be simultaneously satisfied. In other words, if we consider the BGK model with a velocity-dependent collision frequency and we take for f_R the local equilibrium form (2.20), then the $A^{\alpha}(\mathbf{v})$ do not correspond to conserved quantities.

Here, we are going to reformulate the BGK model in a slightly different way. We assume that

$$f_R(\mathbf{r}, \mathbf{v}; t) = f_B(\mathbf{r}, \mathbf{v}; t)$$
$$= a(\mathbf{r}, t) \exp[\mathbf{b}(\mathbf{r}, t) \cdot \mathbf{V}(\mathbf{r}, t) - c(\mathbf{r}, t)\, V^2(\mathbf{r}, t)] \tag{2.22}$$

where

$$\mathbf{V}(\mathbf{r}, t) = \mathbf{v} - \mathbf{u}(\mathbf{r}, t) \tag{2.23}$$

and a, $\mathbf{b}$, and c are field variables that are determined by requiring the kinetic equation to verify the physical conditions (2.5). Moreover, once the functional form (2.22) has been assumed for $f_R(\mathbf{r}, \mathbf{v}; t)$, Eqs. (2.5) automatically imply the H-theorem, Eq. (2.7). This can be easily seen from the relation

$$\int d\mathbf{v}\, \zeta(\mathbf{r}, \mathbf{v}; t)[f(\mathbf{r}, \mathbf{v}; t) - f_B(\mathbf{r}, \mathbf{v}; t)] \log f_B(\mathbf{r}, \mathbf{v}; t) = 0 \tag{2.24}$$

that follows from Eqs. (2.5).

In our model, we will keep the collision frequency as given by Eq. (2.3), i.e., the same expression as it had in the Boltzmann equation. For Maxwell molecules, Eq. (2.14), the distribution (2.22) reduces to the local equilibrium one, Eq. (2.20). The case of VHP interaction, Eq. (2.17), is studied in Appendix A, where it is shown that conditions (2.5) lead to the following set of equations:

$$2dn \frac{k_B T}{m} = D\left(d \frac{k_B T}{m} + \frac{b^2}{4c^2} + \frac{d}{2c}\right) \tag{2.25}$$

$$2 \frac{\mathbf{J}}{m} = \frac{D}{2c}\left(d \frac{k_B T}{m} + \frac{b^2}{4c^2} + \frac{d+2}{2c}\right) \mathbf{b} \tag{2.26}$$

$$n\left(d \frac{k_B T}{m}\right)^2 + \Phi = \frac{D}{4c^2}\left[\left(\frac{b^2}{c} + d\right)(d+2) + (b^2 + 2dc) d \frac{k_B T}{m} + \frac{b^4}{4c^2}\right] \tag{2.27}$$

In these expressions

$$D = a e^{b^2/4c} \left(\frac{\pi}{c}\right)^{d/2} \tag{2.28}$$

and we have introduced the heat flux

$$\mathbf{J}(\mathbf{r}, t) = \frac{m}{2} \int d\mathbf{v}\, V^2(\mathbf{r}, t)\, \mathbf{V}(\mathbf{r}, t) f(\mathbf{r}, \mathbf{v}; t) \tag{2.29}$$

and the local function

$$\Phi(\mathbf{r}, t) = \int d\mathbf{v}\, V^4(\mathbf{r}, t) f(\mathbf{r}, \mathbf{v}; t) \tag{2.30}$$

The presence of $\mathbf{J}(\mathbf{r}, t)$ and $\Phi(\mathbf{r}, t)$ in Eqs. (2.25)–(2.27) indicates that in order to identify the reference state in the VHP model we need up to the fourth moment in velocity space of the distribution function. The local

equilibrium distribution f_l only requires the knowledge up to the second velocity moment, while the exact reference distribution function in the Boltzmann equation, given by Eq. (2.4), is a functional of all the moments of $f(\mathbf{r}, \mathbf{v}; t)$.

Up to now, everything has been general in the sense that no particular physical situation has been considered. In the following sections, we will deal with the application of this formalism to a homogeneous and isotropic system.

3. HOMOGENEOUS AND ISOTROPIC GAS

Let us consider a spatially homogeneous gas with an isotropic distribution of velocities. In this case, the distribution function depends only on the modulus of the velocity, and the densities of the conserved quantities take their equilibrium values. So, the local equilibrium function reduces to the (total) equilibrium one. As a consequence, the BGK model for Maxwell molecules becomes trivial and leads to

$$f(v, t) = f^{\text{eq}}(v) + e^{-\zeta_M t}[f(v, 0) - f^{\text{eq}}(v)] \tag{3.1}$$

The system presents an exponential relaxation towards equilibrium at all times. That means that the model is too rough to describe the complicated and interesting behavior observed in the solutions of the Boltzmann equation.[1] One could think that this is a general feature of the BGK model, but we will see it is not the case. What makes the above description so limited is the fact that the evolution of the distribution function appears as controlled by the average of the conserved quantities. The VHP model, which incorporates higher moments, allows a much richer description of the system.

It is convenient to go over to the energy representation. We introduce the dimensionless variable

$$x = \frac{mv^2}{2k_B T} \tag{3.2}$$

and the distribution function

$$\begin{aligned} F(x, t) &= \frac{1}{n} \int d\mathbf{v}_1 \, \delta\left(x - \frac{mv_1^2}{2k_B T}\right) f(v_1, t) \\ &= \left(\frac{2\pi k_B T}{m}\right)^{d/2} \frac{x^{d/2-1}}{\Gamma(d/2)} \frac{1}{n} f(v, t) \end{aligned} \tag{3.3}$$

The corresponding equilibrium expression is

$$F^{eq}(x) = \frac{x^{d/2-1}}{\Gamma(d/2)} e^{-x} \tag{3.4}$$

while the reference distribution defined in Eq. (2.22) takes the form

$$F_B(x, t) = \frac{v(t)}{\Gamma(d/2)[\theta(t)]^{d/2}} x^{d/2-1} e^{-x/\theta(t)} \tag{3.5}$$

with the definitions

$$v(t) = \frac{a(t)}{n} \left[\frac{\pi}{c(t)}\right]^{d/2} \tag{3.6}$$

$$\theta(t) = \frac{m}{2k_B Tc(t)} \tag{3.7}$$

Upon writing (3.5), we have used the fact that for an isotropic system it is $\mathbf{b} = 0$. This can be seen in the following way. If the system is isotropic, the collision frequency does not depend on the direction of $\mathbf{v}$, and, thus, Eqs. (2.5) imply that f_B must also be independent of it. In particular, for the VHP model, one can reach this result from Eq. (2.26). For an isotropic system it is $\mathbf{J} = 0$ and, then, $\mathbf{b} = 0$.

In the BGK approximation, the distribution function $F(x, t)$ obeys the equation

$$\frac{\partial}{\partial t} F(x, t) = -\zeta(x, t)[F(x, t) - F_B(x, t)] \tag{3.8}$$

For a homogeneous and isotropic system, the VHP collision frequency, Eq. (2.17), becomes time independent and reads

$$\zeta_{VHP}(x) = \zeta_0 \left(1 + \frac{2}{d} x\right) \tag{3.9}$$

where $\zeta_0 = C_{VHP} n d k_B T/m$. Then, the formal solution of Eq. (3.8) yields

$$F(x, t) = e^{-\zeta_{VHP}(x)t} F(x, 0) + \zeta_{VHP}(x) \int_0^t ds\, e^{-\zeta_{VHP}(x)(t-s)} F_B(x, s) \tag{3.10}$$

The function $F_B(x, t)$ depends on time through $v(t)$ and $\theta(t)$, which are functions of the moment $\Phi(t)$ defined in (2.30). More precisely, $v(t)$ and $\theta(t)$ are given by Eqs. (2.25) and (2.27) with $\mathbf{b} = 0$, i.e.,

$$2 = \nu(t)[1 + \theta(t)] \tag{3.11}$$

$$\frac{d}{d+2} + M_2(t) = \nu(t)\,\theta(t)\left[\frac{d}{d+2} + \theta(t)\right] \tag{3.12}$$

where we have introduced

$$M_2(t) = \frac{\Phi(t)}{d(d+2)\,n(k_B T/m)^2} \tag{3.13}$$

In general, we define normalized moments $M_n(t)$ as

$$M_n(t) = \frac{\int d\mathbf{v}\, v^{2n} f(v,t)}{\int d\mathbf{v}\, v^{2n} f^{\text{eq}}(v)} = \frac{\Gamma(d/2)}{\Gamma(n+d/2)} \int_0^\infty dx\, x^n F(x,t) \tag{3.14}$$

From this expression and the conservation laws, it follows that $M_0(t) = M_1(t) = 1$. On the other hand, Eqs. (3.11) and (3.12) lead to a quadratic equation for $\theta(t)$, whose positive solution is

$$\theta(t) = \frac{(d+2)\,M_2(t) - d + \{[3d + 8 + (d+2)\,M_2(t)] - 32(d+2)\}^{1/2}}{4(d+2)} \tag{3.15}$$

As $M_2(t)$ must be positive, we can establish a bound for $\theta(t)$:

$$\theta(t) > \theta_{\min} = \frac{-d + (9d^2 + 16d)^{1/2}}{4(d+2)} \tag{3.16}$$

In Fig. 1 we have plotted θ and ν as functions of M_2 for $d = 3$. It is seen that when M_2 takes the equilibrium value, $M_2 = 1$, it is $\nu = \theta = 1$, i.e., these parameters also take their equilibrium values and, so, the reference distribution function coincides with the equilibrium distribution. Nevertheless, as we will see in the next section, these values are not conserved in time unless $M_n = 1$ for all n. In other words, conservation of M_2 implies that the system is at equilibrium.

To study the time evolution of the system let us introduce

$$R(x,t) = \frac{F(x,t)}{F^{\text{eq}}(x)} \tag{3.17}$$

satisfying the equation

$$R(x,t) = e^{-\zeta_{\text{VHP}}(x)t} R(x,0) + \zeta_{\text{VHP}}(x) \int_0^t ds\, e^{-\zeta_{\text{VHP}}(x)(t-s)} R_B(x,s) \tag{3.18}$$

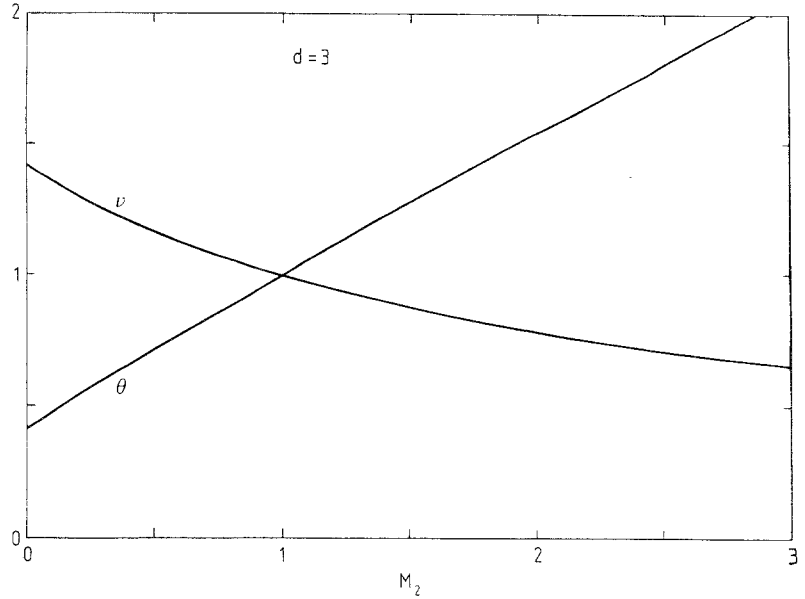

Fig. 1. Dependence of the parameters v and θ defining the reference distribution function, on the second moment M_2 for the three-dimensional VHP interaction in the BGK model.

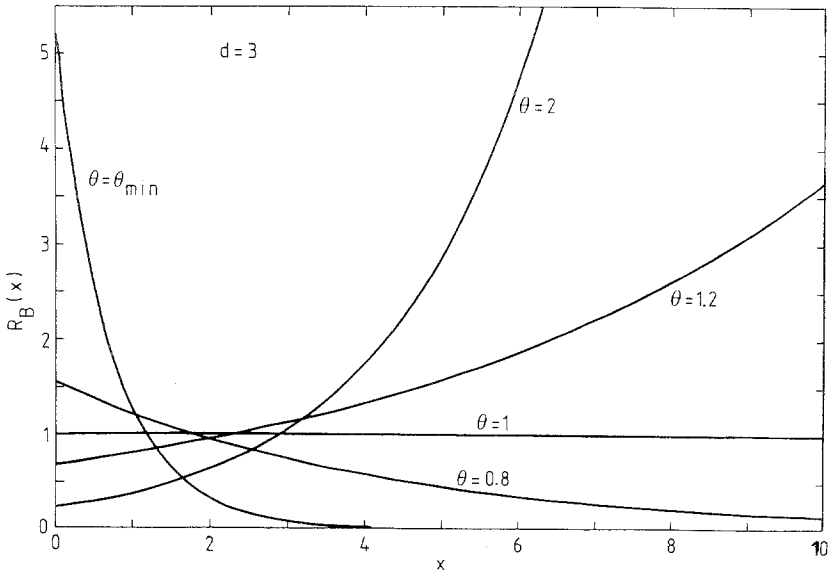

Fig. 2. Graph of the reference function $R_B(x)$ versus x for several values of the time-dependent parameter θ in the case $d = 3$.

where

$$R_B(x,t)=\frac{F_B(x,t)}{F^{eq}(x)}=\frac{2}{[1+\theta(t)][\theta(t)]^{d/2}}\exp\left\{\left[1-\frac{1}{\theta(t)}\right]x\right\} \tag{3.19}$$

Notice that Eq. (3.18) is a closed equation for the function R, as θ is a functional of R through M_2, according to Eq. (3.15).

It is interesting to know how the shape of $R_B(x)$ changes with θ. In Fig. 2, we represent $R_B(x)$ as a function of x for several values of θ. The curves correspond to the three-dimensional case, for which $\theta_{\min}\simeq 0.418$. For $\theta<1$, $R_B(x)$ is a decreasing function of x, while it is an increasing function when $\theta>1$. It is also observed that the slope rapidly increases with x for values of θ greater than one. We will come back to this figure in Section 5.

4. EVOLUTION OF THE MOMENTS

In order to evaluate (3.18), we need $\theta(t)$ or, equivalently, $M_2(t)$. Evolution equations for the moments can be derived from (3.8). For the VHP model, one gets

$$\frac{\partial}{\partial t}M_n(t)=-\zeta_0[M_n(t)-M_{B,n}(t)]$$
$$-\zeta_0\left(1+\frac{2n}{d}\right)[M_{n+1}(t)-M_{B,n+1}(t)] \tag{4.1}$$

with

$$M_{B,n}(t)=\frac{\Gamma(d/2)}{\Gamma(n+d/2)}\int_0^\infty dx\,x^nF_B(x,t)=2\frac{[\theta(t)]^n}{1+\theta(t)} \tag{4.2}$$

For the sake of simplicity, we will take in the following ζ_0^{-1} as the unit of time, so we will take $\zeta_0=1$.

Thus, we have a hierarchy of equations, the evolution of $M_n(t)$ involving the next moment $M_{n+1}(t)$. In fact, Eqs. (3.11) and (3.12) are nothing else but the two first equations of the hierarchy. It must be noticed that Eqs. (4.1) are also valid if one uses the Boltzmann equation, but, then, the moments $M_{B,n}(t)$ must be computed with the reference distribution function (2.4). In this case, each equation of the hierarchy (4.1) would contain all the moments of the distribution function. The main simplification of the BGK approximation is that only $M_2(t)$ or, equivalently, $\theta(t)$ is needed to know the distribution $F_B(x,t)$, and, from it, all the moments $M_{B,n}(t)$.

A glance at Eq. (3.10) shows that $F(x,t)$ is expressed in terms of the initial condition and the values of $F_B(x,s)$ for $0\leqslant s\leqslant t$. In other words,

$F(x, t)$ only depends on the initial moments and the past history of θ. Of course, the same property holds for all the moments $M_n(t)$. Let us make this point explicit. Multiplication of (3.10) by x^n and integration over x yields

$$M_n(t) = P_n(t) + \frac{\Gamma(d/2)}{\Gamma(n+d/2)} \int_0^t ds \int_0^\infty dx\, x^n \zeta_{\mathrm{VHP}}(x) \times e^{-\zeta_{\mathrm{VHP}}(x)(t-s)} F_B(x, s) \tag{4.3}$$

where $P_n(t)$, defined as

$$P_n(t) = \frac{\Gamma(d/2)}{\Gamma(n+d/2)} \int_0^\infty dx\, x^n e^{-\zeta_{\mathrm{VHP}}(x)t} F(x, 0) \tag{4.4}$$

incorporates the initial condition effects. The energy integration in the second term on the right-hand side of Eq. (4.3) can be easily evaluated, and one gets

$$M_n(t) = P_n(t) + 2 \int_0^t ds\, e^{-(t-s)} \frac{[\theta(s)]^{n+1}}{1+\theta(s)} \left[1 + \frac{1}{\theta(s)} + \frac{2(n+t-s)}{d}\right] \times \left[1 + \frac{2}{d}(t-s)\,\theta(s)\right]^{-n-1-d/2} \tag{4.5}$$

Of course, the time derivative of this equation leads to Eq. (4.1).

Equation (4.5) deserves some comments. Taking into account (3.15), we see that all the moments of the distribution function are expressed as a nonlinear and non-Markovian functional of the second moment M_2, plus a term containing all the initial moments. In the case of the Boltzmann equation for Maxwell molecules,[1,6,10] $M_n(t)$ is given by a function of $M_m(0)$ with $m \leqslant n$. That means that, for instance, two different initial distribution functions having the same initial value $M_2(0)$ will evolve in time in such a way that both will always have the same value of $M_2(t)$. This is not true for VHP interaction either in the BGK model or in the Boltzmann equation.

Our aim is to evaluate $R(x, t)$ given by Eq. (3.18). In this equation $\theta(t)$ is given by the solution of Eq. (4.5) taking $n = 0$, 1, or 2. Due to the complexity of the time dependence of θ, we have not been able to find an analytic solution, even for very special and simple initial conditions. This may be a little shocking since the Boltzmann equation for the VHP interaction has been exactly solved for a two-dimensional system.[5] Nevertheless, the following arguments will clarify the reason for this difference.

Let us introduce the Laplace transform of $F(x, t)$ or generating moments function

$$G(z, t) = \int_0^\infty dx\, e^{-zx} F(x, t)$$

$$= \sum_{n=0}^{\infty} (-1)^n \frac{\Gamma(n + d/2)}{n!\, \Gamma(d/2)} M_n(t)\, z^n \tag{4.6}$$

For the reference distribution function (3.5) we have

$$G_B(z, t) = \int_0^\infty dx\, e^{-zx} F_B(x, t) = v(t)[1 + z\theta(t)]^{-d/2} \tag{4.7}$$

The Laplace transform of Eq. (3.8) for the VHP model is

$$\left(\frac{\partial}{\partial t} - \frac{2}{d}\frac{\partial}{\partial z} + 1\right) G(z, t) = \left(1 - \frac{2}{d}\frac{\partial}{\partial z}\right) G_B(z, t)$$

$$= \frac{2}{1 + \theta(t)} \frac{1 + (1 + z)\,\theta(t)}{[1 + z\theta(t)]^{d/2+1}} \tag{4.8}$$

As $\theta(t)$ is a very complicated functional of $G(z, t)$, this equation is very hard to solve. On the other hand, the Boltzmann equation for VHP interaction leads for two-dimensional systems to[1]

$$\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial z} + 1\right) G(z, t) = \frac{1}{z}\{1 - [G(z, t)]^2\} \tag{4.9}$$

The general solution of this equation is

$$G(z, t) = \frac{\psi(z + t) + (z - 1)\, e^{-t}}{(z + 1)\, \psi(z + t) - e^{-t}} \tag{4.10}$$

where $\psi(z)$ is a function depending on the initial conditions, and is determined by setting $t = 0$ in Eq. (4.10). If the initial distribution is singular at some value $x = x_0$, the solution (4.10) shows that the evolution of the system generates new singularities at $2x_0$, $3x_0$,.... This propagation of singularities is not present in the BGK model, as is seen from Eq. (3.8). The distribution function $F_B(x, t)$ is, by definition, a continuous function of x, independently of singularities of $F(x, t)$.

We must point out that the simplicity of Eq. (4.9) is lost when three-dimensional systems are considered. For $d \neq 2$ the analytical solution of the Boltzmann equation for the VHP interaction is not known.

5. INITIAL CONDITIONS

One of the most interesting features found in the solution of kinetic models is the presence of the so-called Tjon effect. For some kind of initial distributions the relaxation towards equilibrium of the high-energy region is not monotonic.[1,2,6,11] The same effect has also been observed in molecular dynamics simulation of dense fluids.[12] Hauge[6] has proposed a criterion to know whether a given initial condition will lead to the Tjon effect. According to it, the effect is expected if

$$M_2(0) > 1 \tag{5.1}$$

with $M_2(t)$ defined by Eq. (3.14). This condition was derived for Maxwell molecules, and, strictly speaking, it cannot be extended to other interactions. Only in the case of Maxwell molecules the behavior of the distribution near equilibrium is mainly governed by the initial value of M_2. Nevertheless, from a practical point of view, the criterion (5.1) has proved to be useful, even for high-density systems.[12]

For VHP interactions we have found in the previous section that the time evolution of $M_2(t)$ depends on all the moments of the initial distribution, and so Hauge's criterion cannot be exact. But we are going to see that, in the BGK model, it is a trustworthy rule for most initial conditions. More precisely, we could say that very often the knowledge of $M_2(0)$ is enough to predict whether there will be Tjon effect and, then, the criterion (5.1) applies. On the other hand, it is possible that $M_2(0) < 1$, but the distribution function exhibits overpopulation at high energies.

From expression (3.19) it is found that $R_B(x)$ is equal to one for an energy x^* given by

$$x^*(\theta) = \frac{\theta}{\theta - 1} \log \left[\frac{1}{2} (1 + \theta)\, \theta^{d/2} \right] \tag{5.2}$$

The value of x^* goes to $\frac{1}{2}(d+1)$ when θ goes to one. Going back to Fig. 2, let us first suppose that $\theta(0) > 1$ and $R(x, 0) < 1$ for $x > x^*[\theta(0)] = x_0$. The BGK equation shows that $R(x, t)$ exponentially tends towards $R_B(x, t)$. This tendency is stronger as we consider higher energies, because $\zeta_{\mathrm{VHP}}(x)$ grows with x. If we assume, as is plausible, that $\theta(t)$ slowly approaches equilibrium, we expect that $R(x, t)$ for $x > x_0$ crosses the unit value before $R(x, t) \simeq R_B(x, t)$. Afterwards, we would have a monotonic decay towards equilibrium. It is also clear from the shape of the curves $R_B(x)$ that the overpopulation effect increases with x. On the other hand, if $\theta(0) < 1$ and $R(x, 0) < 1$ for $x > x_0$, both distributions $R_B(x, t)$ and $R(x, t)$ will approach equilibrium from below and we will have a monotonic behavior. Other possibilities can be analyzed in the same way.

The above qualitative arguments lead to the conclusion that the Tjon effect is expected at high energies if $\theta(0) > 1$. Taking into account Eq. (3.15) and Fig. 1, this result is equivalent to condition (5.1).

In our calculations, we have considered two kinds of initial conditions. The most widely used initial distribution in kinetic models is the so-called (α, β) initial condition:

$$F(x, 0) = F_{\alpha,\beta}(x) = c_\alpha \delta(x - \tfrac{1}{2}\alpha) + c_\beta \delta(x - \tfrac{1}{2}\beta) \tag{5.3}$$

where

$$c_\alpha = \frac{\beta - d}{\beta - \alpha} \tag{5.4}$$

and

$$c_\beta = \frac{d - \alpha}{\beta - \alpha} \tag{5.5}$$

These expressions have been determined from the normalization conditions $M_0(0) = M_1(0) = 1$. Let us take $\beta > \alpha$. Then the positivity of the distribution function leads to

$$0 \leqslant \alpha \leqslant d \leqslant \beta \tag{5.6}$$

The initial moments of the distribution (5.3) are

$$M_n(0) = \frac{\Gamma(d/2)}{2^n \Gamma(n + d/2)} \frac{\alpha^n(\beta - d) + \beta^n(d - \alpha)}{\beta - \alpha} \tag{5.7}$$

In particular, it is

$$M_2(0) = \frac{(d - \alpha)(\beta - d) + d^2}{d(d + 2)} \tag{5.8}$$

and the condition (5.1) for this case reads

$$(d - \alpha)(\beta - d) > 2d \tag{5.9}$$

The other initial condition we have investigated is

$$F(x, 0) = F_\mu(x) = \left(\frac{d}{d-1}\right)^{d/2} \frac{x^{d/2-1}}{\Gamma(d/2)} \exp\left(-\frac{d}{d-1}x\right) \times \left\{\mu x^4 + \left[\frac{d^2}{(d-1)^3(d+2)} - \frac{(d-1)^2(d+4)(d+6)}{2d^2}\mu\right] x^2 + \frac{3d-4}{4(d-1)} + \frac{(d-1)^4(d+2)(d+4)(d+6)}{16d^3}\mu\right\} \tag{5.10}$$

where μ is a parameter. Initial conditions of this sort have been studied in the context of the Boltzmann equation by Cornille and Gervois[11] (Maxwell molecules) and by Ernst[1] (two-dimensional VHP interaction). The initial moments of (5.10) are given by

$$M_n(0) = \left(\frac{d-1}{d}\right)^{n+4} \left\{ \left(n+\frac{d}{2}\right)\left(n+1+\frac{d}{2}\right)\left(n+2+\frac{d}{2}\right)\left(n+3+\frac{d}{2}\right)\mu \right.$$
$$+ \left[\frac{d^4}{(d-1)^5(d+2)} - \frac{(d+4)(d+6)}{2}\mu\right]\left(n+\frac{d}{2}\right)\left(n+1+\frac{d}{2}\right)$$
$$\left. + \left[\frac{d^3(3d-4)}{(d-1)^5} + \frac{(d+2)(d+4)(d+6)}{4}\mu\right]\frac{d}{4} \right\} \tag{5.11}$$

The first moments are $M_0(0) = M_1(0) = 1$, and

$$M_2(0) = 1 + \frac{d-4}{d^2(d+2)} + 2\frac{(d-1)^6(d+4)(d+6)}{d^6}\mu \tag{5.12}$$

and the condition (5.1) becomes

$$\mu > \mu_0 = \frac{d^4(4-d)}{2(d-1)^6(d+2)(d+4)(d+6)} \tag{5.13}$$

For $d=2$ it is $\mu_0 = 1/12$, while for $d=3$, $\mu_0 = 9/4480$. Positivity of $F_\mu(x)$ for all positive values of x requires

$$0 \leqslant \mu \leqslant \mu_{\max} \tag{5.14}$$

where

$$\mu_{\max} = d^4 \frac{2(d^2+3d+4) + [2(d+2)(2d^3+7d^2+7d-20)]^{1/2}}{2(d-1)^5(d+2)(d+3)(d+4)(d+6)} \tag{5.15}$$

i.e., $\mu_{\max} \simeq 0.379$ for $d=2$ and $\mu_{\max} \simeq 0.0525$ for $d=3$.

6. RESULTS

Here, we present the results obtained by numerically solving the equations derived in Sections 3 and 4 with the initial conditions discussed in Section 5. The numerical method employed is outlined in Appendix B. Let us first consider three-dimensional systems. For the (α, β) initial distribution we have studied the cases $(\alpha, \beta) = (1, 4)$, $(1, 9)$, $(1, 16)$, and $(1, 25)$. The last three pairs verify condition (5.9) and, so, overpopulation effect is expected. In the case of the distribution (5.10) we have taken $\mu = \mu_0$ and $\mu = \mu_{\max}$.

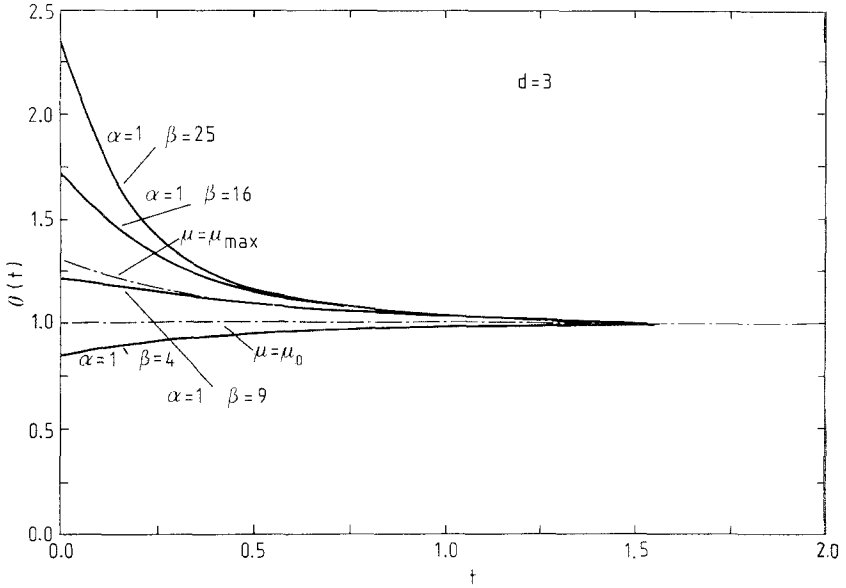

Fig. 3. Time evolution of $\theta(t)$ starting from several initial distributions of the forms given by Eqs. (5.3) and (5.10) in the three-dimensional case.

In Fig. 3 we have plotted the time evolution of $\theta(t)$. Apparently, it presents a monotonic relaxation in all cases and for all times. Nevertheless, some remarks are needed for $\mu = \mu_0$. According to the definition of μ_0, we have in this case $M_2(0) = 1$, and, then, $\theta(0) = 1$, which are their equilibrium values. Nevertheless, $\theta(t)$ does not remain constant, although its variation is not perceptible in the graph because the highest value it takes is roughly 1.004. The evolution of the system is not governed by $M_2(0)$ and the Hauge criterion (5.1) is meaningless. Higher-order moments must be considered. In fact, an analysis of the third initial moment gives a qualitative explanation for the behavior of $\theta(t)$ in this case.

Now, let us study the time evolution of $R(x, t)$ defined by Eq. (3.17). In Fig. 4 we have plotted $R(x, t)$ versus x for the (α, β) initial conditions. The curves are given for three characteristic times. In agreement with the criterion (5.9) the relaxation towards equilibrium is monotonic in the case $(\alpha, \beta) = (1, 4)$. In the other three cases, the high-energy tail of the distribution function has already crossed the equilibrium value at $t = 0.05$, i.e., the system presents the Tjon effect. Besides, the effect is greater as the value of the left-hand side of (5.9) increases. For a given pair (α, β), $R(x, t)$ is an increasing function of x, i.e., the effect shows up sooner and is greater as we consider higher energies. On the other hand, the low-energy region

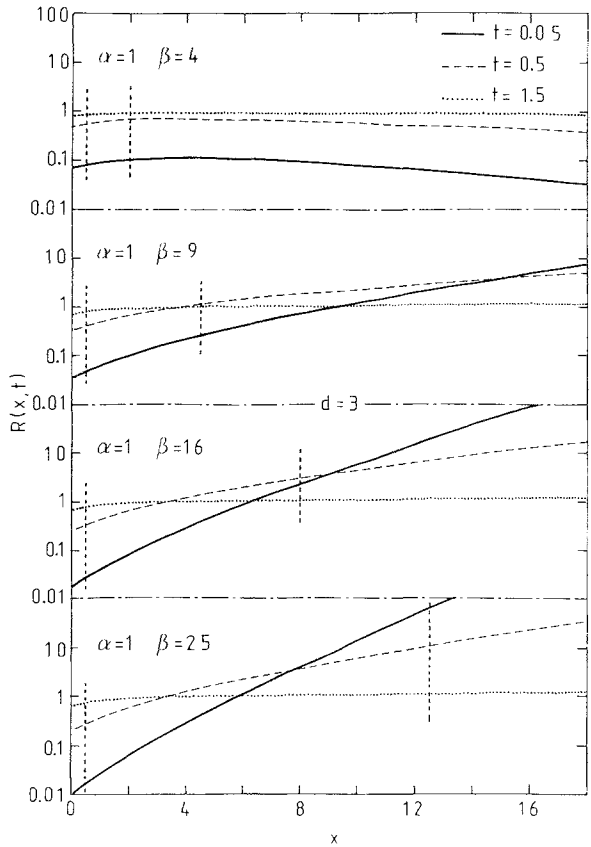

Fig. 4. Logarithmic plot of $R(x, t)$ versus x at three characteristic times for (α, β)-initial distributions. The vertical broken lines indicate the positions of $\frac{1}{2}\alpha$ and $\frac{1}{2}\beta$.

always presents a monotonic behavior. Finally, we notice that the equilibrium relaxation time of $R(x, t)$ is of the same order as that of $\theta(t)$.

As the initial distribution function (5.3) is singular at $x = \frac{1}{2}\alpha$ and $x = \frac{1}{2}\beta$, it is easily seen from Eq. (3.8) that $R(x, t)$ is also singular at these points. We have denoted this by means of vertical broken lines at $\frac{1}{2}\alpha$ and $\frac{1}{2}\beta$ in Fig. 4. It is interesting to study the relaxation of the distribution function in the vicinity of the initial peaks. To do so, we define

$$R_\gamma(t) = \frac{\int_{\frac{1}{2}(\gamma-\Delta x)}^{\frac{1}{2}(\gamma+\Delta x)} dx\, F(x, t)}{\int_{\frac{1}{2}(\gamma-\Delta x)}^{\frac{1}{2}(\gamma+\Delta x)} dx\, F^{\mathrm{eq}}(x)} \tag{6.1}$$

for $\gamma = \alpha$ or β. In Fig. 5 we show the results obtained for the evolution of $R_\alpha(t)$ and $R_\beta(t)$ with a value $\Delta x = 0.045$. We see that the population in the

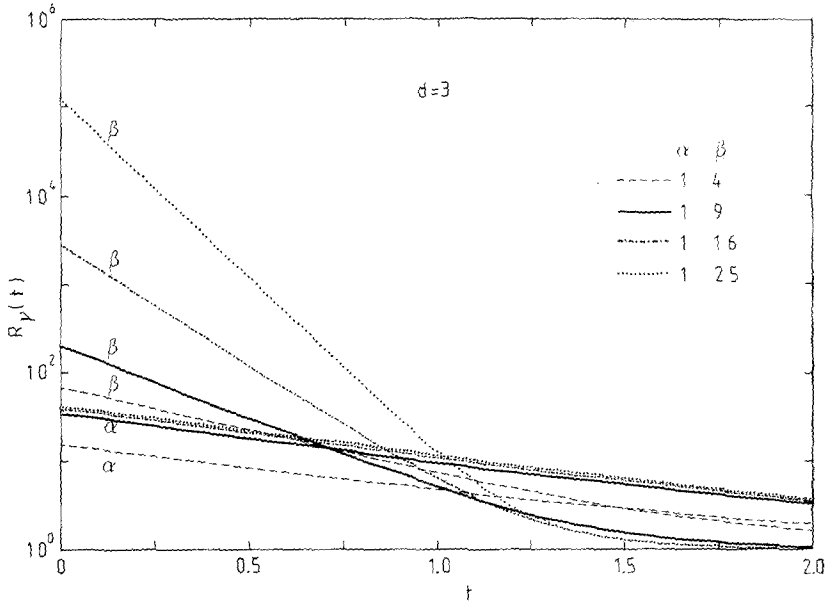

Fig. 5. Time evolution of $R_\alpha(t)$ and $R_\beta(t)$ for the (α, β) initial conditions considered. $R_\gamma(t)$, where $\gamma = \alpha$ or β, represents the relative population of particles with an energy differing from $\frac{1}{2}\gamma$ less than $\frac{1}{2}\Delta x = 0.0225$. Notice that a logarithmic scale has been used.

vicinity of each peak approaches the equilibrium value in a monotonic way in all the cases. Besides, there is a first stage in which the decay is exponential. This can be understood in the following way. The reference distribution function is, by definition, a regular function of x, no matter how singular the true distribution is. So, for the initial conditions under consideration,

$$R_\gamma(t) \gg R_{B,\gamma}(t) = \frac{\int_{\frac{1}{2}(\gamma-\Delta x)}^{\frac{1}{2}(\gamma+\Delta x)} dx\, F_B(x,t)}{\int_{\frac{1}{2}(\gamma-\Delta x)}^{\frac{1}{2}(\gamma+\Delta x)} dx\, F^{eq}(x)} \tag{6.2}$$

for t small. Then, the BGK equation (3.8) leads for short times to

$$R_\gamma(t) \simeq R_\gamma(0) \exp[-\zeta_{VHP}(\tfrac{1}{2}\gamma)t] \tag{6.3}$$

A more careful analysis shows that the exponential behavior lasts longer the smaller the value of Δx is. Expression (6.3) also explains why the slope of $R_\gamma(t)$ increases with the value of γ, since $\zeta_{VHP}(x)$ is an increasing function of x.

The μ-initial conditions (5.10) are analyzed in a similar way. The time evolution of $R(x,t)$ for $\mu = \mu_0$ and $\mu = \mu_{max}$ is represented in Fig. 6. (Notice the logarithmic scale used for $\mu = \mu_{max}$.) In both cases, $R(x,0)$ presents a

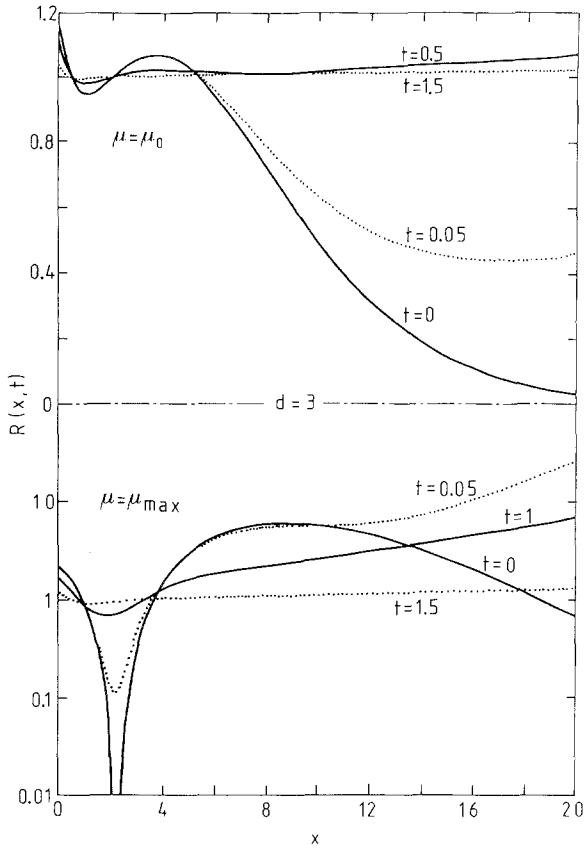

Fig. 6. Plot of $R(x, t)$ versus x at different times starting from μ-initial distributions with $\mu = \mu_0$ and $\mu = \mu_{\max}$ in the case $d = 3$. For $\mu = \mu_{\max}$ a logarithmic scale has been chosen.

maximum, cutting the line $R = 1$ at three points. For $\mu = \mu_0$, there is a slight overpopulation phenomenon at high energies, which appears for times of the order of the equilibrium relaxation time. Let us recall that this case corresponds to $\theta(0) = 1$, higher-order moments making $\theta(t)$ reach a maximum above unity. Concerning the case $\mu = \mu_{\max}$, we observe a nonmonotonic relaxation of $R(x, t)$ in the region $x \gtrsim 10$, that is, the region for which $R_B(x, 0) > R(x, 0)$.

As mentioned before, the Boltzmann equation for the two-dimensional VHP interaction has an exact solution for arbitrary initial conditions.[1,5] As a comparison, we have also numerically solved the BGK equation for $d = 2$, starting from the initial distribution (5.10) with $\mu = 1/15$ and with $\mu = 3/20$. Figure 7 shows the time evolution of the second moment $M_2(t)$ for these

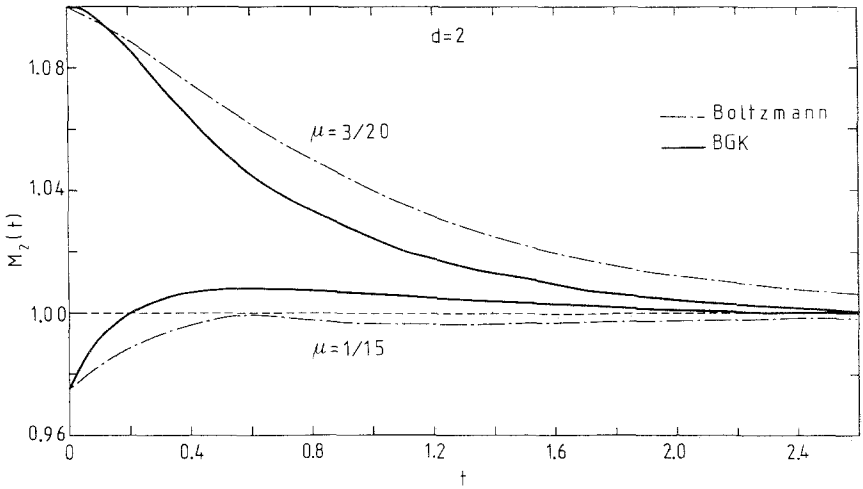

Fig. 7. Time evolution of the second moment $M_2(t)$ for a two-dimensional VHP gas with two different μ-initial distributions according to the Boltzmann equation (broken lines) and to the BGK model (solid lines).

cases both from the Boltzmann equation[1] and from the BGK approximation. In both kinetic equations, the relaxation of $M_2(t)$ is monotonic in the case $\mu = 3/20$ and nonmonotonic in the case $\mu = 1/15$. However, the evolution is faster in the BGK model, in such a way that, for $\mu = 1/15$, $M_2(t)$ overshoots unity and tends finally to equilibrium from above.

Let us now compare the evolution of the two distribution functions. In Fig. 8 we have plotted the function $R(x, t)$ obtained from the Boltzmann equation and the one from the BGK equation for three characteristic times and in the cases $\mu = 1/15$ and $\mu = 3/20$. (Curves corresponding to the Boltzmann equation have been taken from Ref. 1.) In this figure, we observe that, while the qualitative agreement is satisfactory in the low-energy region, this not true when we consider higher energies. In contrast with the Boltzmann solution, the BGK solution at high energies evolves very rapidly, having already crossed the equilibrium value at $t = 0.1$ in the case $\mu = 3/20$. Even more, the BGK solution for $\mu = 1/15$ relaxes in a nonmonotonic way in the high-energy region (although this happens for times greater than those considered in Fig. 8). This is due to the nonmonotonic behavior of the corresponding $M_2(t)$, as observed in Fig. 7. In fact, this is a case where the Hauge criterion (5.1) does not apply: the system described by the BGK model for a two-dimensional VHP interaction presents an overpopulation effect, in spite of being $M_2(0) < 1$.

The reason for this discrepancy between the Boltzmann and the BGK solutions at high energies lies in the approximation (2.22). More precisely,

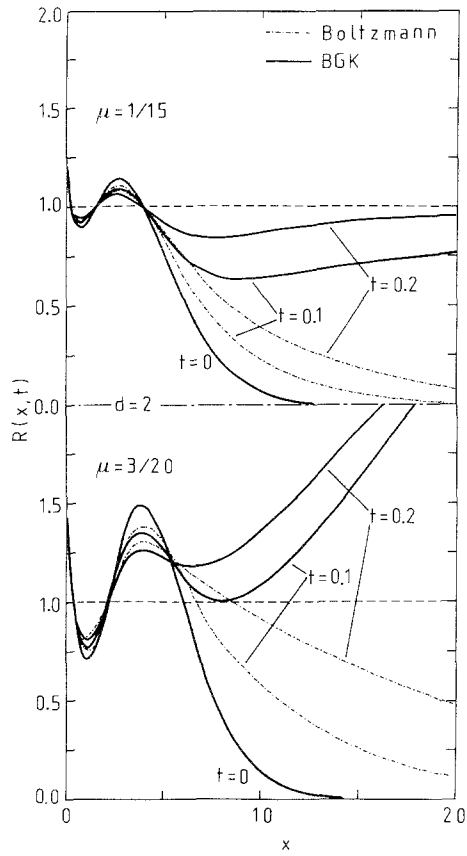

Fig. 8. Plot of $R(x, t)$ versus x at three different times starting from two-dimensional μ-initial distributions with $\mu = 1/15$ and $\mu = 3/20$. The solid lines correspond to the BGK solutions and the dot-dash lines correspond to the Boltzmann solutions. The latter curves have been taken from Ref. 1.

for a homogeneous and isotropic VHP gas, the BGK reference distribution $R_B(x, t)$ is a very rapidly increasing function of x if $\theta(t) > 1$, while the Boltzmann reference function may not be so. Besides, the VHP interaction emphasizes this difference, as the collision frequency increases with the energy. However, we want to point out that we do not consider the BGK model kinetic equation just as an approximation of the Boltzmann equation, but as a model in itself.

ACKNOWLEDGMENT

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APPENDIX A

Here we outline the derivation of Eqs. (2.25)–(2.27). Let us use the notation

$$\langle \varphi(\mathbf{v}) \rangle_t = \int d\mathbf{v}\, \varphi(\mathbf{v}) f(\mathbf{r}, \mathbf{v}; t) \tag{A.1}$$

$$\langle \varphi(\mathbf{v}) \rangle_{Bt} = \int d\mathbf{v}\, \varphi(\mathbf{v}) f_B(\mathbf{r}, \mathbf{v}; t) \tag{A.2}$$

Then, we have

$$\langle 1 \rangle_t = n(\mathbf{r}, t) \tag{A.3}$$

$$\langle \mathbf{v} \rangle_t = n(\mathbf{r}, t)\, \mathbf{u}(\mathbf{r}, t) \tag{A.4}$$

$$\langle V^2(\mathbf{r}, t) \rangle_t = dn(\mathbf{r}, t) \frac{k_B T(\mathbf{r}, t)}{m} \tag{A.5}$$

$$\langle V^2(\mathbf{r}, t)\, \mathbf{V}(\mathbf{r}, t) \rangle_t = 2 \frac{\mathbf{J}(\mathbf{r}, t)}{m} \tag{A.6}$$

$$\langle V^4(\mathbf{r}, t) \rangle_t = \Phi(\mathbf{r}, t) \tag{A.7}$$

where the meaning of the different symbols is given in the main text. Now, we are going to use conditions (2.5), i.e.,

$$\langle \zeta_{\mathrm{VHP}}(\mathbf{r}, \mathbf{v}; t)\, A^\alpha(\mathbf{v}) \rangle_t = \langle \zeta_{\mathrm{VHP}}(\mathbf{r}, \mathbf{v}; t)\, A^\alpha(\mathbf{v}) \rangle_{\mathrm{Bt}} \tag{A.8}$$

Taking into account Eq. (2.6), this is equivalent to

$$\langle \zeta_{\mathrm{VHP}}(\mathbf{r}, \mathbf{v}; t)\, A^\alpha[\mathbf{V}(\mathbf{r}, t)] \rangle_t = \langle \zeta_{\mathrm{VHP}}(\mathbf{r}, \mathbf{v}; t)\, A^\alpha[\mathbf{V}(\mathbf{r}, t)] \rangle_{\mathrm{Bt}} \tag{A.9}$$

Using the expression (2.17), one easily gets

$$\langle \zeta_{\mathrm{VHP}} \rangle_t = C_{\mathrm{VHP}} n^2 2 \frac{k_B T}{m} \tag{A.10}$$

$$\langle \zeta_{\mathrm{VHP}} \mathbf{V} \rangle_t = C_{\mathrm{VHP}} n 2 \frac{\mathbf{J}}{m} \tag{A.11}$$

$$\langle \zeta_{\mathrm{VHP}} V^2 \rangle_t = C_{\mathrm{VHP}} n \left[\Phi + n \left(d \frac{k_B T}{m} \right)^2 \right] \tag{A.12}$$

The calculation of $\langle \zeta_{\mathrm{VHP}} A^{\alpha}(\mathbf{V}) \rangle_{\mathrm{Bt}}$ is simple if one uses the relations

$$\langle \varphi \mathbf{V} \rangle_{\mathrm{Bt}} = \frac{\partial}{\partial \mathbf{b}} \langle \varphi \rangle_{\mathrm{Bt}} \tag{A.13}$$

and

$$\langle \varphi V^2 \rangle_{\mathrm{Bt}} = -\frac{\partial}{\partial c} \langle \varphi \rangle_{\mathrm{Bt}} \tag{A.14}$$

for any dynamical variable $\varphi(\mathbf{v})$. The result is

$$\langle \zeta_{\mathrm{VHP}} \rangle_{\mathrm{Bt}} = C_{\mathrm{VHP}} n a e^{b^2/4c} \left(\frac{\pi}{c}\right)^{d/2} \left(d \frac{k_B T}{m} + \frac{b^2}{4c^2} + \frac{d}{2c}\right) \tag{A.15}$$

$$\langle \zeta_{\mathrm{VHP}} \mathbf{V} \rangle_{\mathrm{Bt}} = C_{\mathrm{VHP}} n a e^{b^2/4c} \left(\frac{\pi}{c}\right)^{d/2} \frac{1}{2c} \left(d \frac{k_B T}{m} + \frac{b^2}{4c^2} + \frac{d+2}{2c}\right) \mathbf{b} \tag{A.16}$$

$$\langle \zeta_{\mathrm{VHP}} V^2 \rangle_{\mathrm{Bt}} = C_{\mathrm{VHP}} n a e^{b^2/4c} \left(\frac{\pi}{c}\right)^{d/2} \frac{1}{4c^2} \times \left[\left(\frac{b^2}{c} + d\right)(d+2) + (b^2 + 2dc) d \frac{k_B T}{m} + \frac{b^4}{4c^2} \right] \tag{A.17}$$

By equating Eqs. (A.10)–(A.12) to Eqs. (A.15)–(A.17), we get Eqs. (2.25)–(2.27).

APPENDIX B

In this appendix we are going to briefly describe the numerical method used to obtain the results presented in Section 6.

The function $\theta(t)$ is the solution of the closed integral equation resulting from taking $n = 0$, 1, or 2 in Eq. (4.5). Concretely, for $n = 1$, we have

$$1 - P_1(t) = 2 \int_0^t ds\, e^{-(t-s)} \frac{[\theta(s)]^2}{1 + \theta(s)} \frac{1 + 1/\theta(s) + 2(1 + t - s)/d}{[1 + (2/d)(t-s)\,\theta(s)]^{d/2+2}} \tag{B.1}$$

Once $\theta(s)$ is known for $s \leqslant t$, Eq. (3.18) allows us to get $R(x, t)$. Equation (3.18) can be written in a recursive form as

$$R(x, t + \Delta t) = e^{-\zeta_{\mathrm{VHP}}(x)\Delta t} R(x, t) + \zeta_{\mathrm{VHP}}(x) \int_t^{t+\Delta t} ds\, e^{-\zeta_{\mathrm{VHP}}(x)(t+\Delta t - s)} R_B(x, s) \tag{B.2}$$

for any arbitrary time interval Δt. The numerical method employed consists on replacing the right-hand sides of Eqs. (B.1) and (B.2) by the trapezoidal rule approximation. Thus, Eq. (B.1) becomes

$$A_j = \theta_j \left(1 + \frac{2}{d}\frac{\theta_j}{1+\theta_j}\right) \tag{B.3}$$

where

$$A_j \equiv \frac{1-P_1(t_j)}{\Delta t} - e^{-t_j}\frac{\theta_0^2}{1+\theta_0}\frac{1+1/\theta_0+2(1+t_j)/d}{[1+(2/d)\,t_j\theta_0]^{d/2+2}} - 2\sum_{k=1}^{j-1} e^{-(t_j-t_k)}\frac{\theta_k^2}{1+\theta_k}\frac{1+1/\theta_k+2(1+t_j-t_k)/d}{[1+(2/d)(t_j-t_k)\,\theta_k]^{d/2+2}} \tag{B.4}$$

and

$$\theta_k \equiv \theta(t_k), \qquad t_k \equiv k\,\Delta t \tag{B.5}$$

Here, Δt is a sufficiently small time interval. The approximation on Eq. (B.2) yields

$$R(x,t_j) = e^{-\zeta_{\mathrm{VHP}}(x)\Delta t}R(x,t_{j-1}) + \zeta_{\mathrm{VHP}}(x)\frac{\Delta t}{2}\left[e^{-\zeta_{\mathrm{VHP}}(x)\Delta t}R_B(x,t_{j-1}) + R_B(x,t_j)\right] \tag{B.6}$$

where $R_B(x,t_j)$ is given from θ_j, which is the positive root of Eq. (B.3), i.e.,

$$\theta_j = \frac{A_j - 1 + [(A_j+1)^2 + 8A_j/d]^{1/2}}{2(1+2/d)} \tag{B.7}$$

Notice that Eq. (B.3) is consistent with Eq. (B.6) and can be obtained from it. Moreover, Eq. (B.6), which contains all the powers of Δt, is exact up to the order $(\Delta t)^2$. The present method has the advantage of not requiring any discretization on the energy. Thus, it is possible to determine the evolution of $R(x,t)$ for a given value of x without the knowledge of the distribution function for the remaining energies.

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