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Comparison between the Boltzmann and BGK equations for uniform shear flow

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Abstract

The exact fourth-degree moments derived in the preceding paper from the Boltzmann equation for Maxwell molecules under uniform shear flow are compared with those obtained from the BGK and the Gaussian approximations. It is shown that the BGK results are closer to the exact ones than the Gaussian results. However, the deviations become significant as the shear rate increases.

1. Introduction

Although the Boltzmann equation provides the adequate framework for studying general nonequilibrium phenomena in dilute gases, the intricacy of its collision term has made the search for explicit solutions a formidable task. Nevertheless, there exist a few examples of non-homogeneous problems for which a solution in terms of the velocity moments is known for Maxwell molecules [2–5]. In the particular case of uniform shear flow (USF), the exact shear viscosity and viscometric functions are known as nonlinear functions of the shear rate [2,6]. On the other hand, the full velocity distribution function is not known.

The mathematical difficulties embodied in the Boltzmann collision operator have stimulated the use of simplified kinetic models, such as the Bhatnagar-Gross-Krook (BGK) kinetic equation [1]. In this model, it is assumed that the net effect of collisions is to make the distribution function tend to relax toward the local equilibrium distribution with a characteristic time equal to the mean free time. In the case of USF, the elements of the pressure tensor coincide with those obtained from the Boltzmann equation for Maxwell molecules when one chooses conveniently the collision frequency [7]. This fact shows the relevance of the BGK model for computing transport properties far from equilibrium. In addition, the velocity distribution function of the BGK equation for USF

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has been obtained [8]. An interesting question is whether such a distribution is a good representation of the "real" solution of the Boltzmann equation. Comparison with Monte Carlo simulations for hard spheres shows that the BGK solution describes fairly well the shape of the "real" distribution except in the high-velocity region [9]. Since the Monte Carlo method does not provide an explicit solution of the Boltzmann equation, it is interesting to carry out a detailed comparison between the BGK and Boltzmann solutions for moments of degree higher than 2. The objective of this paper is to perform such a comparison by using the exact expressions for the fourth-degree moments derived in the preceding paper [10]. This comparison allows one to infer the degree of reliability of the distribution function obtained from the BGK equation.

The plan of the paper is as follows. In Section 2 we give a brief account of the solution of the BGK equation for USF. The Gaussian approximation consistent with the exact second-degree moments is introduced in Section 3. The comparison between the exact fourth-degree moments and those given by the BGK and the Gaussian approximations is carried out in Section 4. Finally, a few conclusions are presented in Section 5.

2. BGK solution for USF

According to the BGK model, the time evolution of the velocity distribution function $f(\mathbf{r},\mathbf{v},t)$ is given by

$$\frac{\partial}{\partial t}f+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}f+\frac{1}{m}\frac{\partial}{\partial \mathbf{v}}\cdot(\mathbf{F}f)=-\nu(f-f^{\mathrm{LE}})\,, \tag{1}$$

where m is the mass of a particle, $\mathbf{F}$ is an external force, and

$$f^{\mathrm{LE}}(\mathbf{r},\mathbf{v},t)=n(\mathbf{r},t)\left(\frac{m}{2\pi k_B T(\mathbf{r},t)}\right)^{3/2}\exp\left(-\frac{m}{2k_BT(\mathbf{r},t)}[\mathbf{v}-\mathbf{U}(\mathbf{r},t)]^2\right) \tag{2}$$

is the local equilibrium distribution function. Here, n, $\mathbf{U}$, and T are the local density, velocity, and temperature, respectively. In Eq. (1), $\nu(\mathbf{r},t)$ is a velocity-independent collision frequency that depends on position and time through the density and the temperature. All the influence of the interaction model enters into the BGK equation via the collision frequency.

In the USF state, $U_i = ay\delta_{ix}$, n is constant, and T is spatially homogeneous. Consequently, the collision frequency is constant for Maxwell molecules and also for any interaction potential when a thermostat force is introduced to compensate for viscous heating. In either case, the explicit shear-rate dependence of the moments in the long-time limit is known [8]. Let us define the following moments:

$$\begin{aligned}M_{k_1,k_2,k_3}&=\frac{1}{n}\int d\mathbf{V}V_x^{k_1}V_y^{k_2}V_z^{k_3}f\\&=\langle V_x^{k_1}V_y^{k_2}V_z^{k_3}\rangle\,,\end{aligned} \tag{3}$$

where $\mathbf{V} \equiv \mathbf{v} - \mathbf{U}$ is the peculiar velocity. Due to the symmetry of the problem, the nonvanishing moments correspond to $k_1 + k_2$ = even and k_3 = even. In that case, the result is

$$M_{k_1,k_2,k_3} = \sum_{q=0}^{k_1} (-a)^q [1 + (k_1 + k_2 + k_3)\alpha]^{-(q+1)} \frac{k_1!}{(k_1 - q)!} M^{\rm LE}_{k_1-q,k_2+q,k_3} , \tag{4}$$

where

$$M^{\rm LE}_{k_1,k_2,k_3} = \left(\frac{2k_BT}{m}\right)^{(k_1+k_2+k_3)/2} \pi^{-3/2} \Gamma\left(\frac{k_1+1}{2}\right) \Gamma\left(\frac{k_2+1}{2}\right) \Gamma\left(\frac{k_3+1}{2}\right) \tag{5}$$

if k_1, k_2, and k_3 are even, being zero otherwise. In Eq. (4), $\alpha = \frac{2}{3}\sinh^2[\frac{1}{6}\cosh^{-1}(1 + 9a^2)]$ and we have taken ν^{-1} as the unit of time. Up to first order in the shear rate (Navier-Stokes order), the moments behave as

$$M_{k_1,k_2,k_3} = M^{\rm LE}_{k_1,k_2,k_3} - k_1 M^{\rm LE}_{k_1-1,k_2+1,k_3} a + \cdots . \tag{6}$$

Since the Chapman-Enskog solutions to the BGK and Boltzmann equations for Maxwell molecules coincide at the level of Navier-Stokes, it is evident that Eq. (6) is exact.

Eq. (4) can be particularized to get the expressions for the second-degree moments. They are

$$M_{2,0,0} = \frac{k_BT}{m} \frac{1+6\alpha}{1+2\alpha} , \tag{7}$$

$$M_{0,2,0} = M_{0,0,2} = \frac{k_BT}{m} \frac{1}{1+2\alpha} , \tag{8}$$

$$M_{1,1,0} = -\frac{k_BT}{m} \frac{a}{(1+2\alpha)^2} . \tag{9}$$

Eqs. (7)–(9) define the most important transport properties of the problem, namely the nonlinear shear viscosity and viscometric functions. It is remarkable that the above moments coincide exactly with those obtained from the Boltzmann equation for Maxwell molecules [10]. This agreement, however, does not extend to higher-degree moments. An exception is the relation

$$\sum_{q=0}^{k/2} (-1)^q \binom{k}{2q} M_{0,2q,k-2q} = 0 , \tag{10}$$

which holds in both cases [10].

Before closing this section, it must be emphasized that the solution to the BGK equation reaches in the long-time limit a form ("normal" solution) that is independent of the initial conditions. This contrasts with the results derived from the Boltzmann equation for Maxwell molecules, where a singularity arises at a certain critical value of the shear rate [11].

3. Gaussian approximation

In order to put the comparison between the Boltzmann and the BGK equations in an appropriate context, it is convenient to consider the Gaussian approximation for the velocity distribution function consistent with the second-degree moments. This approximation is

$$f(\mathbf{V}) = n\pi^{-3/2}(\det \mathsf{Q})^{1/2}\exp(-\mathsf{Q} : \mathbf{VV}) , \tag{11}$$

where $\mathsf{Q} = \frac{1}{2}mn\mathsf{P}^{-1}$, P being the prescribed pressure tensor. From this expression one can easily get all the velocity moments. In our case, by using Eqs. (7)–(9), their explicit form is

$$M_{k_1,k_2,k_3} = \frac{1}{(1+2\alpha)^{(k_1+k_2+k_3)/2}} \sum_{q=0}^{k_1} \left(-\frac{a}{1+2\alpha}\right)^q (1+3\alpha)^{(k_1-q)/2} \times \frac{k_1!}{q!(k_1-q)!} M^{\mathrm{LE}}_{k_1-q,k_2+q,k_3} . \tag{12}$$

Since the second-degree moments are common in the Boltzmann and BGK equations, the Gaussian approximation (12) is also the same in both descriptions. In addition the exact relation (10) is maintained by this approximation. Further, the Gaussian approximation is exact up to first order in the shear rate (Navier-Stokes order).

4. Comparison of the fourth-degree moments

The explicit shear-rate dependence obtained in Ref. [10] for the fourth-degree moments allows one to carry out a detailed comparison with the corresponding moments given by the BGK equation and the Gaussian approximation. Due to the symmetry of the problem there are in principle 9 independent non-zero moments. However, Eq. (10) with $k = 4$ restricts to 8 the number of relevant moments. Of course, there are many possible choices for the set of independent moments. Here, we take the following set:

$$\{\langle V^4\rangle, \langle V^2V_x^2\rangle, \langle V^2V_y^2\rangle, \langle V_x^4\rangle, \langle V_y^4\rangle, \langle V^2V_xV_y\rangle, \langle V_x^3V_y\rangle, \langle V_xV_y^3\rangle\} . \tag{13}$$

The first five moments of the set are even functions of the shear rate, while the remaining three moments are odd functions. The relationship between these moments and the ones considered in Ref. [10] is

$$\begin{pmatrix} \langle V^4\rangle \\ \langle V^2V_x^2\rangle \\ \langle V^2V_y^2\rangle \\ \langle V_x^4\rangle \\ \langle V_y^4\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ \frac{1}{3} & 1 & 0 & 0 & 0 \\ \frac{1}{3} & 0 & 1 & 0 & 0 \\ \frac{1}{5} & \frac{6}{7} & 0 & \frac{4}{3} & \frac{4}{3} \\ \frac{1}{5} & 0 & \frac{6}{7} & 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} M_{4|0} \\ M_{2|xx} \\ M_{2|yy} \\ M_{0|yyyy} \\ M_{0|zzzz} \end{pmatrix} , \tag{14}$$

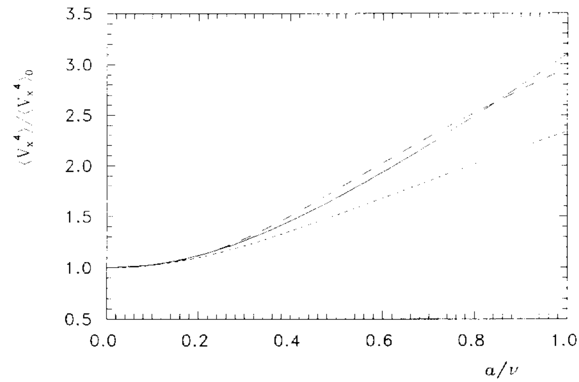

Fig. 1. Shear-rate dependence of $\langle V_x^4\rangle$ relative to its equilibrium value, according to the Boltzmann equation (—), the BGK equation (– – –), and the Gaussian approximation (- - -).

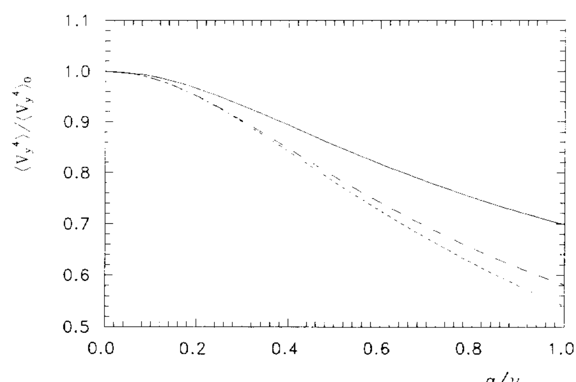

Fig. 2. Same as in Fig. 1, but for $\langle V_y^4\rangle$.

$$\begin{pmatrix} \langle V^2 V_x V_y\rangle \\ \langle V_x^3 V_y\rangle \\ \langle V_x V_y^3\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ \frac{3}{7} & 1 & 0 \\ \frac{3}{7} & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} M_{2|xy} \\ M_{0|xxxy} \\ M_{0|xyyy} \end{pmatrix} . \tag{15}$$

As discussed in Ref. [10], the fourth-degree moments do not reach stationary values, when scaled with respect to the temperature, for shear rates beyond a critical value $a_c \simeq 6.845$. Nevertheless, nonlinear effects are still quite important in the region $a < a_c$. For instance, the generalized shear viscosity for $a = 1$ is about half the Navier-Stokes value. The shear-rate dependence of the moments (13) in the region $0 \leq a \leq 1$ is shown in Figs. 1–8. The exact results obtained from the Boltzmann equation are compared with those obtained from the BGK equation and from the Gaussian approximation. Each moment is normalized with respect to the corresponding first nonzero term in the Chapman-Enskog expansion, which is denoted by $\langle\cdots\rangle_0$.

Fig. 1 shows that the BGK equation reproduces quite well the exact behavior of $\langle V_x^4\rangle$ over the range of shear rates considered. It is interesting to note that the deviation from equilibrium is slightly overestimated by the BGK model for shear rates smaller than about 0.8. On the other hand, the Gaussian approximation, according to which $\langle V_x^4\rangle = 3\langle V_x^2\rangle^2$, systematically underestimates the exact value. These conclusions cannot

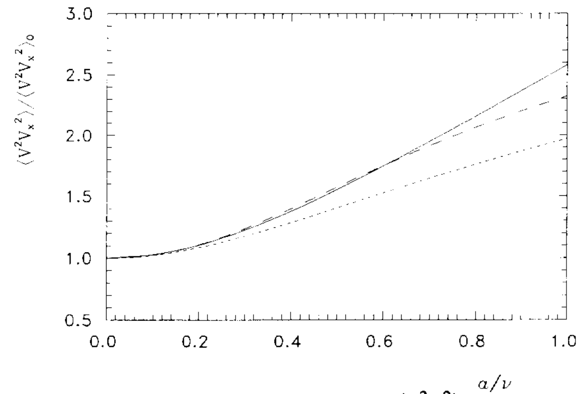

Fig. 3. Same as in Fig. 1, but for $\langle V^2 V_x^2 \rangle$.

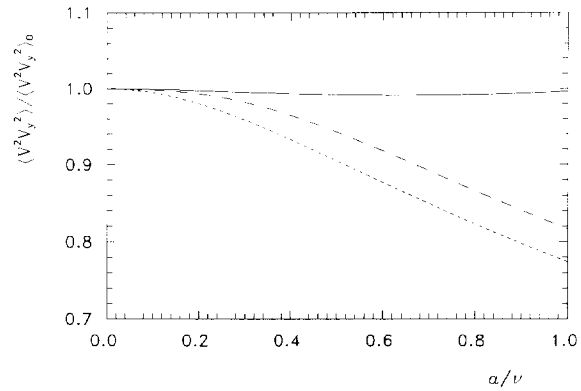

Fig. 4. Same as in Fig. 1, but for $\langle V^2 V_y^2 \rangle$.

be extended to the remaining fourth-degree moments. Thus, we see in Fig. 2 that the predictions for $\langle V_y^4 \rangle$ obtained from the BGK and the Gaussian approximations clearly deviate from the Boltzmann result. It seems paradoxical that the Gaussian approximation gives a larger deviation from equilibrium for $\langle V_y^4 \rangle$ than the exact value. This only means that, as happened for $\langle V_x^4 \rangle$, $\langle V_y^4 \rangle$ is larger than $3\langle V_y^2 \rangle^2$. Consequently, the tail of the actual velocity distribution function is expected to decay more slowly than predicted by the Gaussian approximation.

The remaining three even moments considered are plotted in Figs. 3–5. They provide information about the correlations induced by the shear flow among the components of the velocity. We observe that the moment $\langle V^2 V_x^2 \rangle$ behaves in a similar way as the moment $\langle V_x^4 \rangle$. In particular, the behavior predicted by the BGK model is quite good for shear rates smaller than about 0.6. However, the agreement is very poor in the case of $\langle V^2 V_y^2 \rangle$. Quite surprisingly, the Boltzmann equation shows that this moment is practically insensitive to the value of the shear rate in the range $0 < a < 1$. Some of the main effects observed in the previous figures are present again in Fig. 5. Although the BGK approximation is remarkably better than the Gaussian approximation, both fail to describe well the population of high-velocity particles.

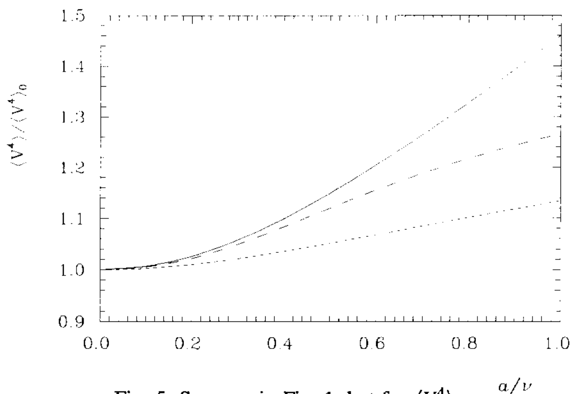

Fig. 5. Same as in Fig. 1, but for $\langle V^4\rangle$.

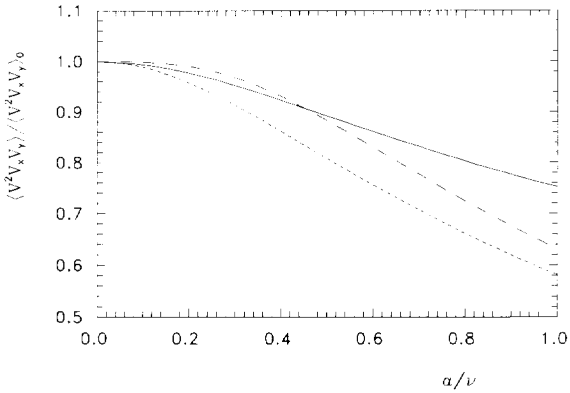

Fig. 6. Shear-rate dependence of $\langle V^2 V_x V_y\rangle$ relative to its Navier-Stokes value, according to the Boltzmann equation (—), the BGK equation (– – –), and the Gaussian approximation (- - -).

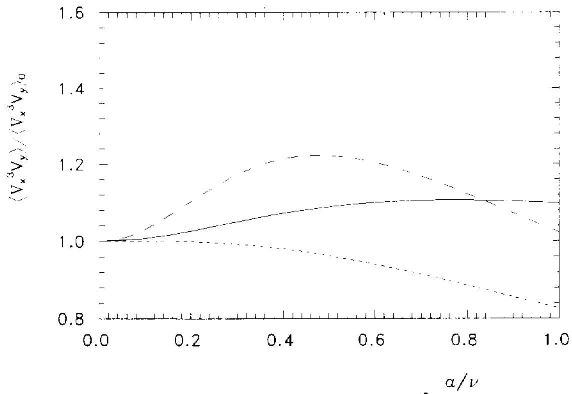

Fig. 7. Same as in Fig. 6, but for $\langle V_x^3 V_y\rangle$.

Finally, the three odd moments are shown in Figs. 6–8. Although they are negative, what is plotted in the figures is their values relative to the Navier-Stokes approximation, so that the ratio is positive. Figs. 6 and 7 exhibit a feature similar to the one observed in Figs. 1 and 3, namely the BGK equation overestimates the exact (absolute) value for small shear rates but it underestimates that value for large shear rates. In all the cases, the Gaussian approximation underestimates the corresponding exact value. The BGK

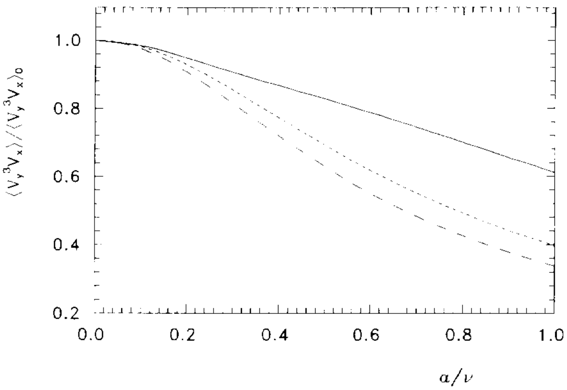

Fig. 8. Same as in Fig. 6, but for $\langle V_x V_y^3 \rangle$.

prediction for $\langle V_x V_y^3 \rangle$ is worse than in the two previous cases. As a matter of fact, this is the only moment for which the Gaussian approximation is better than the BGK one.

5. Concluding remarks

One of the main advantages of the knowledge of exact solutions for specific situations is the possibility of testing approximations. For a dilute gas, the BGK model is frequently used as an approximation of the Boltzmann equation. In the case of the uniform shear flow state, the Ikenberry-Truesdell [2] solution of the Boltzmann equation for Maxwell molecules provides the explicit expressions of the rheological properties over the whole range of shear rates. These transport properties happen to coincide exactly with those obtained from the BGK model for the same problem [7]. Consequently, it is necessary to go beyond the level of hydrodynamic quantities (i.e. second-degree moments) in order to elucidate the degree of reliability of the BGK model. The recent derivation of explicit expressions for the fourth-degree moments from the Boltzmann equation [10] gives the possibility of carrying out the comparison with the BGK results. This has been the main objective addressed in this paper.

Such a comparison is illustrated by Figs. 1–8. In addition, the Gaussian approximation is also considered. We observe that, in general, the BGK predictions are reasonably good for not too large shear rates (say $a \leq 0.2$), especially for moments in which the component V_x is the most relevant one. In particular, the BGK approximation is exact up to first order in the shear rate (Navier-Stokes order). However, it does not give, in general, good estimates for the Burnett (second order) and super-Burnett (third order) coefficients. For instance, the Burnett coefficient of $\langle V^2 V_x^2 \rangle$ is estimated with a deviation of about 1.7%, while for $\langle V^2 V_z^2 \rangle$ this coefficient does not have the same sign as the exact one. Anyway, the results predicted by the BGK model are closer to the exact ones than those obtained from the Gaussian approximation.

It is evident that the comparison between the Boltzmann and the BGK equations at the level of fourth-degree moments is not sufficient to assess the "quality" of the velocity distribution function obtained from the BGK approximation. Nevertheless, the exact agreement for the second-degree moments suggests that the BGK distribution reproduces well the behavior in the region of thermal velocities. Further, since the fourth-degree moments obtained from the BGK approximation are generally smaller than the exact ones, the high-velocity population is possibly underestimated by the BGK approximation. These expectations have been recently confirmed by computer simulations [9,12].

In summary, we conclude that, in general, the BGK model is a good approximation of the Boltzmann equation at the level of transport properties, which are related to the lower-degree velocity moments, although it becomes less reliable as the degree of the moments increases.

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References

[1] P.L. Bhatnagar, E.P. Gross, and M. Krook, Phys. Rev. A 94 (1954) 511.
[2] E. Ikenberry and C. Truesdell, J. Rat. Mech. Anal. 5 (1956) 1; C. Truesdell, J. Rat. Mech. Anal. 5 (1956) 55.
[3] E.S. Asmolov, N.K. Makashev, and V.I. Nosik, Sov. Phys.-Dokl. 24 (1979) 892.
[4] V. Garzó and A. Santos, J. Chem. Phys. 97 (1992) 2039.
[5] C. Marín, V. Garzó, and A. Santos, J. Stat. Phys. (1994), to be published.
[6] C. Truesdell and R.G. Muncaster, Fundamentals of Maxwell's Kinetic Theory of a Simple Monatomic Gas (Academic Press, New York, 1980).
[7] R. Zwanzig, J. Chem. Phys. 71 (1979) 4416.
[8] A. Santos and J.J. Brey, Physica A 174 (1991) 355.
[9] J. Gómez Ordóñez, J.J. Brey, and A. Santos, Phys. Rev. A 41 (1990) 810.
[10] A. Santos and V. Garzó, Exact moment solution of the Boltzmann equation for uniform shear flow, Physica A 213 (1995) 409, preceding paper.
[11] A. Santos, V. Garzó, J.J. Brey and J.W. Dufty, Phys. Rev. Lett. 71 (1993) 3971; 72 (1994) 1392 (Erratum).
[12] J.M. Montanero, A. Santos, and V. Garzó, unpublished.