Dynamics of rarefied granular gases

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(Received 25 June 2001; published 18 January 2002)

This paper presents quite general bidimensional gas-dynamic equations—derived from kinetic theory-which include the *fourth cumulant* $\kappa(\vec{r},t)$ as a dynamic field. The dynamics describes a low-density system of inelastic hard spheres (disks) with normal restitution coefficient r. Two illustrative examples are given and the role of κ in them is discussed. Our general gas-dynamic equations would deal with 9 hydrodynamic fields (which corresponds to 14 in three-dimension). These fields are the standard hydrodynamic fields plus the components p_{ij} of the traceless part of the pressure tensor, the energy flux vector $\vec{Q}$ and the fourth cumulant κ. The present formulation requires no constitutive equations. The two examples are: the well-known homogeneous cooling state and a system, with and without gravity, steadily heated by two parallel walls. In the first case, the dynamics yield a description of the homogeneous cooling state consistent with known results adding extra details mainly about the transient time behavior. The steadily heated system kept in a static state gives rise to quite simple but nontrivial equations. In the case with gravity, it is shown that when κ is included as a dynamic field, the formalism leads to a non-Fourier law already to first order in dissipation. Setting gravity $g=0$ a perturbative solution is shown and favorably compared with observations obtained from molecular dynamics (MD). In both cases, with and without gravity, κ is not homogeneous. An analytic extension suggests a divergent situation for a small negative value of q, which originates in the unavoidable extension of the formalism to exothermic collisions associated with a restitution coefficient larger than one. This divergent behavior is observed in MD.

DOI: 10.1103/PhysRevE.65.021304 PACS number(s): 81.05.Rm, 05.20.Dd, 51.10.+y, 47.70.Nd

I. INTRODUCTION

For almost two decades, many authors have been submitting ever-improving descriptions of granular gases [1–7]. The presence of correlations is one of the sources of difficulties to deal—within statistical mechanics—with granular systems. One specific reason is the inelastic character of the grain-grain collision. In them, the incident collision angle is statistically larger than the angle between the final velocities, making probable that the following collisions in the same neighborhood are correlated. When the density is not low enough, correlations will appear [8]. The study of rarefied granular gases escapes these difficulties and Boltzmann's molecular chaos assumption can be taken as valid.

For granular gases, the velocity distribution function is either flatter or more peaked than a simple Maxwellian and, for large velocities, it decays more slowly than a Maxwellian. It seems that the flatness of the distribution was noticed in the study of homogeneous cooling [4] and it is presently described by a negative kurtosis or fourth cumulant κ, as in Refs. [9–12]. Much theoretical work to characterize the long velocity tail has also been undertaken [10,13–15].

In the case of the inelastic hard-sphere model for granular systems, the particle dynamics is defined by the collision rule, which introduces a constant restitution coefficient r associated with the normal relative velocity, $\vec{c}\,'_{\rm ab}\cdot\hat{n}=-r\vec{c}_{\rm ab}\cdot\hat{n}$, while the tangential component of the relative velocity remains unchanged, $\vec{c}\,'_{\rm ab}\cdot\hat{t}=\vec{c}_{\rm ab}\cdot\hat{t}$. In Boltzmann's equation, only the gain term changes and it does so getting an overall factor r^{-2} and the distribution functions appearing in the gain term depend upon the precollision velocities, which are functions of r.

When the modified Boltzmann's equation is used, the stemming hydrodynamic equations become dependent on the *inelasticity coefficient* $q\equiv(1-r)/2$, ($q=0$ in the perfectly elastic case and $0\leqslant q\leqslant 1/2$) except that the mass and momentum balance equations remain unchanged since mass and momentum are still conserved in every collision.

In the context of Boltzmann's equation, a dissipative gas satisfies the ideal gas equation of state $p=nT$ where the granular temperature T is defined in energy units as the average kinetic energy per particle. If we were to consider the Boltzmann-Enskog equation, then the inelasticity coefficient q would enter through the Enskog collision factor χ, and the equations of state of a normal gas and of a dissipative gas would differ (see in particular [8]), but in the present context, the ideal gas equation of state holds.

Many authors have shown that the fourth cumulant κ is an important aspect of the description of a granular gas. The most economic way of incorporating κ in the formalism consists of defining a moment expansion formalism which goes up to the fourth *scalar* moment or, equivalently, incorporating κ as just one extra dynamic field $\kappa(\vec{r},t)$ in Grad's standard hydrodynamics [16]. Grad's standard formalism using 13 moments in dimension three (8 moments in dimension two) has been quite successful in describing conservative sheared gases [17]. For granular gases we then, define a formalism with 9 moments in the bidimensional case. One of the important goals of the present paper is to show that such formalism, having κ as a dynamic field, recovers known results (e.g., $\kappa \approx -2q$ for the homogeneous cooling state) and produces new ones (e.g., a steady state in which, to lowest order, $\kappa \approx 6q$). Additionally, an example where the dependence on time of κ is made explicit and another case, which exemplifies an inhomogeneous κ, are shown. The presence of κ in the formalism affects some of the dynamic fields at second order in q, but in the case of the energy flux, it does so at first order.

Writing the velocity distribution function, $f(\vec{r},\vec{C},t)$, as an expansion in moments of the peculiar velocity $\vec{C}=\vec{c}-\vec{v}(\vec{r},t)$, [where $\vec{v}(\vec{r},t)$ is the hydrodynamic velocity] the fourth cumulant κ is naturally incorporated. Instead of using directly the fourth moment $\langle C^4\rangle$ we use the fourth cumulant $\kappa = \langle C^4\rangle/\langle C^2\rangle^2-(d+2)/d$ (in the bidimensional case $d=2$) as a dynamic field.

In a previous article, we were able to describe granular gases with global area density $\rho_A=0.01$ with qN up to about 40 (N is the number of particles) without introducing κ and up to about $qN=300$ when κ was used [12]. But in Ref. [12], we introduced κ as a static homogeneous quantity. In the present context, it is natural to deal with the fourth cumulant as an extra hydrodynamic field $\kappa(\vec{r},t)$ in the same footing as the other moments. Therefore, in two-dimension, we deal with nine moments and these are the number density n, the hydrodynamic velocity $\vec{v}=(v_x,v_y)$, the granular temperature T, the independent components of the traceless part of the pressure tensor (e.g., p_{xy} and p_{yy}), the energy flux described by Q_x and Q_y, and finally, κ.

Considering a two-dimensional (2D) system with N particles of *unit mass* in a box of width L_y and length L_x—with overall number density $n_0=N/(L_xL_y)$ and reference granular temperature T_0—dimensionless fields F are defined in terms of the physical fields $\overline{F}$ as

$$\overline{n}=n_0 n, \quad \overline{v_i}=\sqrt{T_0}v_i, \quad \overline{T}=T_0T,$$

$$\overline{P}_{ij}=n_0T_0P_{ij}, \quad \overline{Q}_i=n_0T_0^{3/2}Q_i, \quad \overline{\kappa}=\kappa. \tag{1}$$

The dimensionless pressure tensor P_{ij} can be written as $P_{ij}=nT\delta_{ij}+p_{ij}$. The coordinates $\overline{x_k}$ and time $\overline{t}$ are related to the associated dimensionless quantities by $\overline{x_k}=L_y,x_k$ and $\overline{t}=tL_y/\sqrt{T_0}$. In these units, for example, the free flight time for the corresponding elastic gas at equilibrium at temperature T_0, is 1/4 Kn, where

$$\mathrm{Kn}=\sqrt{\frac{\alpha}{N\rho_A}}, \tag{2}$$

ρ_A being the fraction of volume (area really) occupied by the particles in the box and $\alpha=L_x/L_y$ is the aspect ratio of the box. The number Kn is of the same order as the standard Knudsen number.

Using the dimensionless quantities defined above, the distribution function in two dimension takes the form

$$f=\Phi f_M, \quad f_M=\frac{n}{2\pi T}e^{-C^2/2T},$$

$$\Phi=1+\frac{1}{2pT}\left(C_iC_j-\frac{1}{2}\delta_{ij}C^2\right)p_{ij}+\frac{2}{pT}\left(\frac{C^2}{4T}-1\right)\vec{C}\cdot\vec{Q}$$
$$+\left(\frac{1}{2}-\frac{C^2}{2T}+\frac{C^4}{16T^2}\right)\kappa. \tag{3}$$

Replacing the distribution function defined in Eq. (3), in the inelastic hard-sphere version of Boltzmann's equation it is a standard procedure to derive hydrodynamic equations for all the hydrodynamic fields (the moments of the distribution, including κ). In fact, projecting the distribution f, given in Eq. (3), to each one of the nine Hermite polynomials used to define f, yields a set of nine granular-gas dynamic equations for the nine fields (see the Appendix for more details). These fields are all in the same footing and no extra constitutive equations need to be assumed. Since the general equations have a rather complex structure, we have written them in the appendix while two of their simplest applications are in the main body of the present article.

A granular system behaves similar to a gas when

$$\zeta=\frac{q}{\mathrm{Kn}^2}=\frac{qN\rho_A}{\alpha} \tag{4}$$

remains rather small (order 1). This is the condition given in Ref. [13] to characterize the gaseous phase of granular systems. The parameter ζ *plays a decisive role* in the study of granular gases as explained in what follows.

Taking first the general dynamic equations given in the Appendix for the case of a perfectly elastic system reduced to the eight-moment formalism ($q=0$ and $\kappa=0$), and formally expanding each field in powers of Kn, it can be seen that n, $\vec{v}$, and T are order zero, $O(\mathrm{Kn}^0)$, while the other fields are $O(\mathrm{Kn})$. If the 8 moment equations (13 in 3D) are now written keeping terms only up to first order, it is seen that the time derivative of some fields disappear [they are $O(\mathrm{Kn}^2)$] and one gets the standard constitutive equations instead, namely, Newton's law of viscous flow and Fourier's law of heat transport. In the case of granular systems, Knudsen's number cannot be taken to be small without simultaneously making q small because ζ has to be finite. Namely, it is inconsistent to apply a hydrodynamic limit ($\mathrm{Kn}\to 0$) to expressions stemming from Boltzmann's granular equation without simultaneously taking $q\sim\sqrt{\mathrm{Kn}}\to 0$. As we have already shown in [12], Boltzmann's equation is hardly applicable beyond $\zeta\sim 3$.

One feature of the general dynamic equations is that the right-hand sides of them—coming from the collision term in Boltzmann's equation and called J_X in the Appendix—all have a prefactor $(1-q)$. This factor is there because, even though $q=1$ is unphysical, it is seen to correspond to $r=-1$, a value which makes trivial the collision rule previously defined: it corresponds to particles passing through each other without interacting. One can check that, in fact, Boltzmann's collision term is identically zero in such case. It is no trivial statement that the formalism describes a continuous family of systems ranging from elastic spheres, passing through granular systems, to strange systems with r negative and ending with a free gas. Such formalism implies delicate properties for the solutions describing the behavior of granular systems, solutions that remain valid even extended to cases with $r>1$ (exothermic collisions) as we comment later on. In brief, we could say that the common factor $(1-q)$ is a healthy property of our dynamic equations. Beyond the nine dynamic equations, the only extra relation is the equation of state $p=nT$.

In this paper, we illustrate the implications of our general dynamics solving two quite simple particular cases. The first case, seen in Sec. II, is the time-dependent case of homogeneous cooling (due to dissipation) the second one, seen in Sec. III, is the case of a granular system steadily heated by two infinite parallel walls. It is the simplest stationary (inhomogeneous) case. Section IV contains some final comments.

II. HOMOGENEOUS COOLING

If a granular gas is initialized in a homogeneous state with a Maxwellian velocity distribution, it will start cooling homogeneously at least for some time [4,9,10,14,18–21]. In this homogeneous cooling regime, the set of nine equations reduce to only two, one for the temperature T and one for κ. For reasons about to be explained, the temperature T is replaced by a function β, $T=1/\beta^2$, and the equations are

$$\mathrm{Kn}\frac{d\beta}{dt}=\frac{q(1-q)}{1024}(3\kappa+64)^2, \tag{5}$$

$$\frac{\mathrm{Kn}\beta}{1-q}\frac{d\kappa}{dt}=\frac{9q}{256}\kappa^3+\left(-\frac{1}{32}+\frac{1599q}{1024}-\frac{15q^2}{128}(1-q)\right)\kappa^2 -\left(2+\frac{55q}{8}-15q^2(1-q)\right)\kappa-4q+32q^2 \times(1-q). \tag{6}$$

The right-hand side of Eq. (6) vanishes for three different functions $\kappa_i(q)$, $i=1,2,3$. For all of them, a close form can be written. One diverges at $q=0$, the second one takes the value -64 at $q=0$, and a third one, which we call κ_∞, is zero at $q=0$. The latter has a series expansion given below in Eq. (8). These $\kappa_i(q)$ are the three solutions mentioned in Ref. [14]. Accepting this, it is seen that κ goes to a constant exponentially fast with time. Setting κ equal to κ_∞ in the equation for β shows that T satisfies Haff's law of the form $T=1/(1+at)^2$ [2] from $t=0$, suggesting that it is better to eliminate T in favor of $\beta=1/\sqrt{T}$. The natural time variable is not our previous dimensionless variable t, but $t'=1/\mathrm{Kn}t$, which implies that the transient time associated with β and κ (see below) is of the order of a few free flight times.

Solving these equations perturbatively in powers of q—assuming that κ is initially zero—the solution for κ up to second order is,

$$\kappa=-2(1-e^{-2t'})q+\left(\frac{365}{16}-\frac{19e^{-2t'}t'}{2}+\frac{e^{-4t'}}{16}+8e^{-2t'}t'^2 -\frac{183e^{-2t'}}{8}\right)q^2, \tag{7}$$

which, evaluated up to sixth order, in the limit $t\to\infty$, gives

$$\kappa_\infty=-2q+22.8125q^2-104.869q^3+460.276q^4 -1692.06q^5+4138.78q^6+\cdots. \tag{8}$$

The closed form for κ_∞ becomes positive for $q>0.146\,447=1/2-\sqrt{2}/4$. This threshold was given by van Noije and Ernst in Ref. [10] and our κ corresponds to twice their quantity $a_2(d=2)$, correcting one previously given in Ref. [13], and it coincides with the series expansion (bidimensional version) of the expression given in [14]. The dependence of κ on time, Eq. (7) is implicit in Ref. [14], when they write down their Eq. (23) and comment on it in a following paragraph. The existence of a transient period is determined by the initial condition that we have chosen Maxwellian, namely, $\kappa(0)=0$. Closely related is the direct simulation Monte Carlo study of the transient evolution of the fourth moment given in Ref. [20]. Trying to find an analytic solution of Eqs. (5)–(6) with an arbitrary initial value for κ is quite difficult.

The function $\beta(t')$, written up to third order is

$$\beta\approx1+4qt'+\left(-\frac{19t'}{4}-\frac{3e^{-2t'}}{8}+\frac{3}{8}\right)q^2+\left(-\frac{4941}{1024}+\frac{2391t'}{256}+\left(\frac{1239}{256}+\frac{9t'}{32}-\frac{3t'^2}{2}\right)e^{-2t'}-\frac{15}{1024}e^{-4t'}\right)q^3 +\cdots. \tag{9}$$

For small times, the behavior of β is

$$\beta\approx1+4q(1-q)t'-\tfrac{3}{4}(1-5q)^2q^2t'^2+O(q^2t'^3), \tag{10}$$

and, after the exponential terms have decayed, and up to sixth order, β gives Haff's law in the precise form,

$$\beta\approx b_0+b_1t',$$

$$b_0=1+0.375q^2-4.825q^3+28.6349q^4-144.972q^5 +526.670q^6, \tag{11}$$

$$b_1=4q-4.75q^2+9.33\,984q^3-48.7178q^4+220.992q^5 -873.622q^6.$$

One can check that the asymptotic behavior of β just written satisfies Eq. (5) using $\kappa=\kappa_\infty$. The behavior of β was known in the form of Haff's law [2] as in Eq. (11), without the exponentially decaying terms that the general solution exhibits in Eq. (9). If we had used the eight-moment expansion formalism, hence, no κ present, Eq. (5) would again give Haff's law and its exact form would be with $b_0=1$ and $b_1=4q-4q^2$. The inclusion of κ yields $O(q^2)$ corrections and a transient period before Haff's law holds.

In summary, we have seen that both κ and T have a transient time characterized by exponential terms. It is only after that transient that κ becomes constant and Haff's law begins to be satisfied.

III. STEADILY HEATED SYSTEM

In this section, we describe the static solutions of a 2D granular gas between two parallel walls (parallel to the X axis) separated by a distance L_y, both at temperature T_0. There are periodic boundary conditions in the X direction. Using dimensionless quantities, the walls are at temperature $T_0=1$ and the transversal dimensionless coordinate y, which is the only relevant coordinate, is in the range $(-1/2,\ 1/2)$. First, we describe the equations in the case with a dimensionless acceleration of gravity g, (where $g=\overline{g}L_y/T_0$) and then proceed to write down an approximate solution for the case $g=0$. In both cases, there is no hydrodynamic velocity and $p_{xy}=0$, hence, the pressure tensor has the form $\mathbf{P}=\mathrm{diag}[p-p_{yy},p+p_{yy}]$, and p_{yy} is not zero, but, as shown below, it is a $O(q)$ quantity.

A. With gravity

Four of the nine balance equations given in the Appendix become identities: the mass continuity equation, the momentum balance in the direction X, and the p_{xy} and Q_x balance equations. The five nontrivial equations are equations for n,T, $P_{yy}=p+p_{yy}$, Q_y, and κ. The momentum balance in the direction Y reduces to

$$\frac{\partial P_{yy}}{\partial y}=-gn, \tag{12}$$

showing that if $g=0$ the field P_{yy} would be homogeneous, while *the pressure is not*. The five equations can be solved perturbatively using q as a small parameter. It is illustrative to look at the first-order formalism.

Taking into consideration that under the present conditions n,T,p, and P_{yy} are nontrivial when considering $q=0$, while T', $p_{yy}=P_{yy}-p$, Q_y and κ are $O(q)$ we write down the five surviving equations keeping terms up to first order in q.

From the energy balance equation up to first order in q, it is direct to obtain that

$$\frac{\partial Q_y}{\partial y}=\frac{-8q}{\mathrm{Kn}}T^{3/2}n^2. \tag{13}$$

This first-order expression was anticipated in [6] in their Eq. (1) and the explicit form for their sink I. The balance equation associated with p_{yy} then yields

$$p_{yy}=qnT=qp. \tag{14}$$

With these results, the balance associated with κ implies that

$$\kappa=6q+\mathrm{Kn}\frac{n'}{n^3T^{3/2}}Q_y. \tag{15}$$

The term $6q$ comes from two contributions, one is $-2q$ as in the homogeneous cooling case, and the second one is $-\mathrm{Kn}Q_y'/(T^{3/2}n^2)$ which, according to Eq. (13), is $8q$. Namely, when there is no energy flux, κ recovers, to lowest order, the value $-2q$ seen for homogeneous cooling in Eq. (8). Note that if there is gravity (as in the present case) or another external forcing that imposes a nontrivial zero-order density profile, the contribution coming from the second term in Eq. (15) must be included in a first-order description. In fact, according to Eq. (12), at order q^0 the density satisfies $n'=-gn/T$ (at $q=0$, $T=1$), hence, the second term in Eq. (15) acquires a nontrivial first-order contribution coming from the q dependence of the heat flux. A consequence of the this nontrivial contribution to κ is given in what follows.

The balance equation associated with Q_y yields

$$Q_y=-\mathrm{Kn}\sqrt{T}\frac{\partial T}{\partial y}-\mathrm{Kn}\frac{2\kappa T^{3/2}}{n}\frac{\partial n}{\partial y}-\mathrm{Kn}\frac{T^{3/2}}{2}\frac{\partial \kappa}{\partial y}. \tag{16}$$

Some authors assume that κ is uniform. Making such an assumption would eliminate the last term in Eq. (16) and this equation would take the form of the modified Fourier law of the form $Q_y\sim-k\nabla T-\mu\nabla n$ used quite often in the literature [1,7,11,20,22]. Since presently we are dealing with a solution up to $O(q)$, we can check the relative size of the different contributions. It can be seen that the last two terms are of order $O(gq\mathrm{Kn})$ while the first term is $O(q\mathrm{Kn})$. Our conclusion is that the inhomogeneity of κ cannot be neglected in front of κ itself.

According to Eq. (15), κ can be expressed in terms of Q_y. We replace that expression for κ back in Eq. (16) and finally get a different distorted Fourier law,

$$Q_y=-\mathrm{Kn}\sqrt{T}\frac{dT}{dy}+\left(\zeta\frac{T^{3/2}}{n}\frac{dn}{dy}-\frac{\sqrt{T}}{n^4}\frac{dT}{dy}\left(\frac{dn}{dy}\right)^2+\frac{\sqrt{T}}{2n^3}\frac{dT}{dy}\frac{d^2n}{dy^2}\right)\mathrm{Kn}^3. \tag{17}$$

This expression contains ζ instead of q [see Eq. (4)] and it has been expanded in powers of Kn. The three terms which appear multiplied by Kn^3 are of the same order when the dissipation coefficient is sufficiently small. Equation (12) was never used to get Eq. (17) yet it is the correct (first order) expression to be used when gravity is present. In Eq. (17), all terms are order q, either because of the factor dT/dy or because of ζ. The derivatives of n are $O(q^0)$ as n depends on g.

A law of the form $Q_y\sim-k\nabla T-\mu\nabla n$ has been used as a heuristic modified Fourier law, but Eq. (17), on the other hand, is a direct (first-order) implication of Boltzmann's equation with no adjustable parameters and therefore it should be valid in the quasielastic case. Had we not introduced κ as a dynamic field, we would obtain an eight-moment formalism which would lead to an expression like Eq. (16) with only the standard Fourier term because κ in that expression appears in the other two terms. Hence, in the present context (dynamics derived from moment expansions), the form of Q_y given in Eq. (17) is crucially dependent on the fact that κ is incorporated as a dynamic field.

If we go back to our basic dynamic equations of the Appendix, we can check that the presence of κ (in the first-order solution) comes from the term $\nabla(pT\kappa)$ present in the balance for $\vec{Q}$, see Eq. (A1). The contribution of κ to the collisional terms J_X in the Appendix are of higher order.

The second-order version of Eq. (17) contains hundreds of terms with higher derivatives and products of them as it is already true in the present $O(\mathrm{Kn}^3)$ term. Additionally, not even the form of Eq. (16) is valid to higher order.

B. Without gravity

The five balance equations—not to first order but in general—can easily be solved perturbatively using q as small parameter in the case $g=0$. Up to second order, the fields are,

$$n=1+\left(-\frac{4y^2}{\mathrm{Kn}^2}+\frac{1}{3\,\mathrm{Kn}^2}\right)q+\left(\frac{64y^4}{3\,\mathrm{Kn}^4}-\frac{4y^2}{\mathrm{Kn}^4}+\frac{677y^2}{8\,\mathrm{Kn}^2}+\frac{1}{15\,\mathrm{Kn}^4}-\frac{677}{96\,\mathrm{Kn}^2}\right)q^2,$$

$$T=1+\frac{4y^2-1}{\mathrm{Kn}^2}q+\left(-\frac{4y^2}{3\,\mathrm{Kn}^4}+\frac{2}{3\,\mathrm{Kn}^4}+\frac{673}{32\,\mathrm{Kn}^2}-\frac{16y^4}{3\,\mathrm{Kn}^4}-\frac{673y^2}{8\,\mathrm{Kn}^2}\right)q^2,$$

$$Q_y=-\frac{8qy}{\mathrm{Kn}}+\left(\frac{7y}{2\,\mathrm{Kn}}+\frac{16y^2}{3\,\mathrm{Kn}^3}+\frac{20y}{3\,\mathrm{Kn}^3}\right)q^2, \tag{18}$$

$$\kappa=6q+\left(-\frac{795}{16}+\frac{184y^2}{\mathrm{Kn}^2}\right)q^2,$$

$$P_{yy}=1+\left(1-\frac{2}{3\,\mathrm{Kn}^2}\right)q+\left(\frac{2}{5\,\mathrm{Kn}^4}-\frac{27}{32}+\frac{213}{16\,\mathrm{Kn}^2}\right)q^2,$$

$$p=1-\frac{2q}{3\,\mathrm{Kn}^2}+\left(\frac{671+24y^2}{48\,\mathrm{Kn}^2}+\frac{2}{5\,\mathrm{Kn}^4}\right)q^2.$$

We have obtained this solution up to eighth order.

If we eliminate q in favor of ζ, defined in Eq. (4), the expansions have only positive powers of both ζ and Kn, emphasizing that some sort of granular hydrodynamic regime corresponds to $\mathrm{Kn}\to 0$ with ζ kept fixed. Although this is an unrealistic limit, in the sense that in the real world one cannot find restitution coefficients arbitrarily close to unity, it is conceptually interesting. As already mentioned, the condition $\zeta\leqslant 3$ coincides with the criterion given in Ref. [13] to characterize the gaseous regime and it seems that it is the only regime that can possibly be described using Boltzmann's equation.

The eight-moment formalism (no κ) yields a solution quite similar to that shown in Eq. (18). The difference between both solutions for n,T, P_{yy}, and p is of order $O[(q/\mathrm{Kn}^2)]$, while for Q_y the difference is even smaller, $O(q^2/\mathrm{Kn})$.

In the present case, P_{yy} is uniform and dp/dy is a $O(q^2)$ quantity. There is energy flowing from the walls to the center of the system where the temperature has a minimum, making $Q_y(y<0)>0$ and $Q_y(y>0)<0$. The field κ, also up to second order, is not uniform and it has a minimum ($\kappa_{\min}>0$) at the center of the box, namely, the center of the box is the region where the velocity distribution is less peaked.

In the following, we compare our results, the higher-order version of Eq. (18), with molecular dynamics (MD) observations for values of ζ up to 1.6. Since our simulations are strictly Newtonian, wall effects do appear. To keep them small, we need Kn small, and to avoid correlations, we need the density to be small. The only practical possibility is to have a rather large value for N but then q has to be quite small. We use $N=19\,600$, a global area density $\rho_A=0.01$ and the aspect ratio α of the system is chosen to be 1.

The simulations use Newtonian dynamics and particles hitting the walls totally forget their incoming velocity and bounce back with a velocity chosen from a Maxwellian distribution with temperature $T_0=1$. This algorithmic strategy implies that the simulated system has a velocity distribution discontinuous in a region near the walls (the Knudsen layer). This is an effect due to dissipation, in the sense that $\nabla T\neq 0$ because $q\neq 0$, and in 1D it has been shown to be a $O(qN)$ effect [23]. The discontinuity is quite in opposition to the smoothness assumption made in Eq. (3), and for this reason, the present formalism is unable to faithfully describe the behavior of the system near the walls.

To be able to compare our simulational results with our formal predictions, we need to reassess the meaning of quantities like n_0, T_0, and L_y used to define our dimensionless fields in Eq. (1). This is necessary because wall effects are quite different from the behavior of the bulk of the system (to which the theory refers). Once boundary layers are separated, it is necessary to obtain, from the results of the simulations, the extrapolated temperature T_0 at the walls, the number of particles in the bulk, its width, etc. It is with these quantities that the dimensionless fields of Eq. (1) have to be really defined. In the case of n_0 and L_y, because we have chosen a large N, these effects are quite small and, for example, Kn is directly taken from the crude values used in the simulation.

The discontinuity of the distribution function at the walls implies important effects on the observed profiles: the distribution in the central axis has a precise nonvanishing κ in fair agreement with our solution but near the boundaries, the Maxwellian behavior, imposed on the re-entering particles, tends to produce a vanishing cumulant κ. Hence, the observed κ for the distribution near the walls goes almost to zero while the predicted κ (which does not consider the discontinuity) goes on growing. Apparently, when q is larger

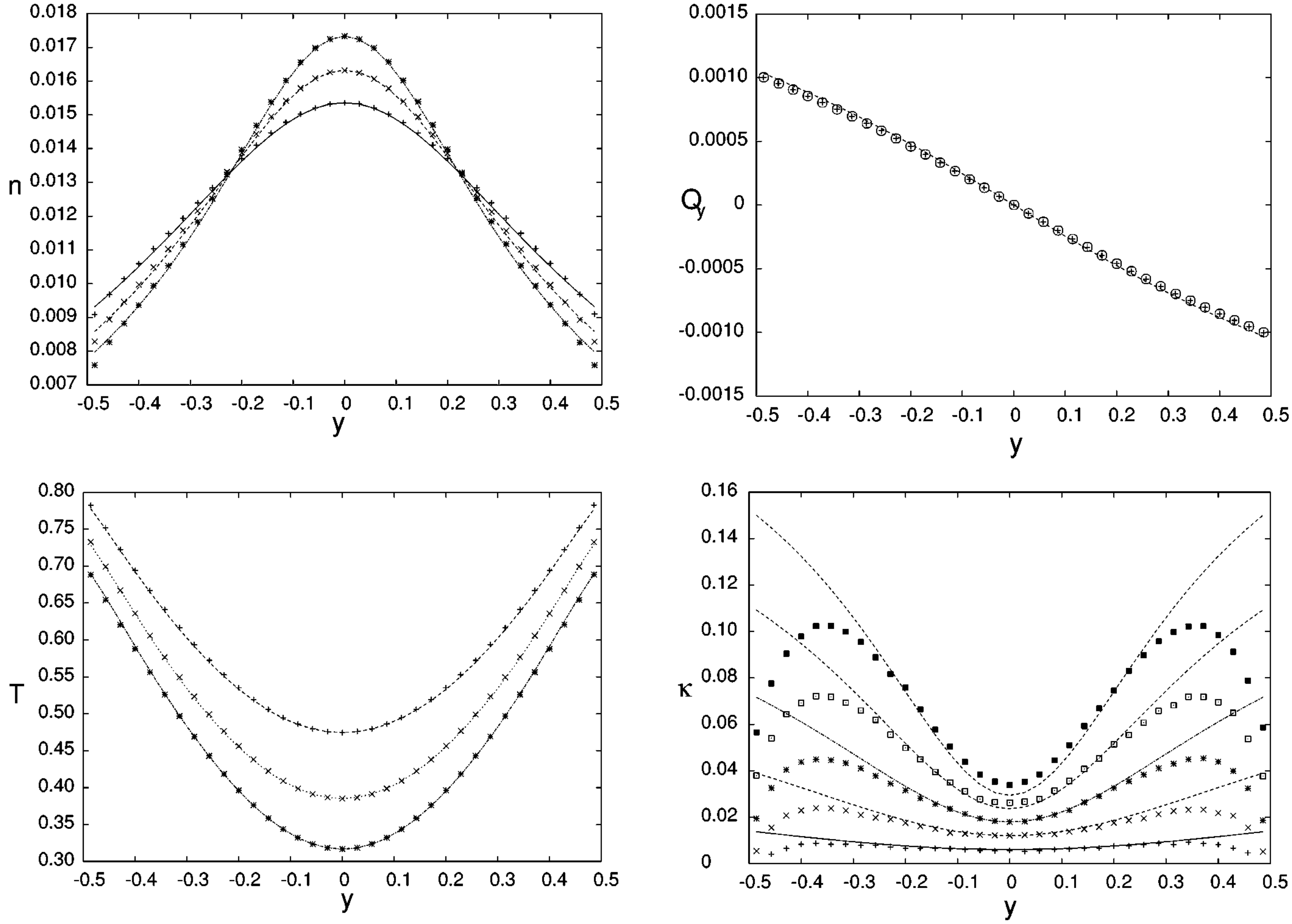

FIG. 1. The dimensionless density n, granular temperature T, energy flux from the walls Q_y, and fourth cumulant κ are shown for a system with $N=19\,600$ particles, area density $\rho_A=0.01$ and Kn$=0.0714$, for different values of ζ. For both, the density and the temperature, the three profiles correspond to $\zeta=0.2$ $(+)$, $\zeta=0.6$ $(\times)$ and $\zeta=1.0$ $(*)$. The profile Q_y corresponds to $\zeta=1.0$. In the case of κ, the values of ζ are: $0.2(+)$, $0.4(x)$, $0.6(*)$, 0.8(open square), 1.0(solid square).

than about 0.004 ($\zeta \geqslant 0.8$) these effects reach the central part of the system introducing an important difference with respect to the theoretical predictions.

To make theory-simulation comparisons we have not used directly the eighth-order expressions, but first we have transformed them using the Padé technique: for each field, we define a function, ratio of two polynomials in ζ (of degrees μ and ν, respectively) such that the series expansion of the rational function coincides with the eighth-order solution. In each case, it is seen that there is a range of values for $[\nu,\mu]$—keeping $\nu+\mu \leqslant 8$—for which the different Padé expressions are numerically almost identical but they differ from the values that takes the eighth-order solution itself, because of the poor convergence of the latter. We found out that it was enough to use $(\mu=2,\nu=2)$ for all fields, except for κ, in which case we had to consider $(\mu=3,\nu=3)$. The use of Padé approximants gives a refined but not radically different fit.

In Fig. 1, we compare the eighth-order solution for n,T, Q_y, and κ with MD results. It can be seen that there is an excellent agreement for the first three fields (n,T, and Q_y). In the case of κ, as discussed before, the agreement is only fair and it badly fails away from the central part of the system.

In Fig. 2, we compare the values of P_{yy} and those of κ at the central part $(y=0)$ for different values of q from MD versus the values predicted by the eighth-order solution. Again, the Padé technique was used. Its application is now essential because of the weak convergence in q. It is seen that κ does not fit well except for quite small values of q and, as mentioned before, this seems to be due to wall effects reaching the central part of the system.

The same kind of effect is observed for $p_{yy}=1/2(P_{yy}-P_{xx})$, an observable that measures the anisotropy between the diagonal components of the pressure tensor. The predicted profile for p_{yy} is a smooth function decreasing from the central part toward the walls. In contrast, the observed profile begins decreasing, as predicted, and then abruptly increases reaching differences, with respect to the predicted profile, of about 20 to 40% in the case of, for example, $q=0.008\,16$ $(\zeta=1.6)$. These important differences take place at approximately the same region where the observed κ profile presents the maximum differences with respect to the theoretical value.

Studying the P_{yy} series up to q^8 using the Padé technique,

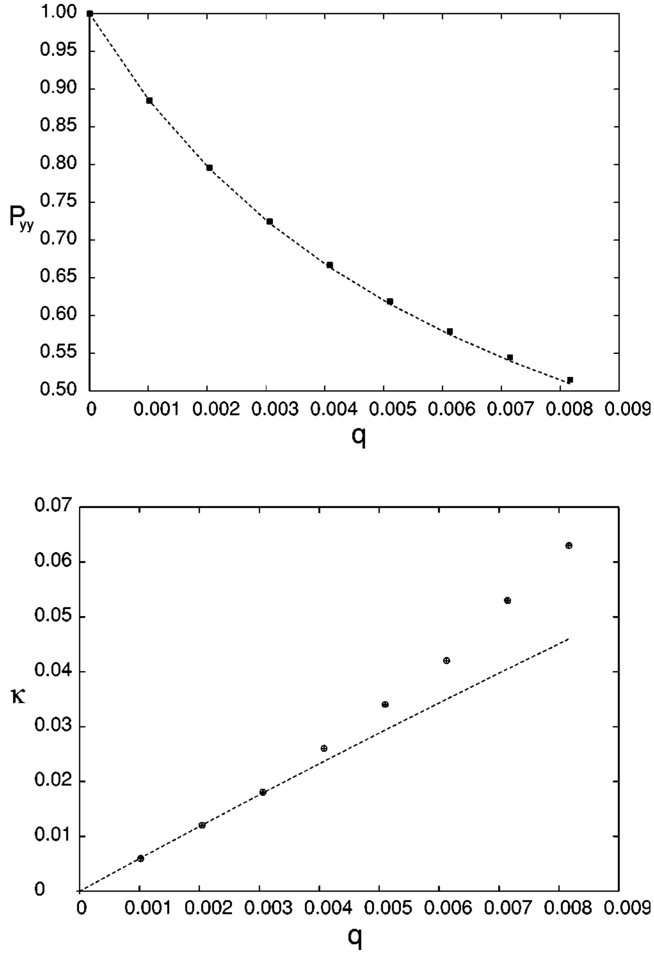

FIG. 2. The values of the two dimensionless fields P_{yy} and κ, evaluated at the center of the system, are shown varying according to the value of the inelasticity coefficient q for a system with $N = 19\,600$ and $\rho_A = 0.01$. In the first case, P_{yy} measured in our simulations is in agreement with the values predicted by our formalism for q as large as $q = 0.008\,164$ ($\zeta = 1.6$). This corresponds to the largest inelasticity coefficient considered. In the case of κ, the field takes values larger and larger than what our theoretical framework predicts, in agreement with similar observations for the anisotropy of the pressure tensor due to wall effects (see text), which for values of $\zeta \geqslant 0.8$ ($q \geqslant 0.004$) seems to reach the central region of the system.

it is possible to detect a systematic pole at a small negative value q_c. P_{yy} is reasonably well approximated by the Padé [1,1] expression

$$P_{yy} = \frac{1 - \frac{1}{15}\zeta + \frac{3499}{160}\mathrm{Kn}^2\zeta}{1 + \frac{3}{5}\zeta + \frac{3339}{160}\mathrm{Kn}^2\zeta},$$

which has a pole at

$$q_c \approx -\frac{1.667\ \mathrm{Kn}^2}{1 + 34.78\ \mathrm{Kn}^2}.$$

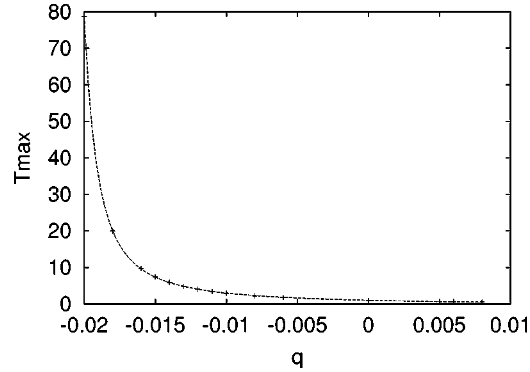

FIG. 3. The dimensionless temperature at the center of a granular system of $N = 5000$ grains is predicted to diverge for inelasticity q less than a critical value. The graph shows the observed temperatures while the continuous line is a fit: $T_{\max} = \exp[-(1 + 31.02q - 0.3829q^2)/(1 + 42.01q)91.98q]$ which is singular at $q = -0.0238$.

For Kn $= 0.1$, the predicted pole is at $q_c \approx -0.012$. Hence, our expansions have a small radius of convergence. The presence of this pole suggests that at some small value, $q < 0$, collisions produce so much extra energy that it cannot be dissipated at the necessary rate to produce a stationary state. Simulations with $N = 5000$ and area density $\rho_A = 0.01$ run for $q = -0.006$, $q = -0.008$,..., $q = -0.022$ produced, beyond $q = -0.020$ a system with ever increasing temperature reaching, in our units, temperatures as high as 10^{12} and not yet stabilized. Results for the temperature at the center of the system and a simple fit are shown in Fig. 3. The divergent behavior does not take place at the predicted value q_c because the temperature profile in the simulation develops immense gradients and a huge discontinuity at the walls making the dissipation far more efficient than the formalism can describe, but our dynamics correctly predicts that such instability exists.

IV. FINAL COMMENTS

We have presented a general rarefied grain-gas dynamics. The formulation, based on moment expansion methods, incorporates the fourth cumulant κ as an extra dynamic variable making this a nine dynamic field formulation in two dimensions (it would be a 14 fields formalism in 3D). Boltzmann's inelastic equation and moment expansion techniques lead to the basic dynamic equations, one for each field. We have discussed the effects of the inclusion of κ in the dynamics of granular gases by means of two simple examples. The simplest one is the homogeneous cooling state, which turns out to coincide with the solution already known, except that extra detail in the transient time dependence is now given. In this first example, it is seen that Haff's law is valid after a transient period and when it holds κ influences the cooling rate by roughly a factor $(1 + 3/32\kappa)$ with respect of a moment expansion formalism which does not include κ. The precise form of Haff's law is affected at second order in the inelasticity coefficient q. Our solution is in close agreement with previous ones given by other authors.

The second example is an inhomogeneous granular gas between two parallel walls kept at constant granular temperature T_0 with and without gravity. The system is not free of complexities even though it is a time-independent steadily heated system. In the case with gravity, the theoretical results show that the cumulant κ couples with the low-order moments implying a distorted Fourier law. The non-Fourier contribution to the heat flux is order q as is the heat flux itself.

In the case with no gravity, theory was compared with the results obtained with MD. The predicted field profiles tend to coincide with the MD observations, except that the fourth cumulant κ deviates more and more from its theoretical value as the dissipation coefficient q gets larger. For small q, the theoretical predictions for κ are in good agreement with MD observations and the inclusion of the second term in Eq. (15) is clearly necessary to account for the observed inhomogeneous κ profile. For large values of q, the wall effects on κ reach the central part of the system introducing important differences with respect to our theoretical predictions, but still, it is evident that κ is quite inhomogeneous. This very simple solution serves to illustrate that only after eliminating q in favor of ζ, it is possible to take the hydrodynamic limit $\mathrm{Kn}\to 0$ (keeping ζ finite).

It is interesting to point out that to lowest order, κ is quite different for different physical regimes. For the homogeneous cooling case, $\kappa_\infty \approx -2q$, while for the steadily heated system seen in Sec. III, we saw that $\kappa \approx 6q + O(qg\,\mathrm{Kn}^2)$ and we corroborated it with simulations.

Another interesting conclusion that came from the analysis of the steadily heated system, is that the analytic behavior of this solution is influenced by a nearby solution corresponding to exothermic collisions with $r>1$. Exothermic collisions imply a singular behavior (no steady solution) when the "inelasticity" q becomes slightly negative. This prediction is qualitatively confirmed by our simulations.

ACKNOWLEDGMENTS

The authors wish to thank Rodrigo Soto for helpful comments and discussions. This work has been partly financed by FONDECYT research Grant Nos. 1990148 (D.R.) and 1000884 (P.C.) and FONDAP Grant No. 11980002.

APPENDIX: MOMENT EXPANSIONS AND DYNAMIC EQUATIONS

Moment expansion methods can summarily be described as follows. The local Maxwellian distribution function $f_M(\vec{r},\vec{c},t)$ is used as the reference function about which an expansion is made. It is written in terms of the peculiar velocity $\vec{C}=\vec{c}-\vec{v}(\vec{r},t)$, where $\vec{v}(\vec{r},t)$ is the hydrodynamic velocity. A set of Hermite polynomials on $\vec{C}$, $H_a(\vec{C})$, are built in the sense that $\int H_a(\vec{C})H_b(\vec{C})f_M(\vec{r},\vec{C},t)d\vec{C}=\delta_{\mathrm{ab}}$. The polynomials H_a are obtained simply deriving a base of orthonormal polynomials starting from $H_0=1$ and from first degree upwards, using the standard method. Then the distribution is written in the form $f(\vec{r},\vec{C},t)=\Sigma_a H_a(\vec{C})R_a(\vec{r},t)f_M(\vec{r},\vec{C},t)$. The coefficients R_a (moments of the distribution) are formally obtained requiring first that f is normalized to the number density: $\int f\,d\vec{c}=n$ and then that the averages $\langle A\rangle \equiv 1/n\int A\,d\vec{c}$ give the formally correct results, namely, it is required that the components of the hydrodynamic velocity are $v_i=\langle c_i\rangle$, the temperature is $T=m/d\langle C^2\rangle$ (the temperature is measured in energy units so that Boltzmann's constant is $k_B=1$), the pressure tensor is $P_{ij}=\langle mnC_iC_j\rangle$, the energy or *heat* flux vector is $Q_i=mn/2\langle C^2C_i\rangle$, and the fourth cumulant is $\kappa=\langle C^4\rangle/\langle C^2\rangle^2-(d+2)/d$. Such requirements totally define the R_a. In such formalism, the collisional contribution to transport is neglected altogether. These are $1/2(4+5d+d^2)$ moments: 14 in 3D and 9 in 2D.

In the present context, the hydrostatic pressure is $p=nT$. The bidimensional distribution—expanded in nine moments as explained above—is the one given in Eq. (3). This distribution is replaced in Boltzmann's (inelastic) equation. Projecting it to the first nine Hermite polynomials yields a set of dynamic equations for the nine moments.

One remarkable feature of the resulting gas-dynamics is that no transport laws are necessary. Their place is taken by dynamic equations for p_{ij}, Q_i, and κ. Namely, these last fields are independent variables in the same footing as the density, the velocity and the temperature fields. Together they satisfy nonlinear coupled differential equations. The complete set of adimensional equations in the present context are

$$\frac{Dn}{Dt}+n\boldsymbol{\nabla}\cdot\vec{v}=0,$$

$$n\frac{D\vec{v}}{Dt}-n\vec{f}+\boldsymbol{\nabla}\cdot\mathbf{P}=0,$$

$$n\frac{DT}{Dt}+\boldsymbol{\nabla}\cdot\vec{Q}+\mathbf{P}:\boldsymbol{\nabla}\vec{v}=J_T,$$

$$\frac{D\mathbf{p}}{Dt}+\mathbf{p}\boldsymbol{\nabla}\cdot\vec{v}+\frac{1}{2}[\boldsymbol{\nabla}\vec{Q}]+[\mathbf{p}\cdot\boldsymbol{\nabla}\vec{v}]+p[\boldsymbol{\nabla}\vec{v}]=J_p,$$

$$\frac{D\vec{Q}}{Dt}+\frac{3}{2}(\vec{Q}\boldsymbol{\nabla}\cdot\vec{v}+\vec{Q}\cdot\boldsymbol{\nabla}\vec{v})+\frac{1}{2}(\boldsymbol{\nabla}\overbrace{\vec{v})\vec{Q}}+T\boldsymbol{\nabla}\cdot\mathbf{p}+3\mathbf{p}\cdot\boldsymbol{\nabla}T-\frac{1}{n}(\boldsymbol{\nabla}\cdot\overbrace{\mathbf{P})\mathbf{p}}+2p\boldsymbol{\nabla}T+\boldsymbol{\nabla}(pT\kappa)=\vec{J}_Q,$$

$$4pT\frac{D\kappa}{Dt}+8(1-\kappa)T\boldsymbol{\nabla}\cdot Q+8(1-\kappa)T\mathbf{p}:\boldsymbol{\nabla}\vec{v}-\frac{8}{n}\vec{Q}\boldsymbol{\nabla}:\mathbf{p}+16\vec{Q}\cdot\boldsymbol{\nabla}T-\frac{8T}{n}\vec{Q}\cdot\boldsymbol{\nabla}n=J_\kappa, \tag{A1}$$

with

$$J_T = -\frac{q(1-q)}{\mathrm{Kn}}\left(\frac{n^2T^{3/2}}{512}(3\kappa+64)^2+\frac{3}{8}\frac{\mathbf{p}:\mathbf{p}}{\sqrt{T}}+\frac{3Q^2}{32T^{3/2}}\right),$$

$$\mathbf{J}_p = \frac{(1-q)(2+3q)}{\mathrm{Kn}}\left(\frac{n\sqrt{T}(\kappa-64)}{32}\mathbf{p}-\frac{[\vec{Q}\vec{Q}]}{64T^{3/2}}\right),$$

$$\vec{J}_Q = -\frac{1-q}{\mathrm{Kn}}\left(n\sqrt{T}\vec{Q}\left\{(2+3q)\frac{\kappa}{64}+(2+15q)\right\}+\frac{1}{2\sqrt{T}}\mathbf{p}\cdot\vec{Q}\right),$$

$$J_\kappa = J_{C^4}-8(2+\kappa)J_T,$$

$$J_{C^4} = \frac{1-q}{\mathrm{Kn}}\left(n^2T^{5/2}\left\{-16q(9-8q(1-q))-\frac{\kappa}{2}(16+207q-120q^2(1-q)),-\frac{\kappa^2}{256}(32+9q+120q^2(1-q))\right\}\right.$$
$$\left.+\left(\sqrt{T}\,\frac{\mathbf{p}:\mathbf{p}}{4}-\frac{Q^2}{16\sqrt{T}}\right)(16-15q+120q^2(1-q))\right), \tag{A2}$$

where $D/Dt \equiv \partial/\partial t+\vec{v}\cdot\boldsymbol{\nabla}$ is the convective derivative, the square brackets have been used to indicate *symmetric traceless part*, namely, $[A]=A_{ij}+A_{ji}-2/d\,\delta_{ij}\Sigma_a A_{aa}$, the first over-brace term indicates contraction of the indices of $\vec{v}$ and $\vec{Q}$ while the second one is to be understood as $(\partial P_{rs}/\partial x_s)p_{kr}$, $\mathbf{p}$ is the symmetric traceless part of the pressure tensor $\mathbf{P}$ and $\vec{f}$ is an external force per unit mass. Since we are dealing with Boltzmann's equation in 2D, then u, the internal energy, is $u=T$ and the hydrostatic pressure obeys the ideal gas equation of state $p=nT$.

All collisional terms have a common factor $(1-q)/\mathrm{Kn}$ because formally making $q=1$ in Boltzmann's equation makes the collisional term identically vanish. This is so because the collision rule for $q=1$ or $r=-1$ is that of particles that pass through each other without interacting.

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