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High-energy tails for inelastic Maxwell models

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Abstract. – Monte Carlo simulations of the spatially homogeneous Boltzmann equation for inelastic Maxwell molecules, performed by Baldassarri *et al.* (cond-mat/0111066), have shown that general classes of initial distributions evolve for large times into a singular nonlinear scaling solution with a power law tail. By applying an asymptotic analysis we derive these results from the nonlinear Boltzmann equation, and obtain a transcendental equation from which the exponents, appearing in the power law tails, can be calculated. The dynamics of this model describes a dissipative flow in v-space, which drives the system to an attractor, the nonlinear scaling solution, with a constant *negative* rate of irreversible entropy production, given by $-\frac{1}{4}(1-\alpha^2)$, where α is the coefficient of restitution.

Introduction. – A classical problem in kinetic theory of possibly overpopulated high-energy tails in velocity distributions [1] has received a new impulse through recent experiments [2] on many-particle systems with inelastic non–energy-conserving interactions. In fact, the stretched exponential overpopulation $\sim \exp[-A|v|^{3/2}]$, observed in laboratory experiments with granular material on vibrating plates, were predicted before [3] on the basis of the nonlinear Boltzmann equation for an inelastic system of hard spheres, driven by Gaussian white noise. These theoretical predictions, as well as the prediction $\sim \exp[-A|v|]$ in the same system *without* energy input [3, 4], have been extensively verified in Direct Monte Carlo Simulations of the nonlinear Boltzmann equation [5, 6].

From the point of view of kinetic theory the intriguing questions are: What is the generic feature causing overpopulated tails, possibly even power law tails, in systems of *inelastic* particles? How does the overpopulation depend on the scattering cross-sections, and on the different forms of energy input [6–10]? The generic feature is the mechanism for overpopulation, and not the specific shape of the tail.

Recently, classes of simplified mathematical models, the so-called inelastic Maxwell models, have been studied in the context of rapid granular flows, *with* and *without* energy input [8–17]. These models are characterized by a nonlinear Boltzmann equation with a collision rate that is independent of the relative kinetic energy of the colliding particles. What harmonic oscillators are for quantum mechanics, and dumb-bells for polymer physics, is what elastic and inelastic Maxwell models are for kinetic theory. For instance, the transport coefficients and spectral properties of the collision operator can be calculated explicitly, the infinite set of moment equations can be solved sequentially, etc.

The question of overpopulated high-energy tails, and how they depend on the interaction models, might also be of interest for fluidized granular matter, as long as the system remains

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spatially homogeneous. This is also suggested by the above experimental and kinetic-theory articles [2–4] on inelastic hard spheres, as well as on inelastic Maxwell models [8–12, 14–17]. It should also be noted here that the macroscopic equations for inelastic Maxwell models, as well as those for the even simpler inelastic BGK or single relaxation time models [18], all lead to nonlinear hydrodynamic equations with qualitatively the same structure and properties, and Haff's law is also obeyed [19].

What type of velocity distributions are observed apparently depends strongly on the type on non-equilibrium (possibly steady) state experiments, performed in laboratories or on computers. One might be able to design laboratory experiments in granular fluids that are able to probe the softer energy dependence of the inelastic pseudo-Maxwell particles. As far as Molecular Dynamics (MD) experiments are concerned, Baldassarri *et al.* [14] have performed molecular-dynamics simulations of a granular *lattice* model with inelastic Maxwellian-type interactions, which supposedly describes the formation of vortex patterns in granular fluids, as long as the clustering instability is suppressed [20]. Moreover, smooth inelastic spheres with a constant coefficient of restitution α (with $0 < \alpha < 1$) are by no means the generally accepted prototypical model for granular fluids. For instance, MD simulations of this system exhibit the spurious inelastic collapse phenomenon, which is an artifact of *constant* α. For physical reasons α should approach unity for vanishing impact velocities.

Finally, from the point of view of non-equilibrium (steady) states, the structure of velocity distributions in dissipative systems, including the high-energy tail, is a subject of continuing research, as the universality of Gibbs' state of thermal equilibrium is lacking outside thermal equilibrium, and a possible classification of generic structures would be of great interest in many fields of non-equilibrium statistical mechanics.

After this explanation of the possible relevance of inelastic Maxwell models for different fields of research, we concentrate on the kinetic theory for these models, in particular on the simplest case, the freely cooling one without energy input. By shear coincidence two groups, Krapivsky and Ben-Naim on the one hand [15], and the present authors on the other hand [17], published preprints, essentially simultaneously, about the existence of power law tails in these models. The research of both groups has been carried out without any knowledge about each other's research activities. Moreover, at the same time, Baldassarri *et al.* [16] have found an exact scaling solution $\tilde{f}(c,t)$ of that equation for $d = 1$, defined as $f(v,t) \sim (1/v_0^d(t))\tilde{f}(v/v_0(t))$, which has the form $\tilde{f}(c) = (2/\pi)/(1+c^2)^2$. It does have a power law tail $(1/c^4)$, and $v_0^2(t) = \langle v^2\rangle_t = \exp[-2\gamma t]$, with $\gamma \sim (1-\alpha^2)$. The quantity $\langle v^2\rangle_t$ is the second moment of $f(v,t)$. More interestingly, they solve the spatially homogeneous Maxwell-Boltzmann equation for $d = 2$ using MC simulations [21], and observe that an initially Maxwellian distribution approaches for long times a scaling form $\tilde{f}(c)$ on which the MC data could be collapsed when plotting $v_0^d(t)f(v,t)$ as a function of $v/v_0(t)$.

We interpret this observation as strong evidence for the existence of interesting limiting behavior when coupled limits are taken, *i.e.* the transformed or rescaled distribution function, $\tilde{f}(c,t)$, approaches a scaling form in the coupled limit as $t \to \infty$ and $v \to 0$, with $v/v_0(t) = c$ kept constant, *i.e.*

$$\lim_{t\to\infty} \tilde{f}(c,t) = \lim_{t\to\infty} (v_0(t))^d f(v_0(t)c,t) = \tilde{f}(c). \tag{1}$$

The existence of such scaling solutions is a surprising result. The Boltzmann equation for this model with dissipative interactions does not obey an H-theorem (the dynamics corresponds to a contracting flow in v-space), but the spectrum of eigenvalues (negative of decay rates) is *non-positive*, and the solutions of the nonlinear closed set of coupled equations for the standard moments $\langle v^n\rangle_t$ for $n > 1$ are all decaying. On the other hand, the eigenvalue spectrum of the transformed kinetic equation for $\tilde{f}(c,t)$ is *non-negative*, and the corresponding equations for some of the higher moments $\langle c^n \rangle_t$ of $\tilde{f}(c,t)$ —their number depends on the coefficient of restitution and on the dimensionality— are linearly unstable, and drive the solution into the singular scaling form in the limit as $t \to \infty$. The detailed analysis of this approach for d-dimensional systems can be found in ref. [22].

To illustrate the singular nature of this scaling state, it is of interest to calculate the entropy S, or H-function, $H = \int f \ln f$ for this contracting flow in one-dimension, for which the scaling solution is explicitly known, *i.e.*

$$
\begin{aligned}
S(t) &= -H(t) = -\int \mathrm{d}c\, \tilde{f}(c) \ln \tilde{f}(c) - \gamma t \\
&\sim -\gamma t + \ln(8\pi/e^2) \qquad (t \text{ large}),
\end{aligned}
\tag{2}
$$

where $v_0(t) = \exp[-\gamma t]$ has been used. We note that the entropy keeps decreasing (at a constant positive rate γ, to be calculated in eq. (14)). This is typical for pattern forming mechanisms in configuration space, where spatial order or correlations are building up, as well as in Chaos Theory, where the rate of irreversible entropy production is negative on an attractor [23, 24].

Moreover, there is no fundamental objection against decreasing entropies in an open subsystem, here the inelastic Maxwell particles, interacting with a reservoir. The reservoir is here a sink, formed by the dissipative interactions. The probability is contracting onto an attractor, which is a well-known phenomenon in chaos theory. The simulations of Baldassarri *et al.* [21] suggest that the collapsed distribution function at large times reaches a scaling form $\tilde{f}(c)$ in any dimension. If that is indeed the case, the rate of entropy production becomes $\mathrm{d}\gamma = (1/4)(1-\alpha^2)$, which is independent of the dimensionality. In dimensions $d \geq 2$ no explicit solution is known, and the constant term on the right-hand side of (2) cannot be calculated.

The goal of this article is to derive the power law from the dominant small-k singularity in the Fourier transform $\tilde{\phi}(k,t)$ of the rescaled velocity distribution function $\tilde{f}(c,t)$ in any dimension, and to calculate the exponents appearing in the algebraic tails. Here $\tilde{\phi}(c,t)$ is the generating function of the rescaled moments $\langle c^n \rangle_t$. When $\tilde{f}(c,t)$ develops a tail $\sim A/|c|^{a+d}$, then the moments with $n > a$ become divergent, and so does the n-th derivative of the corresponding generating function at $k=0$, *i.e.* $\tilde{\phi}(k,t)$ develops a singularity at $k=0$ as $t \to \infty$. Suppose the dominant small-k singularity of $\tilde{\phi}(k,t)$ is $\sim |k|^a$, where a is different from an even integer (even powers of k represent contributions that are regular at small k), then its inverse Fourier transform scales as $1/c^{a+d}$ at large c.

By applying Bobylev's Fourier transform method to the nonlinear Boltzmann equation for pseudo-Maxwell particles in arbitrary dimensions [25], we obtain a nonlinear equation for $\tilde{\phi}(k,t)$, from which we determine the dominant small-k singularity, and derive a transcendental equation for the exponent a in the power law tail $\sim 1/|c|^{a+d}$ of the scaling solutions $\tilde{f}(c)$. The amplitude is left undetermined. For this solution to be physically acceptable, A must be positive. Our method cannot guarantee that, and similarity solutions of Maxwell models are not guaranteed to be positive either. The methods used in refs. [15, 17] are similar in spirit, in the sense that they derive a transcendental equation for the exponent of the power law by a self-consistent method, but the mathematical details of the analysis are quite different.

Dominant small-k singularity. – The Boltzmann equation for the d-dimensional inelastic Maxwell model reads

$$
\partial_t f(v_1,t) = \int_n \int \mathrm{d}v_2 \left[\tfrac{1}{\alpha} f(v_1^{**}) f(v_2^{**}) - f(v_1) f(v_2) \right]. \tag{3}
$$

Here $\int_n(\cdots) = (1/\Omega_d)\int \mathrm{d}n(\cdots)$ is an average over a d-dimensional solid angle where $\Omega_d = 2\pi^{d/2}/\Gamma(\frac{1}{2}d)$. The velocities v_i^{**} with $i,j = \{1,2\}$ denote the d-dimensional *restituting* velocities, and v_i^* the corresponding *post-collision* velocities. They are defined as

$$\begin{aligned} v_i^{**} &= v_i - \tfrac{1}{2}(1+\tfrac{1}{\alpha})v_{ij}\cdot nn \\ v_i^{*} &= v_i - \tfrac{1}{2}(1+\alpha)v_{ij}\cdot nn, \end{aligned} \tag{4}$$

where $v_{ij} = v_i - v_j$, n is a unit vector along the line of centers of the interacting particles, and $a\cdot b$ is a scalar product of two d-dimensional vectors a and b. In one-dimension, the tensorial product nn can be replaced by 1. From the normalization of f it follows that the loss term reduces to $-f(v_1,t)$, *i.e.* the collision frequency is unity, and the dimensionless time t counts the average number of collisions per particle. Application of Bobylev's Fourier transform method to the Boltzmann equation for this case [11,25] yields the transformed equation

$$\partial_t\phi(k,t) = \int_n \phi(k_+,t)\phi(k_-,t) - \phi(k,t), \tag{5}$$

where the n-average is defined above, and the k-vectors are defined as

$$\begin{aligned} k_+ &= pk\cdot nn\,, \qquad & |k_+|^2 &= p^2k^2(\hat{k}\cdot n)^2\,, \\ k_- &= k - k_+\,, \qquad & |k_-|^2 &= k^2[1-q(\hat{k}\cdot n)^2]\,, \end{aligned} \tag{6}$$

where $p = \frac{1}{2}(1+\alpha)$ and $q = p(2-p)$ are positive numbers, and we have used the relation $\phi(0,t) = 1$. In one-dimension this equation simplifies to

$$\partial_t\phi(k,t) = \phi(pk,t)\phi((1-p)k,t) - \phi(k,t), \tag{7}$$

where $k_+ = pk$ and $k_- = (1-p)k$. We first illustrate our analysis for the one-dimensional case. Consider the equation for the rescaled Fourier transform $\tilde{\phi}(\kappa,t) = \phi(k,t)$ with $\kappa = v_0(t)k$. The scaling solution is the limiting form $\tilde{\phi}(\kappa,\infty) = \Phi(\kappa)$ for $t\to\infty$ at fixed $\kappa = v_0(t)k$. It satisfies the nonlinear equation

$$-\gamma k d\Phi(k)/\mathrm{d}k + \Phi(k) = \Phi(pk)\Phi((1-p)k), \tag{8}$$

where the exponent γ in $v_0(t) = v_0(0)\exp[-\gamma t]$ is still to be determined.

The requirement that the total energy be finite imposes the lower bound $a > 2$ on the exponent. We therefore make the ansatz that the dominant small-k singularity has the form

$$\Phi(k) = 1 - \tfrac{1}{2}\langle(k\cdot c)^2\rangle + A|k|^a, \tag{9}$$

insert this in eq. (8), and equate the coefficients of equal powers of k. This yields

$$a = \frac{1-p^a-(1-p)^a}{p(1-p)}. \tag{10}$$

The smallest root of this equation, satisfying $a > 2$, is $a = 3$, and A is left undetermined. Consequently, the scaling solution has a power law tail, $\tilde{f}(c) \sim 1/c^4$.

For general dimension we proceed in the same way as in the one-dimensional case, and obtain the equation for the scaling solution

$$-\gamma k d\Phi(k)/\mathrm{d}k + \Phi(k) = \int_n \Phi(k_+)\Phi(k_-). \tag{11}$$

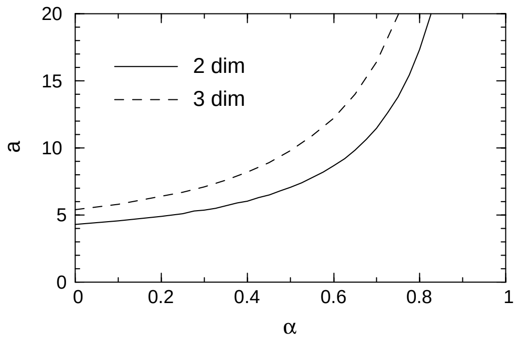

Fig. 1 – Non-trivial solution $a(\alpha)$ of eq. (15) as a function of α for 2 and 3 dimensions.

Inserting the ansatz (9) into (11), and equating the coefficients of equal powers of k^s with $s = \{2, a\}$ yields

$$s\gamma\langle|k\cdot c|^s\rangle = \int_n \langle|k\cdot c|^s - |k_+\cdot c|^s - |k_-\cdot c|^s\rangle. \tag{12}$$

In order to carry out the angular $\hat{c}$-average in $\langle|q\cdot c|^s\rangle$ with $q = \{k, k_+, k_-\}$ we choose q as polar axis, and denote $q\cdot c = q\, c\, \hat{q}\cdot\hat{c} = q\, c\, \cos\theta$, then $\langle|q\cdot c|^s\rangle = |q|^s\langle|c|^s\rangle K_s^{(d)}$, where $K_s^{(d)}$ is the average of $|\cos\theta|^s$ over a d-dimensional solid angle, which equals

$$K_s^{(d)} = \Gamma(\tfrac{1}{2}(s+1))\,\Gamma(\tfrac{1}{2}d)/\Gamma(\tfrac{1}{2}(s+d))\,\Gamma(\tfrac{1}{2}). \tag{13}$$

Finally we carry out the angular n-averages using (6), and obtain

$$\begin{aligned}\int_n |k_+|^s &= k^s p^s K_s^{(d)},\\ \int_n |k_-|^s &= k^s \int_n [1 - q(\hat{k}\cdot n)^2]^{s/2} \equiv k^s L_s^{(d)}(q).\end{aligned} \tag{14}$$

Insertion of these results in (12) for $s = 2$ yields

$$\gamma = \frac{1}{d}p(1-p) = \frac{1}{4d}(1-\alpha^2). \tag{15}$$

The exponent 2γ enters in Haff's law [19] for the granular temperature, *i.e.* $T(t) \sim v_0^2(t) \sim \exp[-2\gamma t]$, where time is measured in mean free times between collisions. To obtain the standard form of Haff's law $T(\tau) \sim 1/\tau^2$ for Maxwell molecules in terms of the external/laboratory time τ we refer to ref. [11]. For the exponent a, featuring in the power law tail of the scaling function $\tilde{f}(c) \sim 1/c^{a+d}$, we obtain from (12) for $s = a$ the transcendental equation

$$a = \frac{1 - p^a K_a^{(d)} - L_a^{(d)}(q)}{\frac{1}{d}p(1-p)}. \tag{16}$$

Here $a = 2$ is always a trivial solution, as follows from (12). The two most interesting cases are $d = 2, 3$, where

$$\begin{aligned}L_a^{(2)}(q) &= \frac{2}{\pi}\int_0^{\pi/2} d\theta[1 - q\cos^2\theta]^{a/2},\\ L_a^{(3)}(q) &= \int_0^1 \mathrm{d}x[1 - qx^2]^{a/2}.\end{aligned} \tag{17}$$

We look for the smallest solution $a(\alpha)$ of this transcendental equation with $a > 2$. The numerical solutions for $d = 2, 3$ are shown in fig. 1 as a function of α. If $p = \frac{1}{2}(1+\alpha) \uparrow 1$, the root $a(\alpha)$ moves to ∞, as it should, which is consistent with a Maxwellian tail distribution for the elastic case.

The simulations of the two-dimensional Maxwell-Boltzmann equation for the tail exponent, $a(\alpha = 0)+2$, show a *slow* approach to the theoretical value 6.2 [21]. However, at large velocities the statistical errors in the simulations become very large, and make a quantitative comparison with the analytical results difficult, specially for larger α-values.

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