

Velocity distributions in homogeneous granular fluids: the free and the heated case

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Abstract Non-Gaussian properties (cumulants, high energy tails) of the single particle velocity distribution for homogeneous granular fluids of inelastic hard spheres or disks are studied, based on the Enskog-Boltzmann equation for the unforced and heated case. The latter is in a steady state. The non-Gaussian corrections have small effects on the cooling rate, and on the stationary temperature in the heated case, at all inelasticities. The velocity distribution in the heated steady state exhibits a high energy tail $\sim \exp(-Ac^{3/2})$, where c is the velocity scaled by the thermal velocity and $A \sim 1/\sqrt{\epsilon}$ with ϵ the inelasticity. The results are compared with molecular dynamics simulations, as well as direct Monte Carlo simulations of the Boltzmann equation.

1 Introduction

Most theories for rapid granular flows are based on the assumption that the particle velocities are distributed according to a Gaussian or Maxwell distribution. Since granular particles collide inelastically, this assumption is not obvious. In fact, granular systems are typically in far from equilibrium states in the sense that an external driving force is necessary to maintain a stationary or periodic state. Only in systems of nearly elastic particles states close to equilibrium may be expected.

Deviations from Gaussian behavior in rapid granular flows have been studied in several contexts. Using molecular dynamics simulations, Goldhirsch et al. [1] measured the flatness or kurtosis of the velocity distribution function (VDF), defined by $\langle v^4 \rangle / \langle v^2 \rangle^2$, in a freely evolving fluid of inelastic hard spheres or disks (IHS), and found a broadening of the VDF when transitions to shearing or clustered states occurred. Brey et al. [2] measured higher

cumulants for the same system in the homogeneous cooling state (HCS) through direct Monte Carlo simulation of the Boltzmann equation, assuming that the Boltzmann equation remains meaningful for large inelasticity, $\epsilon = 1 - \alpha^2$, where α is the coefficient of normal restitution. These investigators have compared their simulation results with the theoretical results of the present paper, available through Ref. [3]. Several groups performed computer simulations of gas-fluidized or vibrated beds of grains, measured cumulants of the VDF [4], and observed power law behavior of the high energy tails [4, 5].

Analytic results derived from the Boltzmann equation are scarce. Wilkinson and Edwards [6] studied the VDF in the steady state of a Lorentz gas of independent granular particles, moving in a random array of fixed *inelastic* hard sphere scatterers, *driven* through gravity. They found that for small inelasticities, the VDF behaves dominantly as $\exp(-Av^4)$ with $A \sim \epsilon/g^2$, where g is the gravitational acceleration. Their VDF shows an underpopulation of the high energy tail as compared to the Maxwell distribution.

Goldshstein and Shapiro [7] solved the Boltzmann equation for the freely evolving IHS gas in the HCS by an expansion in Sonine polynomials. We return to their method below. For the same case, Esipov and Pöschel [8] determined the asymptotic form of the VDF at *large* velocities by obtaining a self-consistent solution of the nonlinear Boltzmann equation of the form $\mathcal{A} \exp[-Av/v_0(t)]$, showing an overpopulated tail distribution. Here $v_0(t)$ is the time dependent thermal velocity and $A \sim 1/\epsilon$. The coefficient $\mathcal{A}$ is left undetermined. The explicit form of the high energy tail for this case has been obtained in Ref. [9]. In fact, this asymptotic form of the VDF seems to have a more universal significance, as it is also found in systems of independent particles colliding with a dissipative (moving) container wall [10]. We shall return to this point in the conclusions. An enhanced population for large energies was also found by Brey et al. [11] from a BGK model kinetic equation for an undriven granular gas. This model shows algebraically decaying tails, as was found in fluidized beds of grains, with diverging velocity moments of degree $\geq 2/\epsilon$. The algebraic tail is obtained in both studies [5, 11] from an average $\int_0^\infty dx P(x) \exp(-xv^2)$ of a Gaussian distribution. Sela and Goldhirsch [12] have numerically obtained a perturbative solution of the Boltzmann equation for inelastic hard spheres to orders of $\mathcal{O}(\epsilon)$, $\mathcal{O}(\epsilon k)$, $\mathcal{O}(k^2)$. The order $\mathcal{O}(\epsilon)$ estimates the deviation from Gaussian behavior of the homogeneous solution and contributes to the rate of homogeneous cooling.

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The VDF has been studied for another type of granular flows, namely the uniformly heated IHS fluid, also referred to as random acceleration model, where each particle is subject to a random white force. This system possesses a spatially homogeneous steady state. The heated IHS fluid models properties of rapidly vibrated granular layers [13–16] and gas-fluidized beds of grains [4]. The one-dimensional version of this model has been studied in Refs. [13–15].

Peng and Ohta [16], and Trizac et al. [17] have carried out molecular dynamics simulations of two-dimensional heated IHS systems, and measured the high energy tails and fourth cumulants of the VDF. Recently, Santos et al. [18] have measured the same properties by direct Monte Carlo simulation of the new Boltzmann equation, where the Boltzmann collision term is supplemented with a Fokker-Planck diffusion term to account for the random accelerations, as proposed in section 3.

The goal of the present paper is to determine on the basis of the Enskog-Boltzmann equation the VDF of the homogeneous IHS fluid in the freely evolving (section 2) and uniformly heated case (section 3), as well as the corresponding high energy tails in section 4. The results are compared with existing simulation results (section 5), obtained either from molecular dynamics or direct Monte Carlo simulations of the Boltzmann equation.

The nonlinear Enskog-Boltzmann equation for the IHS system is solved for the freely evolving and the heated system of hard spheres and disks. To determine the cumulants we expand the VDF in Sonine polynomials, and derive equations for its moments. Before Goldshtein and Shapiro [7] calculated the fourth cumulant for the special case of (i) three dimensions, and (ii) a freely evolving gas. Unfortunately their result is incorrect (approximately a factor 5 too small at high inelasticity) except to $\mathcal{O}(\epsilon)$, due to an error in their calculations.

Comparing our calculation with the one presented in Ref. [12], we note that the results for the $\mathcal{O}(\epsilon)$ correction to the cooling rate are close. Whereas the calculation in Ref. [12] provides quantitative information on the VDF itself, ours provides quantitative information on its moments, and shows only qualitatively similar behavior of the VDF. The advantage of our method, however, is that it is nonperturbative in the inelasticity, i.e. the moments can be obtained for all values of the coefficient of restitution.

To discuss the high energy tail of the VDF we use an asymptotic method for solving the nonlinear Boltzmann equation, employed by Krook and Wu [19] to study the formation of Maxwellian tails in elastic systems with rapidly decreasing differential scattering cross sections at large impact energies. In doing so we obtain the tail distributions for the *free* and the *heated* case. The former one coincides with the result of Esipov and Pöschel [8].

Our starting point is the nonlinear Enskog-Boltzmann equation [20] for the single particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ in a dense system of inelastic hard spheres in d dimensions. In the absence of external forces, the *homogeneous* solution $f(\mathbf{v}, t)$ of this equation obeys

$$\begin{aligned} \partial_t f(\mathbf{v}_1, t) &= \chi \sigma^{d-1} \int d\mathbf{v}_2 \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \\ &\times \left\{ \frac{1}{\alpha^2} f(\mathbf{v}_1^{**}, t) f(\mathbf{v}_2^{**}, t) - f(\mathbf{v}_1, t) f(\mathbf{v}_2, t) \right\} \\ &\equiv \chi I(f, f). \end{aligned} \quad (1)$$

The prime on the $\hat{\sigma}$ integration denotes the condition $\mathbf{v}_{12} \cdot \hat{\sigma} > 0$, where $\hat{\sigma}$ is a unit vector along the line of centers of the colliding spheres at contact. In *direct* collisions of inelastic hard spheres with a coefficient of normal restitution α , the initial relative velocity $\mathbf{v}_{12}$ follows the inelastic reflection law $\mathbf{v}_{12}^* \cdot \hat{\sigma} = -\alpha \mathbf{v}_{12} \cdot \hat{\sigma}$. The gain term in (1) describes the *restituting* collisions, i.e. the precollision velocities $(\mathbf{v}_1^{**}, \mathbf{v}_2^{**})$ yield $(\mathbf{v}_1, \mathbf{v}_2)$ as postcollision ones with $\mathbf{v}_{12}^{**} \cdot \hat{\sigma} = -(1/\alpha) \mathbf{v}_{12} \cdot \hat{\sigma}$. Total momentum is conserved in a binary collision, and consequently in direct collisions

$$\begin{aligned} \mathbf{v}_1^* &= \mathbf{v}_1 - \frac{1}{2}(1 + \alpha)(\mathbf{v}_{12} \cdot \hat{\sigma})\hat{\sigma} \\ \mathbf{v}_2^* &= \mathbf{v}_2 + \frac{1}{2}(1 + \alpha)(\mathbf{v}_{12} \cdot \hat{\sigma})\hat{\sigma}, \end{aligned} \quad (2)$$

whereas $\mathbf{v}_i^{**}(\alpha) = \mathbf{v}_i^*(1/\alpha)$ in restituting collisions. The factor $1/\alpha^2$ in the gain term originates from the Jacobian $d\mathbf{v}_1^{**} d\mathbf{v}_2^{**} = (1/\alpha) d\mathbf{v}_1 d\mathbf{v}_2$ and from the length of the collision cylinder $|\mathbf{v}_{12}^{**} \cdot \hat{\sigma}| dt = (1/\alpha) |\mathbf{v}_{12} \cdot \hat{\sigma}| dt$.

Note that for the spatially homogeneous case, the only difference between the Enskog-Boltzmann equation for dense systems and the Boltzmann equation for dilute systems, is the presence of the factor $\chi(n)$, which is the pair correlation function of hard spheres or disks at contact. It accounts for the increased collision frequency in dense systems, caused by excluded volume effects.

For later reference we will also quote the equation for the rate of change of the average $\langle \psi \rangle = (1/n) \int d\mathbf{v} \psi(\mathbf{v}) f(\mathbf{v}, t)$, where the density $n = \int d\mathbf{v} f(\mathbf{v}, t)$. From (1) it follows as

$$\begin{aligned} \frac{d\langle \psi \rangle}{dt} &= \frac{\chi \sigma^{d-1}}{2n} \int d\mathbf{v}_1 d\mathbf{v}_2 \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) f(\mathbf{v}_1, t) f(\mathbf{v}_2, t) \\ &\times \Delta[\psi(\mathbf{v}_1) + \psi(\mathbf{v}_2)], \end{aligned} \quad (3)$$

where $\Delta\psi(\mathbf{v}_i) = \psi(\mathbf{v}_i^*) - \psi(\mathbf{v}_i)$ is the ψ change in a direct collision.

In the next section we study the solution of (1) for a freely evolving fluid. In the subsequent section a uniformly heated system of inelastic particles will be considered.

2 Homogeneous cooling state

For the freely evolving granular fluid, Goldshtein and Shapiro [7] have shown that Eq. (1) admits an isotropic scaling solution, describing the homogeneous cooling state, with a single particle distribution function depending on time only through the temperature $T(t)$ as

$$f(\mathbf{v}, t) = \frac{n}{v_0^d(t)} \tilde{f}\left(\frac{\mathbf{v}}{v_0(t)}\right), \quad (4)$$

where the thermal velocity $v_0(t)$ is defined in terms of the temperature by $T(t) = \frac{1}{2} m v_0^2(t)$, with

$$\frac{1}{2} dn T(t) = \int d\mathbf{v} \frac{1}{2} m v^2 f(\mathbf{v}, t), \quad (5)$$

and m the particle mass. Choosing $\psi = \frac{1}{2}mv_1^2$ in Eq. (3) we obtain for the rate of change of the temperature

$$\frac{dT}{dt} = -\frac{\mu_2}{d} m \chi n \sigma^{d-1} v_0^3 \equiv -2\gamma \omega_0 T. \quad (6)$$

Here ω_0 is the Enskog collision frequency for elastic hard spheres, defined as the average loss term in Eq. (1),

$$\omega_0 = \chi n \sigma^{d-1} \left\langle \int' d\hat{\sigma} (\mathbf{v}_{12} \cdot \hat{\sigma}) \right\rangle_0 = \frac{\Omega_d}{\sqrt{2\pi}} \chi n \sigma^{d-1} v_0, \quad (7)$$

where $\langle \dots \rangle_0$ denotes an average over Maxwellian velocity distributions for $\mathbf{v}_1$ and $\mathbf{v}_2$ at temperature $T = \frac{1}{2}mv_0^2$ and $\Omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface area of a d -dimensional unit sphere. The second equality in (6) defines the *time independent* dimensionless cooling rate as $\gamma \equiv (\sqrt{2\pi}/d\Omega_d)\mu_2$, where

$$\mu_p \equiv - \int d\mathbf{c}_1 c_1^p \tilde{I}(\tilde{f}, \tilde{f}) \quad (8)$$

are the moments of the dimensionless collision integral

$$\begin{aligned} \tilde{I}(\tilde{f}, \tilde{f}) \equiv & \int d\mathbf{c}_2 \int' d\hat{\sigma} (\mathbf{c}_{12} \cdot \hat{\sigma}) \\ & \times \left\{ \frac{1}{\alpha^2} \tilde{f}(c_1^{**}) \tilde{f}(c_2^{**}) - \tilde{f}(c_1) \tilde{f}(c_2) \right\}, \end{aligned} \quad (9)$$

with $\mathbf{c} = \mathbf{v}/v_0(t)$. Using Eqs. (4) and (6), the scaling form $\tilde{f}(c)$ satisfies the integral equation

$$\frac{\mu_2}{d} \left(d + c_1 \frac{d}{dc_1} \right) \tilde{f}(c_1) = \tilde{I}(\tilde{f}, \tilde{f}). \quad (10)$$

In the limit of small dissipation, the solution of (10) approaches a Maxwellian, i.e. $\tilde{f}(c) \approx \phi(c) \equiv \pi^{-d/2} \exp(-c^2)$. Therefore, a systematic approximation of the isotropic function $\tilde{f}(c)$ can be found by expanding it in a set of Sonine polynomials, i.e.

$$\tilde{f}(c) = \phi(c) \left\{ 1 + \sum_{p=1}^{\infty} a_p S_p(c^2) \right\}, \quad (11)$$

which satisfy the orthogonality relations

$$\int d\mathbf{c} \phi(c) S_p(c^2) S_{p'}(c^2) = \delta_{pp'} \mathcal{N}_p, \quad (12)$$

where $\delta_{pp'}$ is the Kronecker delta and $\mathcal{N}_p$ a normalization constant. For general dimensionality d , the first few Sonine polynomials are

$$S_0(x) = 1$$

$$S_1(x) = -x + \frac{1}{2}d$$

$$S_2(x) = \frac{1}{2}x^2 - \frac{1}{2}(d+2)x + \frac{1}{8}d(d+2). \quad (13)$$

The coefficients a_p are polynomial moments of the scaling function:

$$a_p = \frac{1}{\mathcal{N}_p} \int d\mathbf{c} S_p(c^2) \tilde{f}(c) \equiv \frac{1}{\mathcal{N}_p} \langle S_p(c^2) \rangle. \quad (14)$$

In particular $a_1 = (2/d)\langle S_1(c^2) \rangle = 0$, because the temperature definition (5) implies $\langle c^2 \rangle = \frac{1}{2}d$. Moreover, a_2 is

proportional to the fourth cumulant of the scaling form $\tilde{f}(c)$, i.e.

$$a_2 = \frac{4}{d(d+2)} [\langle c^4 \rangle - \frac{1}{4}d(d+2)] = \frac{4}{3} [\langle c_x^4 \rangle - 3\langle c_x^2 \rangle^2], \quad (15)$$

where we have used the relation, $\langle c_x^4 \rangle = 3\langle c^4 \rangle/[d(d+2)]$, valid for any isotropic distribution $\tilde{f}(c)$.

To determine the coefficients a_p we construct a set of equations for the moments

$$\langle c^p \rangle \equiv \int d\mathbf{c} c^p \tilde{f}(c), \quad (16)$$

by multiplying (10) with c_1^p ($p = 1, 2, \dots$) and integrating over $\mathbf{c}_1$. For the moments μ_p , defined in Eq. (8), we obtain

$$\begin{aligned} \mu_p &= -\frac{\mu_2}{d} \int d\mathbf{c} c^p \left(d + c \frac{d}{dc} \right) \tilde{f}(c) \\ &= \frac{\mu_2}{d} p \langle c^p \rangle, \end{aligned} \quad (17)$$

where the second line has been obtained by partial integration. For $p = 2$ the above equation reduces to a trivial identity because of the definition of temperature.

The quantities μ_2 , μ_p and $\langle c^p \rangle$ all depend on the unknown scaling function $\tilde{f}(c)$. To calculate a_2 from (17) we set $p = 4$, approximate the scaling form by $\tilde{f}(c) = \phi(c) \{1 + a_2 S_2(c^2)\}$, and evaluate μ_2 , μ_4 and $\langle c^4 \rangle$. The procedure is explained in more detail in the appendix and yields for general dimensionality d :

$$a_2 = \frac{16(1-\alpha)(1-2\alpha^2)}{9 + 24d + 8\alpha d - 41\alpha + 30(1-\alpha)\alpha^2}. \quad (18)$$

This result for a_2 is plotted in Fig. 1 as a function of α .

In principle one can continue this approximation scheme by setting $\tilde{f}(c) = \phi(c) \{1 + a_2 S_2(c^2) + a_3 S_3(c^2)\}$, and then using (17) for $p = 4$ and $p = 6$ to obtain two coupled equations for a_2 and a_3 , and solve the resulting equations to obtain better approximations for a_2 and a_3 than the previous ones, i.e. a_2 in (18) and $a_3 = 0$. As a_2 is already quite small, we do not calculate any higher coefficients a_p ($p \geq 3$) in (11).

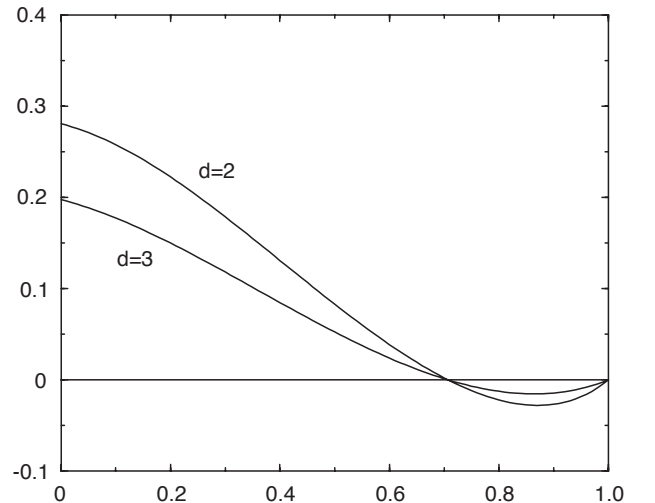


Fig. 1. Fourth cumulant a_2 versus α for homogeneous cooling solution in a freely evolving fluid

For the three-dimensional case Goldshtein and Shapiro [7] have calculated the coefficient a_2 and find the result

$$a_2^{\text{GS}} = \frac{16(1-\alpha)(1-2\alpha^2)}{401-337\alpha+190(1-\alpha)\alpha^2}. \quad (19)$$

This result is only correct to linear order in $1-\alpha$ as the authors made an error in their algebraic calculations¹. Their coefficient $|a_2^{\text{GS}}| \lesssim 0.04$ for all $\alpha \in (0, 1)$, whereas the correct coefficient obeys $|a_2| \lesssim 0.2$ for all α . However, the conclusion of Ref. [7] that the homogeneous scaling form is well approximated by a Maxwellian remains valid for a large range of coefficients of restitution (say $0.6 \lesssim \alpha < 1$). For these values we have $|a_2| \lesssim 0.04$ in three dimensions and $|a_2| \lesssim 0.024$ in two dimensions. Our result for a_2 has been quantitatively confirmed by the Direct Simulation Monte Carlo results of Brey et al. [2]. This will be discussed in section 5.

To obtain the time dependence of the temperature, it is convenient to introduce the new time variable τ representing the average number of collisions suffered per particle in a time t , and defined as $d\tau = \omega_0(T(t))dt$. This yields

$$\tau = \frac{1}{\gamma} \ln(1 + \gamma t/t_0). \quad (20)$$

Here $t_0 = 1/\omega_0(T_0)$ is the mean free time at the initial temperature $T(0) = T_0$. Next we find from Eq. (6)

$$T(t) = T_0 \exp(-2\gamma\tau) = \frac{T_0}{(1 + \gamma t/t_0)^2}. \quad (21)$$

In Eq. (A.6) of the appendix, we derive for the cooling rate $\gamma \equiv (\sqrt{2\pi}/d\Omega_d)\mu_2$:

$$\gamma = \gamma_0 \left\{ 1 + \frac{3}{16}a_2 \right\}, \quad (22)$$

where $\gamma_0 = (1-\alpha^2)/2d$. Sela and Goldhirsch [12] have performed a numerical perturbation expansion of the Boltzmann equation to first order in $\epsilon = 1 - \alpha^2$ and found the result $\gamma = \gamma_0(1 - 0.0258\epsilon + \mathcal{O}(\epsilon^2))$, which is close to the result $\gamma = \gamma_0(1 - 3\epsilon/128 + \mathcal{O}(\epsilon^2)) = \gamma_0(1 - 0.0234\epsilon + \mathcal{O}(\epsilon^2))$, obtained here. The method of appendix A also enables us to calculate the average collision frequency $\omega = \omega[\tilde{f}]$ in the homogeneous scaling state with the result

$$\omega = \omega_0 \left\{ 1 - \frac{1}{16}a_2 \right\}, \quad (23)$$

where the Enskog frequency ω_0 is defined in (7). Since the contribution from a_2 to γ and ω are small for all α , (22) and (23) are very well approximated by γ_0 and ω_0 , respectively.

3

Uniformly heated system

To study this system we start from the stochastic equations of motion

$$\frac{d\mathbf{v}_i}{dt} = \frac{\mathbf{F}_i}{m} + \hat{\xi}_i, \quad (24)$$

where $\mathbf{F}_i$ is the force due to collisions and $\hat{\xi}_i$ is the random acceleration due to external forcing, which is assumed

to be Gaussian white noise and uncorrelated for different particles, i.e.

$$\langle \hat{\xi}_{i\alpha}(t) \hat{\xi}_{j\beta}(t') \rangle = \xi_0^2 \delta_{ij} \delta_{\alpha\beta} \delta(t - t'), \quad (25)$$

where ξ_0^2 is the strength of the correlation. The validity of the above equations is based on the following assumptions: (i) the system is thermodynamically large, so that the condition $\sum_i \hat{\xi}_i(t) = 0$, imposed in computer simulations to guarantee momentum conservation in finite systems, can be ignored; (ii) the time between random kicks is small compared to the mean free time t_0 , and therefore much smaller than the characteristic cooling time t_0/γ [see Eq. (21)].

The Enskog-Boltzmann equation for the single particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ of a system heated in this way is corrected with a Fokker-Planck diffusion term (see e.g. Ref. [22]), representing the change of the distribution function caused by the small random kicks, and reads in the spatially homogeneous case:

$$\partial_t f(\mathbf{v}_1, t) = \chi I(f, f) + \frac{\xi_0^2}{2} \left(\frac{\partial}{\partial \mathbf{v}_1} \right)^2 f(\mathbf{v}_1, t). \quad (26)$$

The diffusion coefficient ξ_0^2 is proportional to the rate of energy input $\frac{d}{2}\xi_0^2$ per unit mass. The equation for the temperature balance can be derived from Eq. (26) in a similar fashion as in Eq. (6) for the cooling granular fluid, and reads

$$\frac{dT}{dt} = m\xi_0^2 - 2\gamma\omega_0 T. \quad (27)$$

We are looking for a stationary solution of (26), where the heating exactly balances the loss of energy due to collisions, and the temperature becomes time independent. Again it is convenient to introduce a scaled distribution function by

$$f(\mathbf{v}) = \frac{n}{v_0^d} \tilde{f} \left(\frac{\mathbf{v}}{v_0} \right), \quad (28)$$

where now the thermal velocity v_0 is time independent. Stationarity of $\tilde{f}$ then requires

$$\tilde{I}(\tilde{f}, \tilde{f}) + \frac{\xi_0^2}{2v_0^3 \chi n \sigma^{d-1}} \left(\frac{\partial}{\partial \mathbf{c}_1} \right)^2 \tilde{f}(c_1) = 0. \quad (29)$$

By multiplying this equation by c_1^p and integrating over $\mathbf{c}_1$, we obtain the following set of equations which couple the moments $\langle c^{p-2} \rangle$ of the distribution to the moments μ_p of the collision term, defined in Eq. (8):

$$\frac{\xi_0^2}{2v_0^3 \chi n \sigma^{d-1}} p(p+d-2) \langle c^{p-2} \rangle = \mu_p. \quad (30)$$

For $p = 2$ we recover the energy balance of Eq. (27), yielding for the stationary value of the thermal velocity in terms of μ_2 :

$$v_0 = \left(\frac{d\xi_0^2}{\mu_2 \chi n \sigma^{d-1}} \right)^{1/3}. \quad (31)$$

Note that in order to obtain a finite temperature in the limit $\alpha \rightarrow 1$, the α limit should be taken together with

¹ In the unpublished appendices to their article, Eq. (E.10) should read $A_2 = 96 + 90a_2$.

the limit $\xi_0^2 \rightarrow 0$. The above expression is used to write Eq. (30) in the form

$$\frac{\mu_2}{2d} p(p+d-2) \langle c^{p-2} \rangle = \mu_p. \quad (32)$$

Since $a_1 = 0$ by definition of the temperature, i.e. $\langle c^2 \rangle = \frac{1}{2}d$, the first correction to Gaussian behavior is coming from a_2 . To calculate it, we take $p = 4$ in Eq. (32), use expression (A.8) for μ_4 , and solve for a_2 to finally obtain the result

$$a_2 = \frac{16(1-\alpha)(1-2\alpha^2)}{73+56d-24\alpha d-105\alpha+30(1-\alpha)\alpha^2}. \quad (33)$$

This function is shown in Fig. 2 for the two- and three-dimensional case. Again we find only small corrections to a Maxwellian distribution ($a_2 < 0.086$ in two dimensions and 0.067 in three). Therefore to a good approximation, μ_2 is given by its zeroth order approximation and the stationary temperature is found from Eqs. (31) and (A.6) as

$$T_0 = m \left(\frac{d\xi_0^2 \sqrt{\pi}}{(1-\alpha^2)\Omega_d \chi n \sigma^{d-1}} \right)^{2/3}. \quad (34)$$

4

High energy tails

In this section we will derive the asymptotic solution of the Enskog-Boltzmann equation (29) for high velocities in case the granular fluid is uniformly heated. Esipov and Pöschel [8] have given a similar derivation for a freely evolving gas and found a high energy tail $\tilde{f}(c) \sim \exp(-Ac)$. The derivation in both cases proceeds along similar lines [19]. If particle 1 is a fast particle ($c_1 \gg 1$), the dominant contributions to the collision integral are collisions where particle 2 is typically in the thermal range, so that $\mathbf{c}_{12}$ in the collision integral $\tilde{I}(\tilde{f}, \tilde{f})$ in (9) can be replaced by $\mathbf{c}_1$. The gain term $\tilde{I}_g$ of the collision integral $\tilde{I}$ can then be neglected with respect to the loss term $\tilde{I}_l$, as will be verified a posteriori at the end of this section. The collision integral $\tilde{I}(\tilde{f}, \tilde{f})$ then reduces to $\tilde{I}_l \approx -\beta_1 c_1 \tilde{f}(c_1)$, with

$\beta_1 = \pi^{(d-1)/2} / \Gamma(\frac{1}{2}(d+1))$ as given in Eq. (A.3) of the appendix, and Eq. (10) simplifies to

$$\frac{\mu_2}{d} \left(d + c \frac{d}{dc} \right) \tilde{f}(c) = -\beta_1 c \tilde{f}(c). \quad (35)$$

The first term on the left hand side can be neglected with respect to the right hand side, and the large c solution has the form

$$\tilde{f}(c) \sim \mathcal{A} \exp \left(-\frac{\beta_1 d}{\mu_2} c \right), \quad (36)$$

where $\mathcal{A}$ is an undetermined integration constant. For $c \gg 1$ this solution corresponds to a tail which is overpopulated when compared to $\exp(-c^2)$ if $c \gtrsim 1/\epsilon$.

To determine the high energy tail of $\tilde{f}(c)$ for the uniformly heated system, we proceed in a similar fashion and use (31) to write Eq. (29) as

$$\tilde{I}(\tilde{f}, \tilde{f}) + \frac{\mu_2}{2d} \left(\frac{\partial}{\partial \mathbf{c}_1} \right)^2 \tilde{f}(c_1) = 0. \quad (37)$$

For large velocities c_1 , the collision integral can again be replaced by $-\beta_1 c_1 \tilde{f}(c_1)$, and Eq. (37) reduces to

$$-\beta_1 c \tilde{f}(c) + \frac{\mu_2}{2d} \left(\frac{d^2}{dc^2} + \frac{d-1}{c} \frac{d}{dc} \right) \tilde{f}(c) = 0, \quad (38)$$

where we have used isotropy of the distribution function. Inserting solutions of the form $\tilde{f}(c) \propto \exp(-Ac^B)$, we obtain the large c solution with $B = \frac{3}{2}$ and $A = \frac{2}{3} \sqrt{\frac{2d\beta_1}{\mu_2}}$, which is the only solution that vanishes for $c \rightarrow \infty$. Again we find an enhanced population for high energies.

To show that for $c_1 \gg 1$ the gain term can be neglected with respect to the loss term, we use the asymptotic collision dynamics

$$\begin{aligned} \mathbf{c}_1^{**} &= \mathbf{c}_1 - \frac{1}{2}(1+\alpha^{-1})(\mathbf{c}_1 \cdot \hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}} \\ \mathbf{c}_2^{**} &= \mathbf{c}_2 + \frac{1}{2}(1+\alpha^{-1})(\mathbf{c}_1 \cdot \hat{\boldsymbol{\sigma}})\hat{\boldsymbol{\sigma}}, \end{aligned} \quad (39)$$

where we have replaced $\mathbf{c}_{12}$ by $\mathbf{c}_1$. If $|\mathbf{c}_1 \cdot \hat{\boldsymbol{\sigma}}| \gg 1$, as is typically the case, $\mathbf{c}_2$ in (39) can be neglected and we have

$$\begin{aligned} \mathbf{c}_1^{**} &= c_1 \sqrt{1 - \frac{1}{4}(1+\alpha^{-1})(3-\alpha^{-1})(\hat{\mathbf{c}}_1 \cdot \hat{\boldsymbol{\sigma}})^2} \\ \mathbf{c}_2^{**} &= \frac{1}{2}(1+\alpha^{-1})c_1 |\hat{\mathbf{c}}_1 \cdot \hat{\boldsymbol{\sigma}}| \gg 1, \end{aligned} \quad (40)$$

where $\hat{\mathbf{c}}_1$ is a unit vector. To demonstrate that $\tilde{f}(c) \sim \exp(-Ac^B)$ is a consistent large c solution, both in the freely evolving case with $B = 1$ and in the heated case with $B = \frac{3}{2}$, we compare the factor $\tilde{f}(c_1^{**})\tilde{f}(c_2^{**})$ in $\tilde{I}_g$ with the factor $\tilde{f}(c_1)\tilde{f}(c_2)$ in $\tilde{I}_l$ for large c , i.e.

$$\frac{\tilde{f}(c_1^{**})\tilde{f}(c_2^{**})}{\tilde{f}(c_1)\tilde{f}(c_2)} \sim \exp \left\{ -A[(c_1^{**})^B + (c_2^{**})^B - c_1^B] \right\}. \quad (41)$$

The exponent is proportional to c_1^B and *strictly* negative for $\alpha < 1$ and $B < 2$, except for grazing collisions, where it vanishes. This happens inside a small θ interval J of length $\mathcal{O}(1/c_1)$ near $\theta = \pi/2$, where $|\mathbf{c}_1 \cdot \hat{\boldsymbol{\sigma}}| = c_1 \cos \theta \sim \mathcal{O}(1)$. Outside this interval the factor in (41) vanishes exponentially fast. Inside the interval J the factor in (41) is $\mathcal{O}(1)$. The contribution of this interval to the gain term

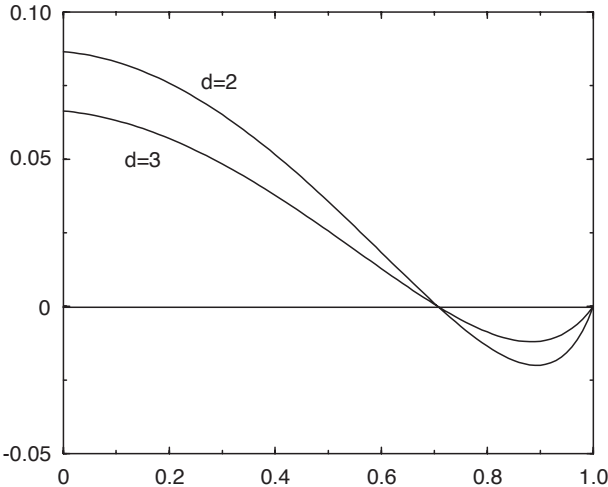


Fig. 2. Fourth cumulant a_2 versus α for the stationary state of a uniformly heated system

can be estimated as $\int_J d\theta c_1 \cos \theta \tilde{f}(c_1) \simeq \tilde{f}(c_1)/c_1$, where $c_1 \cos \theta \sim \mathcal{O}(1)$. Consequently, $\tilde{I}_g/\tilde{I}_l \sim 1/c_1^2$ for large c_1 .

In summary we have shown that $\tilde{f}(c) \sim \exp(-Ac^B)$ is a consistent large c solution of the Boltzmann Eqs. (10) and (29) with $B = 1$ and A given in (36) for the freely evolving fluid, and $B = \frac{3}{2}$ and A given below (38) for the heated fluid.

5

Comparison with simulations

In Refs. [1, 21], the undriven fluid of inelastic hard disks has been studied by molecular dynamics simulations. As long as the system is spatially homogeneous, measurements of the temperature decay confirm the validity of the homogeneous cooling law (21) where the cooling rate γ is given by its zeroth order approximation $\gamma_0 = \epsilon/2d$. Also in the initial homogeneous state, the measured number of collisions C among N particles in a time t is consistent with $\tau = 2C/N$ where τ is given by Eq. (20), implying that the collision frequency ω is very well approximated by its Enskog value ω_0 .

So far, molecular dynamics simulations have not been able to obtain sufficient statistical accuracy to determine the fourth moment or the high energy tail of the velocity distribution. Such measurements are possible, however, by means of the Direct Simulation Monte Carlo method for the Enskog-Boltzmann equation. Using this method, Brey et al. [2] have solved the nonlinear Boltzmann equation (1) for homogeneously cooling inelastic hard spheres ($d = 3$) and measured the fourth and sixth moment of the distribution $\tilde{f}(c)$. Again the measured temperature decay shows no deviations of the cooling rate γ from its Gaussian value γ_0 . Fig. 5 of Ref. [2] compares their simulation data for the fourth cumulant a_2 with (18), first derived in [3], and shows quantitative agreement. In particular, the fourth cumulant is predicted to vanish for $\alpha = 1/\sqrt{2}$, which is very close to the value observed in the simulations. Also note that the simulation results disagree with the prediction of Ref. [7]. Moreover, the approximation $\tilde{f}(c) = \phi(c)\{1 + a_2 S_2(c^2)\}$ shows good agreement with the simulation data for the functional form of $\tilde{f}$ (see Figs. 7 and 8 of Ref. [2]). This second Sonine approximation is qualitatively similar to the form presented in Fig. 3 of Ref. [12], calculated numerically to order $\mathcal{O}(\epsilon)$.

It is also interesting to compare our theoretical predictions with recent molecular dynamics results of Peng and Ohta [16] on the *heated* granular fluid. These authors have measured the temperature relaxation $T(t)$ in a fluid of N inelastic hard disks of mass $m = 2$ at an area fraction $\phi = \frac{1}{4}\pi\sigma^2 N/L^2 \simeq 0.16$ and heating rate $\xi_0^2 = (\delta V)^2/3\tau_H \simeq 1.67 \times 10^{-4}$, where the randomly added velocity components are sampled from a uniform distribution on the interval $(-\delta V, \delta V)$ where $\delta V = 10^{-3}$, measured in system length L per unit time, and $\tau_H = 2 \times 10^{-3}$ is the period between random kicks. For the pair distribution of hard disks at contact, χ , we use the approximate form [23] $\chi = (1 - \frac{7}{16}\phi)/(1 - \phi)^2 \simeq 1.32$. The steady state temperature predicted by Eq. (34) then becomes $T_0 = 1.15 \times 10^{-3}$ for $\alpha = 0.8$. The simulations

yield $T_0^{\text{sim}} \simeq 1.21 \times 10^{-3}$ (see Fig. 1 of Ref. [16]), in fair agreement with the Enskog theory.

Moreover, Eq. (34) predicts that T_0 depends on the heating rate $\xi_0^2 = (\delta V)^2/3\tau_H$ and inelasticity $\epsilon = 1 - \alpha^2$, as

$$T_0 = c_0 \left(\frac{(\delta V)^2}{\tau_H(1 - \alpha^2)} \right)^{2/3} \equiv c_0 \zeta^\lambda. \quad (42)$$

The measurements show an exponent $\lambda = 0.65 \pm 0.01$. The theoretical prediction (34) gives $c_0 \simeq 0.092$, which is again in fair agreement with the simulation result of Ref. [16] $c_0^{\text{sim}} \simeq 0.099$.

Eq. (27) also gives a prediction for the approach of $T(t)$ to T_0 . By observing that $\omega_0 \propto \sqrt{T}$ and *linearizing* Eq. (27) around T_0 , one obtains the solution $T(t) = T_0 + T_1 \exp(-t/\tau_0)$ with $\tau_0 = 2T_0/3m\xi_0^2$. For the parameters $\phi = 0.16$ and $\alpha = 0.8$ of Fig. 1 in Ref. [16] this yields $\tau_0 = 2.3$, and their simulations yield $\tau_0^{\text{sim}} = 1/b' = 2.6$.

Next, we compare the collision frequency ω_0 in (7) from the Enskog theory for elastic hard disks with the collision frequency ω^{sim} , measured in Ref. [16]. If there are C binary collisions among N particles in a time t , then the collision frequency is $2C/Nt$. The simulation results at $\alpha = 0.2, 0.4, 0.6, 0.7$ are respectively $\omega^{\text{sim}} \simeq 2.93, 1.67, 1.49, 1.49$, and the Enskog predictions for the same α values are $\omega_0 \simeq 1.17, 1.22, 1.33, 1.44$. The Enskog frequency $\omega_0 \sim \sqrt{T_0}$ decreases according to (42) with increasing $\epsilon = 1 - \alpha^2$, whereas ω^{sim} increases strongly with ϵ . The simulation results for ω^{sim} suggest that the Enskog theory gives reasonable predictions for $\alpha > 0.6$. Similar conclusions have been obtained by Orza et al. [21] for the homogeneous cooling state of a freely evolving fluid of inelastic hard disks. The deviations at larger inelasticities are probably caused by clustering and the onset of kinetic collapse, which strongly increases the collision frequency.

Finally, the overpopulation in the high energy tail $\sim \exp(-Ac^{3/2})$, with A given below (38), of the steady state distribution function has also been observed in the simulations by Peng and Ohta [16], but their statistical accuracy is too low to make any quantitative comparison. Preliminary results by Santos et al. [18] obtained by direct Monte Carlo simulation of the Boltzmann equation show quantitative agreement with our predictions for the fourth cumulant (33) and for the high energy tail.

6

Conclusions and outlook

We have investigated non-Gaussian behavior in granular fluids of smooth inelastic hard spheres or disks, both in the absence of an external forcing and in a system uniformly heated by random accelerations. In a freely evolving granular fluid, we find for all inelasticities very small corrections to the cooling rate and the collision frequency due to non-Gaussian characteristics of the homogeneous cooling state. As a consequence, such deviations have never been observed in computer simulations on homogeneous systems. Our result for the fourth cumulant has been confirmed by the computer simulations of Brey et al. [2] for the free case and by preliminary results of Santos et al. [18] for the heated case. These authors used the Direct Simulation Monte Carlo method to obtain an accurate

homogeneous solution of the nonlinear Enskog-Boltzmann equation.

Quantitative information on the high energy tail $\sim \exp[-Av/v_0(t)]$ in the freely evolving granular fluid is not yet available. However, it is interesting to observe that this asymptotic form has a more *universal* significance in the presence of dissipative interactions. It describes the high energy tail in an *unforced* Lorentz gas of independent particles, moving in a random array of fixed *inelastic* scatterers. It also occurs in a system of *independent* particles colliding with the moving wall of a container, as shown by Jarzynski and Swiatecki [10]. What are the common features in these problems? There exists a VDF that changes through collisions: of identical particles (freely evolving granular gas), of particles with an inelastic static environment (unforced inelastic Lorentz gas), or of particles with a moving wall, or more generally, of particles with a slowly changing random environment (random potential). Let the average energy per particle, E , change according to

$$\frac{dE}{dt} = \omega_0(t)\Delta E, \quad (43)$$

where $\omega_0 \sim nv_0$ is the typical collision frequency with $v_0 \sim \sqrt{E}$, and let the change in energy, ΔE , (gain or loss) in a single collision be *small* compared to E ($\epsilon \sim \Delta E/E \ll 1$). These conditions are satisfied for the cases of Ref. [10], the freely evolving granular gas (see Eq. (6) where $\Delta E \sim -2\gamma T$), and the unforced inelastic Lorentz gas. We *conjecture* that systems satisfying the above conditions have a *universal* tail distribution $\sim \exp[-Av/v_0(t)]$, that changes *adiabatically* on a time scale t_0/ϵ , much larger than the mean free time t_0 between collisions.

Long range spatial correlations in the velocity-velocity and density-density correlation functions, $G(r)$, measured in one- [13–15] and two-dimensional [16] simulations of heated granular fluids, are currently being analyzed for the two- and three-dimensional case by fluctuating hydrodynamics with external noise [17]. The analysis indicates that static structure factors diverge as $S(k) \sim 1/k^2$ at small wavenumbers k , corresponding to long range spatial correlations $G(r) \sim \ln r$ in two and $G(r) \sim 1/r$ in three dimensions. The approach of adding *external* noise has some similarity with the Edwards-Wilkinson model [24] for the growth of a granular surface on which particles are impinging at random. Here also structure factors $S(k) \sim 1/k^2$ have been found.

7

Appendix

In this appendix we calculate the quantities μ_2, μ_4 and $\langle c^4 \rangle$, which are required in (17) to calculate the coefficient a_2 in (11) by setting $\hat{f}(c) = \phi(c) \{1 + a_2 S_2(c^2)\}$, where $\phi(c)$ is the Maxwellian. In fact, the moment $\langle c^4 \rangle$ in (16) requires only moments of the Gaussian distribution. A straightforward calculation gives

$$\begin{aligned} \langle c^4 \rangle &= \int d\mathbf{c} c^4 \phi(c) \{1 + a_2 S_2(c^2)\} \\ &= \frac{1}{4}d(d+2) \{1 + a_2\}. \end{aligned} \quad (A.1)$$

Next we consider the moments μ_p ($p = 2, 4$) in (8). With

the help of Eq. (3) it can be transformed into

$$\begin{aligned} \mu_p &= -\frac{1}{2} \int d\mathbf{c}_1 \int d\mathbf{c}_2 \int' d\hat{\boldsymbol{\sigma}} (\mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}}) \phi(c_1) \phi(c_2) \\ &\quad \times \{1 + a_2 [S_2(c_1^2) + S_2(c_2^2)] + \mathcal{O}(a_2^2)\} \Delta(c_1^p + c_2^p), \end{aligned} \quad (A.2)$$

where the operator Δ is defined below Eq. (3). In the following, terms of $\mathcal{O}(a_2^2)$ will be neglected. For $\alpha \gtrsim 0.6$ this is a safe approximation as can be checked from the results Eqs. (18) and (33) for a_2 .

To evaluate (A.2) we introduce center of mass and relative velocities by $\mathbf{c}_1 = \mathbf{C} + \frac{1}{2}\mathbf{c}_{12}$ and $\mathbf{c}_2 = \mathbf{C} - \frac{1}{2}\mathbf{c}_{12}$. Moreover, we need the angular integral

$$\begin{aligned} \beta_n &\equiv \int' d\hat{\boldsymbol{\sigma}} (\hat{\mathbf{c}}_{12} \cdot \hat{\boldsymbol{\sigma}})^n = \frac{1}{2}\Omega_d \frac{\int' d\hat{\boldsymbol{\sigma}} (\cos \theta)^n}{\int' d\hat{\boldsymbol{\sigma}}} \\ &= \frac{1}{2}\Omega_d \frac{\int_0^{\pi/2} d\theta (\sin \theta)^{d-2} (\cos \theta)^n}{\int_0^{\pi/2} d\theta (\sin \theta)^{d-2}} = \pi^{\frac{d-1}{2}} \frac{\Gamma(\frac{n+1}{2})}{\Gamma(\frac{n+d}{2})}, \end{aligned} \quad (A.3)$$

where $\hat{\mathbf{c}}_{12} = \mathbf{c}_{12}/|\mathbf{c}_{12}|$ is a unit vector. Using the relations between Gaussian moments, it is straightforward to derive the relations:

$$\begin{aligned} \langle \mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}} C^2 \Delta C^n c_{12}^m \rangle_0 &= \frac{1}{4}(d+n) \langle \mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}} \Delta C^n c_{12}^m \rangle_0 \\ \langle \mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}} C^4 \Delta C^n c_{12}^m \rangle_0 &= \frac{1}{16}(d+n)(d+n+2) \\ &\quad \times \langle \mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}} \Delta C^n c_{12}^m \rangle_0, \end{aligned} \quad (A.4)$$

where

$$\begin{aligned} \langle \psi(\mathbf{c}_{12}, \mathbf{C}) \rangle_0 &\equiv \int d\mathbf{c}_{12} \frac{1}{(2\pi)^{d/2}} \exp(-\frac{1}{2}c_{12}^2) \\ &\quad \times \int d\mathbf{C} \left(\frac{2}{\pi}\right)^{d/2} \exp(-2C^2) \psi(\mathbf{c}_{12}, \mathbf{C}) \end{aligned} \quad (A.5)$$

denotes a Gaussian average over $\mathbf{c}_{12}$ and $\mathbf{C}$. The above formulas are very helpful in evaluating the moments μ_p in (A.2). With the help of (A.3) and (A.4) one finds

$$\begin{aligned} \mu_2 &= \frac{1}{4}(1 - \alpha^2) \beta_3 \langle c_{12}^3 \rangle_0 \{1 + \frac{3}{16}a_2\} \\ &= \frac{1}{2}(1 - \alpha^2) \frac{\Omega_d}{\sqrt{2\pi}} \{1 + \frac{3}{16}a_2\}. \end{aligned} \quad (A.6)$$

To calculate μ_4 we need the quantity

$$\begin{aligned} \Delta(c_1^4 + c_2^4) &= 2(1 + \alpha)^2 (\mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}})^2 (\mathbf{C} \cdot \hat{\boldsymbol{\sigma}})^2 \\ &\quad + \frac{1}{8}(\alpha^2 - 1)^2 (\mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}})^4 \\ &\quad + (\alpha^2 - 1)(\mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}})^2 C^2 \\ &\quad + \frac{1}{4}(\alpha^2 - 1)(\mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}})^2 c_{12}^2 \\ &\quad - 4(1 + \alpha)(\mathbf{c}_{12} \cdot \hat{\boldsymbol{\sigma}})(\mathbf{C} \cdot \hat{\boldsymbol{\sigma}})(\mathbf{C} \cdot \mathbf{c}_{12}). \end{aligned} \quad (A.7)$$

One finds after long and tedious calculations

$$\mu_4 = \beta_3 \langle c_{12}^3 \rangle_0 \{T_1 + a_2 T_2\}, \quad (A.8)$$

with

$$\begin{aligned} T_1 &= \frac{1}{4}(1 - \alpha^2)(d + \frac{3}{2} + \alpha^2) \\ T_2 &= \frac{3}{128}(1 - \alpha^2)(10d + 39 + 10\alpha^2) \\ &\quad + \frac{1}{4}(1 + \alpha)(d - 1). \end{aligned} \quad (A.9)$$

For the homogeneous cooling solution, inserting the results (A.1), (A.6) and (A.8) into (17) for $p = 4$ yields

a closed equation for a_2 . Neglecting again small contributions $\mathcal{O}(a_2^2)$, we solve for a_2 , and the result in (18) is recovered. Eq. (33) corresponding to uniform heating is found by inserting (A.6) and (A.8) into (32) for $p = 4$.

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