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Breakdown of the Sonine expansion for the velocity distribution of granular gases

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Abstract. – The velocity distribution of a granular gas is analyzed in terms of the Sonine polynomials expansion. We derive an analytical expression for the third Sonine coefficient a_3. In contrast to frequently used assumptions this coefficient is of the same order of magnitude as the second Sonine coefficient a_2. For small inelasticity the theoretical result is in good agreement with numerical simulations. The next-order Sonine coefficients a_4, a_5 and a_6 are determined numerically. While these coefficients are negligible for small dissipation, their magnitude grows rapidly with increasing inelasticity for $0 < \varepsilon \lesssim 0.6$. We conclude that this behavior of the Sonine coefficients manifests the breakdown of the Sonine polynomial expansion caused by the increasing impact of the overpopulated high-energy tail of the distribution function.

Introduction. – The velocity distribution of granular gases deviates from the Maxwell distribution, as described by Goldshtein and Shapiro [1]. This deviation depends on the coefficient of restitution ε, which quantifies the loss of energy for a collision of two particles i and j:

$$\vec{v}_i' = \vec{v}_i - \frac{1+\varepsilon}{2}\left[(\vec{v}_i - \vec{v}_j)\cdot\vec{e}\right]\vec{e}, \qquad \vec{v}_j' = \vec{v}_j + \frac{1+\varepsilon}{2}\left[(\vec{v}_i - \vec{v}_j)\cdot\vec{e}\right]\vec{e}. \tag{1}$$

Here $\vec{v}_i'$ and $\vec{v}_j'$ stand for the post-collisional velocities where the unit vector of the relative particle position at the collision instant is $\vec{e} \equiv (\vec{r}_i - \vec{r}_j)\,/\,|\vec{r}_i - \vec{r}_j|$.

The deviation from the Maxwell distribution may be described by a Sonine polynomials expansion [1–3]. This expansion is applicable to the main part of the velocity distribution, excluding the high-energy tails, which is known to be overpopulated with respect to the Maxwell distribution, *i.e.*, it decays as $\exp[-\text{const}\ v]$ [4].

Whereas non-Maxwellian velocity distributions are not surprising for non-equilibrium systems, the case of granular gases in the homogeneous cooling state (HCS) is special: It may be shown [4] that the distribution function $f(\vec{v})$ factorizes into a time-independent function $\tilde{f}(\vec{v}/v_T) \equiv \tilde{f}(\vec{c})$ and a prefactor which depends on the thermal velocity v_T. In this sense, by rescaling time, to keep v_T constant, a granular gas can be understood as an effectively equilibrium system. Nevertheless, in contrast to a molecular gas, $\tilde{f}(c)$ deviates from the Maxwell distribution. A granular gas heated uniformly by a Gaussian thermostat is equivalent to a gas in the HCS [5], hence the above arguments apply to heated granular gases as well.

So far it was silently accepted that the Sonine coefficients converge to zero with escalating order, so that it is sufficient to keep only the first few of them to achieve acceptable accuracy of the Sonine polynomials expansion. The contribution of the exponential tail to these coefficients was disregarded, *i.e.*, it was assumed that the exponential tail does not noticeably contribute to the coefficients. This assumption was supported by Direct Simulation Monte Carlo (DSMC) of the Boltzmann equation [6], as well as by Molecular Dynamics simulations of Granular Gases [7]. Up to now, however, neither the region of validity of the Sonine expansion, nor the impact of the exponential tail on the convergence of this series is known.

Huthmann, Orza, and Brito [7] derived a system of equations for the Sonine coefficients from the Boltzmann equation and solved it perturbatively with the assumption that the Sonine coefficient a_k is of the order $\mathcal{O}\left(\lambda^k\right)$ with λ being a small parameter. For $\varepsilon \gtrsim 0.6$ they obtained rapid decrease of the Sonine coefficients with escalating order k, while for smaller values of ε the high-order coefficients, $k \geq 3$, were not negligible and could be of the same order as the first non-trivial coefficient a_2. It was not evident, however, whether the Sonine polynomials expansion breaks down for $\varepsilon \lesssim 0.6$, or the perturbative approach based on the conjecture $a_k \sim \lambda^k$ was inadequate.

In the present study we derive the third Sonine coefficient, a_3, and address the relevance of the Sonine polynomials expansion analytically and numerically by means of DSMC. We show that the Sonine coefficients do not decrease with increasing $k \geq 3$ for $\varepsilon \lesssim 0.6$, which makes the Sonine series irrelevant, in the sense that it is not possible to describe the velocity distribution function using only a relatively small set of Sonine coefficients. We conclude that the breakdown of the Sonine expansion is caused by the increasing impact of the exponential tail for large dissipation.

Sonine polynomials expansion. – We consider a Granular Gas of particles of mass m which interact with a constant coefficient of restitution $\varepsilon = \text{const}$ and neglect their rotational degrees of freedom. We assume that the gas is in the HCS at number density $n = N/V$. We also assume that the velocity distribution function $f(\vec{v}, t)$ acquired its scaling form [1,4], *i.e.*

$$f(\vec{v}, t) = \frac{n}{v_T^d(t)} \tilde{f}(\vec{c}) \,, \qquad \vec{c} \equiv \frac{\vec{v}}{v_T(t)} \,, \tag{2}$$

where d is the system dimension and $v_T(t)$ is the thermal velocity due to the temperature $T(t)$,

$$\frac{d}{2} nT = \int \frac{mv^2}{2} f(v) \mathrm{d}\vec{v} = \frac{d}{2} n \frac{mv_T^2}{2} \,. \tag{3}$$

For $\varepsilon = \text{const}$ the Boltzmann equation reduces to two uncoupled equations, for the temperature and for the reduced distribution function $\tilde{f}(c)$ [1,4]. The first equation reads

$$\frac{\mathrm{d}T}{\mathrm{d}t} = -\frac{2}{d} g_2(\sigma) \sigma^{d-1} n v_T T \mu_2 \,, \tag{4}$$

where σ is the particle diameter. For $d = 3$, the contact value of the pair distribution function may be approximated by the Carnahan-Starling relation $g_2(\sigma) = (1 - \eta/2)/(1 - \eta)^3$ with the packing fraction $\eta = n\pi\sigma^3/6$, and

$$\mu_p \equiv -\int \mathrm{d}\vec{c}_1 c_1^p \tilde{I}(\tilde{f}, \tilde{f}) \tag{5}$$

denotes the moments of the dimensionless collision integral [2, 3, 8],

$$\tilde{I}\left(\tilde{f},\tilde{f}\right) \equiv \int d\vec{c}_2 \int d\vec{e}\,\Theta\left(-\vec{c}_{12}\cdot\vec{e}\right)\left|\vec{c}_{12}\cdot\vec{e}\right| \left[\frac{1}{\varepsilon^2}\tilde{f}(\vec{c}_1^{\,\prime\prime})\tilde{f}(\vec{c}_2^{\,\prime\prime}) - \tilde{f}(\vec{c}_1)\tilde{f}(\vec{c}_2)\right]. \tag{6}$$

The Heaviside function $\Theta(x)$ guarantees that only approaching particles collide, $|\vec{c}_{12}\cdot\vec{e}|$ gives the length of the collision cylinder and $\vec{c}_1^{\,\prime\prime}$ and $\vec{c}_2^{\,\prime\prime}$ denote the reduced velocities for the inverse collision, *i.e.*, for the collision which results at the reduced velocities $\vec{c}_1$ and $\vec{c}_2$ [9]. The second equation for the reduced distribution function reads [2, 3].

$$\frac{\mu_2}{d}\left(d + c_1\frac{\partial}{\partial c_1}\right)\tilde{f}\left(\vec{c}_1\right) = \tilde{I}(\tilde{f},\tilde{f}). \tag{7}$$

For the case of elastic collisions, $\varepsilon = 1$, the resulting velocity distribution is the Maxwell distribution. Therefore, for sufficiently large coefficient of restitution, $\varepsilon \to 1$, we may assume that $\tilde{f}(c)$ is close to the Maxwellian, $\phi(c) = \pi^{-d/2}\exp\left[-c^2\right]$. This suggests to expand the (unknown) distribution function $\tilde{f}(c)$ around $\phi(c)$ in terms of orthogonal polynomials $S_p(x)$:

$$\tilde{f}(c) = \phi(c)\varphi(c) = \phi(c)\left[1 + \sum_{p=1}^{\infty} a_p S_p\left(c^2\right)\right]. \tag{8}$$

We chose $S_p(x)$ to be the Sonine polynomials (see, *e.g.*, [9]):

$$S_p(x) = \sum_{n=0}^{p} \frac{(-1)^n (p+1/2)!}{(n+1/2)!(p-n)!n!} x^n. \tag{9}$$

The first few of them, relevant for this study, read

$$\begin{aligned} S_1(x) &= -x + \frac{1}{2}d, \qquad S_2(x) = \frac{1}{2}x^2 - \frac{1}{2}(d+2)x + \frac{1}{8}d(d+2),\\ S_3(x) &= -\frac{1}{6}x^3 + \frac{1}{4}(d+4)x^2 - \frac{1}{8}(d+2)(d+4)x + \frac{1}{48}d(d+2)(d+4). \end{aligned} \tag{10}$$

The expansion coefficients a_k characterize the deviation of the distribution function from the Maxwell distribution, namely, they quantify the deviation of the moments of the distribution function, $\langle c^p\rangle \equiv \int d\vec{c}c^p\tilde{f}(c)$, from the corresponding values for the Maxwell distribution. The equations for the moments may be found multiplying both sides of eq. (7) by c_1^p, integrating over $\vec{c}_1$, and using the orthogonality of the Sonine polynomials. This yields an infinite set of equations [2, 3, 9],

$$d\,\mu_p = \mu_2\, p\,\langle c^p\rangle, \qquad p = 2, 4, \ldots. \tag{11}$$

Since $\langle c^p\rangle$ and μ_p are expressed in terms of the Sonine coefficients, this set of equations can be used to determine the Sonine coefficients and, thus, to find the velocity distribution. To close the set of equations, a cutoff of the series (8) is applied, that is, it is assumed that the Sonine coefficients a_k with $k > k_0$ are negligible.

The first Sonine coefficient vanishes, $a_1 = 0$, according to the definition of temperature [1]. Since $\left\langle c^2\right\rangle = \frac{1}{2}d$, the first equation in eq. (11) for $p = 2$ gives the identity. The second equation in eq. (11) for $p = 4$ allows to find a_2 by expressing $\left\langle c^4\right\rangle$, μ_2 and μ_4 in terms of a_2 and neglecting all other coefficients a_3, $a_4, \ldots$ [1]. Hence the first non-trivial Sonine coefficient is a_2.

Second and third Sonine coefficients. – We write $\tilde{f}(c) = \phi(c)\left[1 + a_2 S_2(c^2) + a_3 S_3(c^2)\right]$ for the velocity distribution function by assuming that $a_4, a_5, \ldots$ are negligible. Further, we write eq. (11) for $p = 4$ and $p = 6$ and express all quantities in these two equations in terms of a_2 and a_3. In particular,

$$\left\langle c^4 \right\rangle = \frac{1}{4} d(d+2)(1+a_2)\,, \qquad \left\langle c^6 \right\rangle = \frac{1}{8} d(d+2)(d+4)(1+3a_2-a_3)\,. \tag{12}$$

To find the moments μ_2, μ_4, and μ_6 we recast eq. (5) using the properties of the collision integral (see, *e.g.*, [9]):

$$\mu_p = -\frac{1}{2}\int d\vec{c}_1 \int d\vec{c}_2 \int d\vec{e}\, \Theta\left(-\vec{c}_{12}\cdot\vec{e}\right)\left|\vec{c}_{12}\cdot\vec{e}\right| \tilde{f}(c_1)\tilde{f}\left(c_2\right) \Delta\left(c_1^p + c_2^p\right)\,, \tag{13}$$

where $\Delta\psi(\vec{c}_i) = \psi\left(\vec{c}_i^{\,\prime}\right) - \psi\left(\vec{c}_i\right)$ denotes the variation of some quantity $\psi\left(\vec{c}\right)$ in a direct collision. The evaluation of integrals of the form of eq. (13) was described in detail in [9]. Using this approach, analytical expressions for μ_2, μ_4, and μ_6 may be obtained, which are rather cumbersome. Since it is expected that $a_2 \gg a_2^2$, $a_3 \gg a_3^2$, $a_2 \gg a_2 a_3$, and $a_3 \gg a_2 a_3$, we keep in these moments only linear terms with respect to a_2 and a_3:

$$\begin{aligned} \mu_2 &= \frac{\pi^{d/2}}{\sqrt{2\pi}\,\Gamma(d/2)}\left(1-\varepsilon^2\right)\left[1 + \frac{3}{16}a_2 + \frac{1}{64}a_3\right], \\ \mu_4 &= \frac{\pi^{d/2}}{\sqrt{2\pi}\,\Gamma(d/2)}\left[T_1 + T_2 a_2 + T_3 a_3\right], \\ \mu_6 &= \frac{\pi^{d/2}}{\sqrt{2\pi}\,\Gamma(d/2)}\left[D_1 + D_2 a_2 + D_3 a_3\right], \end{aligned} \tag{14}$$

where

$$\begin{aligned} T_1 &= \left(1-\varepsilon^2\right)\left(d + \frac{3}{2} + \varepsilon^2\right), \\ T_2 &= \frac{3}{32}\left(1-\varepsilon^2\right)\left(10d + 10\varepsilon^2 + 39\right) + (1+\varepsilon)\,(d-1)\,, \\ T_3 &= \frac{\left(1-\varepsilon^2\right)}{128}\left(10\varepsilon^2 + 97\right) - \frac{(1+\varepsilon)\,(d-1)}{64}\,(21 - 5\varepsilon)\,, \\ D_1 &= \frac{3}{4}\left(1-\varepsilon^2\right)\left[\left(d+\varepsilon^2\right)\left(5+2\varepsilon^2\right) + d^2 + \frac{19}{4}\right], \\ D_2 &= \frac{3}{256}\left(1-\varepsilon^2\right)\left[1289 - 4\left(d+\varepsilon^2\right)\left(311+70\varepsilon^2\right) + 172d^2\right] + \frac{3}{4}B(\varepsilon), \\ D_3 &= -\frac{3}{1024}\left(1-\varepsilon^2\right)\left[2537 + 4\left(d+\varepsilon^2\right)\left(583+70\varepsilon^2\right) + 236d^2\right] - \frac{9}{16}B(\varepsilon), \\ B &= (1+\varepsilon)\left[(d-3)\left(3+4\varepsilon^2\right) + 2\left(d^2-\varepsilon\right)\right]\,. \end{aligned} \tag{15}$$

For $a_3 = 0$, the above equations for μ_2 and μ_4 coincide with the equivalent equations in [2,3].

Substituting eqs. (12), (14) and (15) into eqs. (11) for $p = 4$ and $p = 6$ we obtain the Sonine coefficients a_2 and a_3 in linear approximation. For $d = 3$, the result reads

$$\begin{aligned} a_2 &= -\frac{16}{b(\varepsilon)}\left(240\varepsilon^8 - 480\varepsilon^7 + 3312\varepsilon^6 - 7424\varepsilon^5 + 3510\varepsilon^4 - 364\varepsilon^3 + 895\varepsilon^2 + 1934\varepsilon - 1623\right), \\ a_3 &= -\frac{128}{b(\varepsilon)}\left(80\varepsilon^8 - 160\varepsilon^7 + 816\varepsilon^6 - 1600\varepsilon^5 + 154\varepsilon^4 + 1548\varepsilon^3 - 669\varepsilon^2 - 386\varepsilon + 217\right), \end{aligned} \tag{16}$$

$$b(\varepsilon) = 2800\varepsilon^8 - 5600\varepsilon^7 + 34800\varepsilon^6 - 84480\varepsilon^5 - 4410\varepsilon^4 + 25716\varepsilon^3 + 112155\varepsilon^2 - 172458\varepsilon + 214357.$$

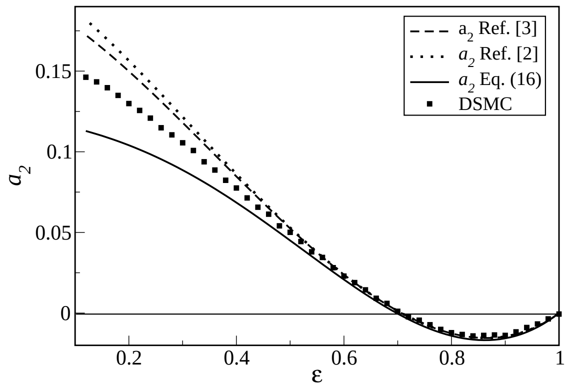

Fig. 1 – The second Sonine coefficient a_2 *vs.* the coefficient of restitution ε as given by eq. (16), where a_2 and a_3 are taken into account, $a_2(\varepsilon)$ from the linear theory, where only a_2 is taken into account [2], and $a_2(\varepsilon)$ from the corresponding non-linear theory [3], together with DSMC results.

DSMC simulations. – To check the predictions of the theory and to study the behavior of higher Sonine coefficients we perform Monte Carlo simulations of the Boltzmann equation (DSMC) using 2×10^7 particles of unit mass. The coefficient of restitution was varied in the interval $\varepsilon \in (0.1, 1)$ in steps of 0.01. To obtain smooth data, for each value of ε we performed 80 simulations and recorded the velocities of the particles when the system had reached a state with a scaling distribution function, eq. (2). From these snapshots we computed the temperature and the moments of the reduced distribution functions evaluating the averages

$$T = \frac{1}{3N} \sum_{i=1}^{N} \vec{v}_i \cdot \vec{v}_i \,, \qquad \left\langle c^{2k} \right\rangle = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{\vec{v}_i \cdot \vec{v}_i}{2T} \right)^k . \tag{17}$$

The Sonine coefficients can be computed using the relation (see, *e.g.*, [9])

$$\left\langle c^{2k} \right\rangle = \frac{(2k+1)!!}{2^k} \left(1 + \sum_{p=1}^{k} (-1)^p \frac{k!}{(k-p)!p!} a_p \right) . \tag{18}$$

Figure 1 shows a_2 as given by eq. (16) (which takes a_3 into account), a_2 as follows from the linear theory [2] and a_2 due to a non-linear theory [3] together with DSMC results. All approaches agree fairly well with the simulation results for small inelasticity, $\varepsilon \lesssim 0.6$, and deviate noticeably for larger dissipation. Figure 2 (left) shows a_3 due to eq. (16) together with the DSMC results. Again we see that the predictions of the new theory are in good agreement with the numerical results for $\varepsilon \gtrsim 0.6$. Similar numerical investigations of a_3 have been done by Montanero and Santos [5] for a uniformly heated granular gas and for HCS by Brey *et al.* [6] for $\varepsilon > 0.7$ and of a_3, a_4, a_5 by Nakanishi [10] for $\varepsilon > 0.9$.

Higher Sonine coefficients. – In fig. 2 (right) we present the high-order Sonine coefficients as functions of the coefficient of restitution $a_4(\varepsilon)$, $a_5(\varepsilon)$, and $a_6(\varepsilon)$. These coefficients are very small for $\varepsilon \lesssim 0.6$, which indicates the relevance of the Sonine expansion. For larger inelasticity, however, the absolute values of a_p, $p = 4, 5, 6$ increase with increasing p. Hence, fig. 2 suggests that for large inelasticity, $\varepsilon \lesssim 0.6$, the Sonine expansion is not relevant in the sense that one needs an infinite number of Sonine coefficients to describe the velocity

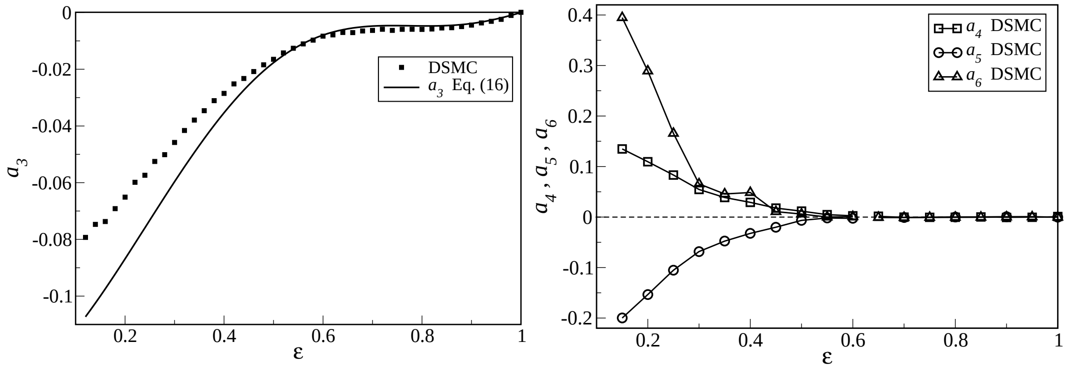

Fig. 2 – Left: the coefficient a_3 over the coefficient of restitution ε due to eq. (16) and to DSMC. Right: high-order Sonine coefficients as functions of ε (symbols). The lines guide the eye.

distribution for $c \in (0, \infty)$. A similar result was reported in [7], where the Sonine coefficients were found from the Boltzmann equation under the assumption $a_k \sim \lambda^k$ ($\lambda \ll 1$).

What is the reason for the breakdown of the Sonine expansion with increasing inelasticity? This happens due to the increasing impact of the overpopulated tail of the velocity distribution function [4], which reads for $c \gg 1$ [2,4]:

$$\tilde{f}(c) \sim Be^{-bc}\,; \qquad b = \frac{\pi^{(d-1)/2}d}{\Gamma\left(\frac{d+1}{2}\right)\mu_2}\,, \tag{19}$$

where μ_2 was defined above, while the prefactor B is unknown. For small ε the overpopulation starts at velocities not significantly larger than the thermal velocity. In this case the contribution to the moments $\langle c^{2k} \rangle$ from the exponential tail rapidly grows with increasing k, which entails the growth of a_k and ultimately, the breakdown of the Sonine expansion. Simulations show that the main part of the distribution with $c \sim 1$ has a crossover to the tail part, eq. (19), at $c \sim c^*$ [11], that is, the overpopulation of the tail starts at $c^* \sim b \sim 1/(1-\varepsilon^2)$ [11,12].

The breakdown of the Sonine expansion may be also understood from a simple mathematical argument: The Sonine expansion, eq. (8), contains only even powers of the scaled velocity c. The tail of the distribution decaying as $\exp[-c]$, however, cannot be represented by any finite series in even powers of c for the infinite interval (c^*, ∞). Hence, for any value of $\varepsilon < 1$, the presence of the exponential tail renders the Sonine expansion *irrelevant* for $c \to \infty$.

We illustrate this for $\varepsilon \lesssim 1$, where the tail starts at rather large velocity $c^* \gg 1$, and only high-order terms of the Sonine expansion, sensitive to large c, are affected. The corresponding high-order Sonine coefficients a_p are large. This follows from eqs. (8), (19) for $c \gg 1$:

$$\varphi(c) = \frac{\tilde{f}(c)}{\phi(c)} = 1 + \sum_{p=1}^{\infty} a_p S_p(c^2) \sim B\exp\left[-bc + c^2\right] \sim B\exp\left[c^2\right] = B\sum_{p=1}^{\infty}\frac{c^{2p}}{p!}\,, \tag{20}$$

while the Sonine polynomials may be approximated by their leading-order terms:

$$S_p \approx \frac{(-1)^p c^{2p}}{p!}\,, \qquad \text{thus} \qquad a_p \to (-1)^p B \quad \text{for} \quad p \gg 1\,. \tag{21}$$

Hence, even for $\varepsilon \lesssim 1$, the coefficients a_p do not converge to zero for $p \to \infty$ and an infinite number of terms is needed to describe the velocity distribution in the interval $c \in (c^*, \infty)$. The function $\tilde{f}(c)$ itself, however, is extremely small for these velocities. For larger inelasticity, that is, smaller ε, the value of c^* does not significantly exceed the thermal velocity. In this case, as shown above, already smaller Sonine coefficients such as a_3 to a_6 are large.

Nevertheless, the Sonine expansion remains a valuable tool for describing the main part of the velocity distribution, $\tilde{f}(c)$, for $c < c^*$ which is the range of interest in most cases. When considering the expansion up to a_6, the range $\varepsilon \in (0.6, 1)$ seems to be a safe interval for applying the Sonine expansion. For higher-order expansions, however, the range of validity may be restricted to a smaller interval. A more quantitative discussion will be given in [11]

Conclusion. – We derived the first two non-trivial Sonine coefficients as functions of the coefficient of restitution, $a_2(\varepsilon)$ and $a_3(\varepsilon)$, and show that a_3 is not negligible as compared to a_2 as it was assumed in previous theories. We show that for small inelasticity, $0.6 \lesssim \varepsilon < 1$, a_k with $k \geq 4$ are significantly smaller than a_2, a_3 and may be neglected. For this interval of ε the obtained theoretical values of a_2 and a_3 are in a good agreement with numerical results. We also find numerically the coefficients a_4, a_5, and a_6 for a wide range of the restitution coefficient, $0.1 \leq \varepsilon \leq 1$. For large inelasticity, $0 < \varepsilon \lesssim 0.6$, the high-order Sonine coefficient are of the same order as a_2, a_3 and, hence, may not be neglected. The increase and the subsequent saturation of the absolute value of the Sonine coefficients with escalating order is caused by the overpopulated tail. Its contribution to the moments of the distribution function and thus to the Sonine coefficients grows rapidly with increasing inelasticity and with the order of the moments, ultimately undermining the applicability of the Sonine polynomial expansion. The results of our study, addressed to granular gases in homogeneous cooling state, may be applied as well to driven granular gases with a Gaussian thermostat.

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