On the first Sonine correction for granular gases

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We consider the velocity distribution for a granular gas of inelastic hard spheres described by the Boltzmann equation. We investigate both the free of forcing case and a system heated by a stochastic force. We propose a new method to compute the first correction to Gaussian behavior in a Sonine polynomial expansion quantified by the fourth cumulant \( a_2 \). Our expressions are compared to previous results and to those obtained through the numerical solution of the Boltzmann equation. It is numerically shown that our method yields very accurate results for small velocities of the rescaled distribution. We finally discuss the ambiguities inherent to a linear approximation method in \( a_2 \).

Most theories of rapid granular flows consider a granular gas as an assembly of inelastic hard spheres and assume uncorrelated binary collisions described by the Boltzmann equation, with a possible Enskog correction to account for excluded volume effects. The deviations from the Maxwellian velocity distribution may be accounted for by an expansion in Sonine polynomials, and it is often sufficient to retain only the leading term in this expansion, quantified by \( a_2 \), the fourth cumulant of the velocity distribution. The purpose of this paper is to discuss the ambiguities—common to both approaches—encountered performing computations up to linear order in \( a_2 \), neglecting not only higher order Sonine contributions but also terms in \( a_k^2 \), \( k = 2, 3 \). Such an ambiguity has first been mentioned by Montanero and Santos.

Within the framework of the Boltzmann equation, the one-particle velocity distribution function \( f(\mathbf{v};t) \) for a homogeneous system free of forcing obeys the relation

\[
\partial_t f(\mathbf{v}_1; t) = I(f, f),
\]

where the collision integral reads

\[
I(f, f) = \sigma^{d-1} \int_{\mathbb{R}^d} d\mathbf{v}_2 \int d\mathbf{\hat{r}} \theta(\mathbf{\hat{r}} \cdot \mathbf{v}_{12}) (\mathbf{\hat{r}} \cdot \mathbf{v}_{12}) \left[ \frac{1}{\alpha^2} f(v^*_1; t)f(v^*_2; t) - f(\mathbf{v}_1; t)f(\mathbf{v}_2; t) \right].
\]

In Eq. (2), \( \sigma \) is the diameter of the particles, \( \theta \) the Heaviside distribution, \( \mathbf{v}_{12} = \mathbf{v}_1 - \mathbf{v}_2 \) the relative velocity of two particles, \( \mathbf{v}_{12} = v_{12}/v_{12}, \mathbf{v}_{12} = |\mathbf{v}_{12}| \), and \( \mathbf{\hat{r}} \) a unit vector joining the centers of the grains. The space dimension is \( d \).

The precollisional velocities \( \mathbf{v}_1^* \) and the postcollisional ones \( \mathbf{v}_i \) are related by

\[
\mathbf{v}_1^* = \mathbf{v}_1 - \frac{1+\alpha}{2\alpha} (\mathbf{v}_{12} \cdot \mathbf{\hat{r}}) \mathbf{\hat{r}},
\]

\[
\mathbf{v}_2^* = \mathbf{v}_2 + \frac{1+\alpha}{2\alpha} (\mathbf{v}_{12} \cdot \mathbf{\hat{r}}) \mathbf{\hat{r}},
\]

with \( \alpha \in [0, 1] \) the restitution coefficient. If energy is supplied to the system, an additional forcing term is present in Eq. (4), but the general arguments and method presented below remain valid. To be more specific, we shall also consider the situation where the system is driven into a non equilibrium steady state by a random force acting on the particles. With this energy feeding mechanism, coined “stochastic thermostat”, the Fokker-Planck term \( \xi_0^2 \nabla f \) should be added to the right-hand side (r.h.s.) of Eq. (4), where \( \xi_0 \) is related to the amplitude of the random force acting on the grains.

We are searching for an isotropic scaling solution \( \tilde{f}(c) \) of Eq. (2). The requirement of a time independent behavior with respect to the typical velocity \( v_0(t) = \sqrt{2(v^2)/d} \) imposes that

\[
f(\mathbf{v}; t) = \frac{n}{v_0(t)} \tilde{f}(c),
\]

where \( n \) is the number of particles.

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where the rescaled velocity is given by $c = v/v_0(t)$ and the angular brackets $\langle \cdot \rangle$ denote the average over $f(v;t)$. The presence of the density $a$ on the r.h.s. of Eq. (4) ensures that $\int df c f = 1$ and $\int dc^2 f(c) = d/2$. This scaling function describing the homogeneous cooling state satisfies the time-independent equation (2, 4, 8)

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

(5)

where

$$\mu_p = -\int_{\mathbb{R}^d} dc_1 c_1^p \tilde{I}(\tilde{f}, \tilde{f}),$$

(6)

and

$$\tilde{I}(\tilde{f}, \tilde{f}) = \int_{\mathbb{R}^d} dc_2 \int d\tilde{\sigma} \theta(\tilde{\sigma} \cdot \tilde{c}_{12})(\tilde{\sigma} \cdot c_{12}) \left[ \frac{1}{\alpha^2} f(c_1^*) f(c_2^*) - f(c_1) f(c_2) \right].$$

(7)

It is useful to consider the hierarchy of moment equations obtained by integrating Eq. (5) over $c_1$ with weight $c_1^p$ [4]

$$\mu_p = \frac{\mu_2}{d} p(c^p).$$

(8)

The solution of Eq. (5) is non-Gaussian in several respects. The high energy tail is overpopulated compared to the Maxwellian [4], a generic although not systematic feature for granular gases (a particular heating mechanism leading to an under-population at large velocities has been studied in [8]). Deviation from Gaussian behavior may also be observed at thermal scale or near the velocity origin. To study the latter correction, it is convenient to resort to a Sonine expansion for the distribution function $\tilde{f}(c)$ [10]

$$\tilde{f}(c) = M(c) \left[ 1 + \sum_{i \geq 1} a_i S_i(c^2) \right],$$

(9)

where $M(c) = \pi^{-d/2} \exp(-c^2)$ is the Maxwellian, and $S_i(c^2)$ the Sonine polynomials (that may be found in [15]; the first few are recalled in [3]). Due to the constraint $\langle c^2 \rangle = d/2$ the first correction $a_1$ vanishes [8], and for our purposes it is sufficient to know $S_2(x) = x^2/2 - (d + 2)x/2 + d(d + 2)/8$. From Eq. (10) and making use of the orthogonality of the Sonine polynomials with respect to a Gaussian measure, one may relate the coefficient $a_2$ to the kurtosis of the velocity distribution

$$\langle c^4 \rangle = \frac{d(d+2)}{4}(a_2 + 1),$$

(10)

so that, upon taking $p = 4$ in Eq. (5), we get

$$\mu_4 = (d+2)(1+a_2)\mu_2.$$  

(11)

In the following analysis, we will only retain the first correction in the expansion [2]: $\tilde{f} = M(1 + a_2 S_2)$. Computing $\mu_2$ and $\mu_4$ to linear order in $a_2$ with this functional ansatz [and further linearizing Eq. (11)], one deduces $a_2$ [4, 8]. This approach is nonperturbative in the restitution coefficient. However, since the high energy tail of $M(1 + a_2 S_2)$ is very distinct from that of the exact solution of Eq. (5), computing $a_2$ from relation (8) with $p > 4$ is expected to give a poor estimate, all the worse as $p$ increases. With this in mind, it appears that the limit of vanishing velocity of the rescaled Boltzmann equation (5) contains an interesting piece of information:

$$\mu_2 \tilde{f}(0) = \lim_{c_1 \to 0} \tilde{I}(\tilde{f}, \tilde{f}).$$

(12)

The main steps to compute this limit are given in appendix. Up to a geometrical prefactor, the loss term of $\lim \tilde{I}$ on the r.h.s. reads $\tilde{f}(0)(c_1)$ and is thus of lower order than the quantities appearing in (11). Working at linear order in $a_2$, one may therefore expect to achieve a better accuracy when computing the various terms (except may be the gain term) appearing in (12) than in (11). In the context of ballistic annihilation, a related remark lead to analytical predictions for the decay exponents of the dynamics and non-Gaussian features of the velocity statistics, in excellent agreement with the numerical simulations [15, 16]. In the present situation, the gain term of $\tilde{I}$ in (12) cannot be written as a collisional moment, so that the situation is less clear and deserves some investigation. We propose to
compare the value of \(a_2\) following this route to the standard one of Refs. 4, 8, 14. Evaluating (12) at first order in \(a_2\), we obtain:

\[
a_2 = \frac{4(\alpha^2 + 1)^2(\alpha^2 - 1)}{A(\alpha, d)}. \tag{13}
\]

where

\[
A(\alpha, d) = 5 + d(2 - d) + 8\alpha(\alpha^2 + 1)(d - 1) - \alpha^2(23 - 6d + d^2) + \alpha^4(3 + 6d + d^2) + \alpha^6(-1 + 2d + d^2) - \sqrt{2}(\alpha^2 + 1)^3(\alpha^2 - 1)(3 + 4d + 2d^2)/4. \tag{14}
\]

In Fig. 1, we compare this result with the analytical expression of van Noije and Ernst 4. We also display the fourth cumulant \(a_2\) obtained by Monte Carlo simulations from the numerical solution of the nonlinear Boltzmann equation (1) (so called DSMC technique 20, 21). Our expression appears more accurate at small inelasticity, but less satisfying close to elastic behavior. The smallest root of \(a_2 = 0\) obtained with Eq. (13) is \(\alpha^* = (\sqrt{2} - 1)^{1/2} \approx 0.643\ldots\). This root differs from the value \(\alpha^{**} = 1/\sqrt{2} \approx 0.707\ldots\) obtained upon solving (11) (both \(\alpha^*\) and \(\alpha^{**}\) do not depend on space dimension \(d\)). The inset shows that the exact root is located in the interval \(\alpha^*, \alpha^{**}\), and seems closer to \(\alpha^{**}\).

In order to understand the discrepancy close to the elastic limit shown in Fig. 1, it is useful to study the first Sonine correction \(\bar{f}(c_i)/M(c_i) = 1 + a_2S_2(c_i^2)\). The result for \(\alpha = 0.8\) where our method seems to be the less accurate is shown in Fig. 2 and in Fig. 3 for \(\alpha = 0.5\).

In spite of the imprecision of our analytical expression for \(a_2\) seen in Fig. 1, Fig. 2 shows that the limit method is very accurate for small velocities, but turns to quickly become more imprecise for bigger velocities. This suggests that computing the fourth cumulant from the limit of vanishing velocities gives more weight to this region which leads to a better behavior of the Sonine expansion for small velocities. On the other hand, the traditional route yields a global interpolation for all velocities. The good precision of our result for small velocities and the lower accuracy for higher velocities is confirmed in Fig. 3. Exploiting the above qualitative interpretation of the limit method, we expect to achieve a good accuracy using Eq. (13) in order to find the first moment 16:

\[
\langle |c| \rangle = \frac{\sqrt{\pi}}{2} \left( 1 - \frac{a_2}{8} \right). \tag{15}
\]

Indeed, we suppose that the function \(a_2\) obtained from the limit method gives a precise description of the rescaled velocity distribution for small velocities. Thus our \(a_2\) is likely to describe more accurately a low order velocity moment than a high order one. This is confirmed by Fig. 4.
As emphasized by Montanero and Santos, a certain degree of ambiguity is present when evaluating an identity such as (11) or (12) to first order in $a_2$. According to the way we rearrange the terms $\mu_4$, $\mu_2$, and $(d+2)(1+a_2)$ in say Eq. (11) and subsequently apply a Taylor series expansion in $a_2$, we obtain different predictions for $a_2(\alpha)$. For instance van Noije and Ernst did expand the relation (11), whereas Montanero and Santos also considered other possibilities such as $\mu_4/\mu_2 = (d+2)/(1+a_2)$ (this leads to a result which turns out to be fairly close to the one in [4]) and also $\mu_4/(1+a_2) = (d+2)\mu_2$. For small $\alpha$ in the latter case, the resulting $a_2$ turns out to be 20% lower than the previous ones, and very close to the exact (within Boltzmann’s equation framework) numerical results, for all the values of the restitution coefficient $\delta$. We push further this remark and show in Fig. 5 the eight simplest different possible functions $a_2(\alpha)$ obtained upon rearranging the terms of Eq. (11) and expanding the result to first
FIG. 4: First rescaled velocity moment $\langle |c| \rangle$ as a function of the restitution coefficient. DSMC is done for $10^5$ particles and approximately 500 collisions for each particle.

FIG. 5: The eight possible fourth cumulant $a_2$ obtained from Eq. (11), corresponding to the two-dimensional homogeneous free cooling. We define $\eta = (d+2)(1+a_2)$, then rewrite the equation $\mu_4 = \eta \mu_2$ according to the eight possible different combinations mentioned in the legend, before doing the linear Taylor expansion around $a_2 = 0$. The first curve is the plot of the function $a_2$ obtained by van Noije and Ernst [4], whereas the second one – obtained by Montanero and Santos [8] – is very close to the exact results shown by crosses.

order in $a_2$. A similar ambiguity is present making use of Eq. (12). The corresponding eight different possibilities are plotted in Fig. 6. It appears that the envelope of the curves following from this method is less spread than within the “traditional” route, by a factor of approximately 2. We thus achieve a better accuracy at small $\alpha$.

The dispersion of the curves in Figs. 5 and 6 illustrates the nonvalidity of the linearization approximation at small $\alpha$. However – and concentrating on Fig. 5 – it appears that all curves do not have the same status. Brilliantov and Pöschel have indeed solved analytically the full nonlinear problem [i.e. working again with the distribution function $\tilde{f} = M(1 + a_2 S_2)$ but keeping nonlinear terms in $a_2$], and obtained results that are very close to those of Noije/Ernst,
except for $\alpha < 0.2$ where they found slightly larger fourth cumulants $\beta$. Their result is therefore farther away from the exact one obtained by DSMC (see e.g. Fig. 1 where it appears than the Noije/Ernst expression already overestimates the exact curve). The difference between the DSMC results and those of Brilliantov/Pöschel therefore illustrates the relevance of Sonine terms $a_i$ with $i \geq 3$ in expansion $\beta$. However, some of the curves shown in Fig. 5 lie close to the exact one, which means that it is possible to correct the deficiencies of truncating $f$ at second Sonine order by an ad-hoc linearizing scheme. The agreement obtained is nevertheless incidental, and the corresponding analytical expression should be considered as a semi-empirical interpolation supported by numerical simulations. One should thus emphasize that the right way to compute $a_2$ is to use its definition involving the fourth rescaled velocity cumulant of Eq. (10) because this relation is not sensitive to higher order Sonine terms, nor to nonlinearities, even if this route doesn’t give the most accurate description in the small velocity domain (as seen from Figs. 2 and 3).

For completeness, we now briefly consider the stochastic thermostat situation $\beta$, where the counterpart of Eq. (5) reads

$$\frac{\mu^2}{2d} \nabla^2 c f(c_1) = \lim_{c_1 \to 0} \tilde{I}(\tilde{f}, \tilde{f}).$$

(16)

Considering again the limit $c_1 \to 0$ and retaining only the first correction in the expansion $\beta$, we get

$$\frac{\mu^2}{2\pi^{d/2}} \left[ 2 + a_2 \frac{(d+2)(d+4)}{4} \right] = \lim_{c_1 \to 0} \tilde{I}(\tilde{f}, \tilde{f}).$$

(17)

Given that the r.h.s. is already known from the free cooling calculation, it is straightforward to extend the previous results to the present case. As before, there are 8 possible ways to extract $a_2$ from Eq. (17) working at linear order. The resulting expressions are displayed in Fig. 7. On the other hand, the moment method described in Refs. $\beta$, $\beta$ makes use of the identity $\mu_2(d+2) = \mu_4$, that is a direct consequence of Eq. (16). There are thus 4 possible rearrangements leading to the different cumulants shown in the inset of Fig. 7. For comparison, we have also implemented Monte Carlo simulations in the present heated situation (see the crosses in Fig. 7). It is difficult to compare the dispersion of the curves with both methods (8 possibilities versus 4), since our approach makes use of Eq. (17) which is of higher order in $a_2$ than $\mu_2(d+2) = \mu_4$, the starting point used in Refs. $\beta$, $\beta$. Our method appears here less accurate than for the free cooling, with again an underestimation of $a_2$ at large $\alpha$.

In order to get free from the ambiguities inherent to a linear computation in $a_2$, we have also solved the full nonlinear problem. The computation becomes cumbersome, and since Brilliantov and Pöschel $\beta$ have already initiated this route in 3D for the homogeneous free cooling (thereby providing the calculation of $\mu_2$ and $\mu_4$), we will turn our attention to the 3D situation. First and for the sake of comparison, we have repeated the nonlinear derivation of Ref. $\beta$ for the stochastic thermostat. Second, we have computed the right-hand sides of Eqs. (12) and (17) without any...
linearization, from the form $\tilde{f} = M(1 + a_2 S_2)$. The left-hand sides only require the knowledge of $\mu_2$. For both free and forced situations, we subsequently obtain a polynomial equation of degree 3 for $a_2$ from which we extract the physical root, the two others corresponding to unstable scaling solutions [9]. The results are displayed in Fig. 8. In particular, our approach again suffers from an underestimation of $a_2$ for $\alpha > 0.5$, already observed within the linear computation, and that is thus ascribable to Sonine terms of order 3 or higher. In this respect, it is surprising that these terms do not affect similarly the moment method of Ref. [9] in the same range of inelasticities.

To sum up, using a new approach we obtain the first non-Gaussian correction $a_2$ to the scaled velocity distribution. In view of the above results, we conclude that our approach constitutes an improvement over the previous procedures in the small velocity regime, and our analysis turns to be technically simpler to perform. We have also discussed the
where the function $c$ and

$$
\text{with } \Gamma \text{ the gamma function.}
$$

Within the framework of the Sonine expansion (9), neglecting the coefficients

$$
\lim_{c_1 \to 0} \frac{I(\alpha \pi / 2)}{\Gamma((d + 1)/2)} = \pi^{(d-1)/2} I(I(\alpha / 2)) - \beta \langle c_2 \rangle,
$$

Eq. (A.2) becomes

$$
I = -\beta_1 \langle c_2 \rangle,
$$

where

$$
\beta_1 = \int_{\mathbb{R}^d} d\hat{\sigma} \theta(\hat{\sigma} \cdot \hat{c}_1) (\hat{\sigma} \cdot \hat{c}_2) = \frac{\pi^{(d-1)/2}}{\Gamma((d + 1)/2)},
$$

with $\Gamma$ the gamma function. Within the framework of the Sonine expansion (10), neglecting the coefficients $a_i$, $i \geq 3$, and making use of (10)

$$
\langle c_2 \rangle = \left(1 - \frac{\alpha_2}{8}\right) \frac{\Gamma((d + 1)/2)}{\Gamma(d/2)},
$$

Eq. (A.2) becomes

$$
I = -\frac{S_d M(0)}{2\sqrt{\pi}} \left[1 + \frac{d(d + 2)}{8} \right] \left(1 - \frac{\alpha_2}{8}\right),
$$

where $S_d = 2\pi^{d/2}/\Gamma(d/2)$ is the surface of the $d$-dimensional sphere.

Defining $\beta = (1 + \alpha)/(2\alpha) > 1$, the precollisional rescaled velocities $c_{i}^{*}$ and postcollisional ones $c_{i}$ are related by

$$
c_{i}^{*} = c_1 - \beta (c_{12} \cdot \hat{\sigma}) \hat{\sigma},
$$

$$
c_{2}^{*} = c_2 + \beta (c_{12} \cdot \hat{\sigma}) \hat{\sigma}.
$$

The gain term (A.10) thus becomes

$$
\tilde{I}_g = \frac{1}{\alpha^2} \int_{\mathbb{R}^d} d\hat{\sigma}_1 \theta(\hat{\sigma} \cdot \hat{c}_1) (\hat{\sigma} \cdot \hat{c}_2) \tilde{f} \left[\beta(\hat{c}_2 \cdot \hat{\sigma}) \tilde{f} \right] |c_2 - \beta (c_{12} \cdot \hat{\sigma}) | \hat{\sigma},
$$

where the function $\tilde{f}$ is isotropic. Performing the integration over $c_2$ before that over $\hat{\sigma}$, we choose the $x$ Cartesian coordinate as corresponding to the $\hat{\sigma}$ direction. The velocity $c_2$ is thus written $c_2 = c_x \hat{x} + c_{\perp}$, with $c_x = (c_2 \cdot \hat{\sigma}) \in \mathbb{R}$ and $c_{\perp} = c_2 - c_x \hat{x} \in \mathbb{R}^{d-1}$. Eq. (A.7) becomes

$$
\tilde{I}_g = \frac{1}{\alpha^2} \int_{\mathbb{R}^d} d\hat{\sigma}_1 \theta(c_x) \int_{\mathbb{R}^d} dc_{\perp} \tilde{f} (\beta c_{\perp} \hat{\sigma}) \tilde{f} (c_{\perp} - \beta c_x \hat{\sigma}),
$$

$$
= \frac{S_d}{\alpha^2} \int_0^{\infty} dc_x c_x \int_{\mathbb{R}^{d-1}} dc_{\perp} \tilde{f} (\beta c_{\perp}) \tilde{f} \left(\sqrt{c_{\perp}^2 + c_x^2 (1 - \beta)^2}\right).
$$
Eq. (A.9) is an exact relation within Boltzmann’s framework. Making use of the the Sonine expansion where we retain only the first correction $a_2$, Eq. (A.9) becomes

$$
\tilde{I}_g = \frac{S_d}{\alpha^2 \pi^d} \int_0^\infty dc_x e^{-\beta^2 + (1-\beta)^2} c_x^2 \int_{R^{d-1}} dc_\perp e^{-c_\perp^2} \left[ 1 + a_2 S_2(\beta^2 c_x^2) \right] \left\{ 1 + a_2 S_2 \left[ c_\perp^2 + c_x^2 (1-\beta)^2 \right] \right\}.
$$

(A.10)

With the definition of the second Sonine polynomial $S_2(x) = x^2/2 - (d+2)x/2 + d(d+2)/8$, one sees that Eq. (A.10) may be expressed as a sum of products of the integrals

$$
J_\perp(n) = \int_{R^{d-1}} dc_\perp e^{-c_\perp^2} c_\perp^n,
$$

(A.11a)

$$
J_x(n) = \int_0^\infty dc_x e^{-\left[ \beta^2 + (1-\beta)^2 \right] c_x^2} c_x^n,
$$

(A.11b)

that may be computed using the general relation ($a > 0$)

$$
\int_{R^d} d\mathbf{x} |x|^n e^{-ax^2} = \frac{\pi^{d/2}}{a^{(d+n)/2}} \frac{\Gamma \left[ (d+n)/2 \right]}{\Gamma(d/2)}.
$$

(A.12)

Tedious but technically simple calculations thus lead to

$$
\tilde{I}_g = \frac{S_d M(0)}{2 \sqrt{\pi}} \left[ \frac{2}{1 + \alpha^2} + a_2 D_1(\alpha, d) + a_2^2 D_2(\alpha, d) \right],
$$

(A.13)

where the final expressions $D_1(\alpha, d)$ and $D_2(\alpha, d)$ are too cumbersome to be given here. Finally, the limit $c_1 \to 0$ of Eq. (7) is given by the sums of Eqs. (A.5) and (A.13).

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