Velocity-correlation distributions in thermal and granular hard-core gases

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(Received 24 June 2008; revised manuscript received 27 August 2008; published 14 October 2008)

Collision statistics of hard-core systems (thermal and dissipative) is investigated through the velocity-correlation distributions after n collisions of a tagged hard-core particle: These quantities provide information on the velocity correlations for a given number of collisions. We obtain exact results for arbitrary dimension for the velocity-correlation distribution after the first collision as well as for the velocity-correlation function after an infinite number of collisions. For Gaussian velocity distributions, we show that the decay of the first-collision velocity-correlation distribution for negative argument is always exponential in any dimension; the decay rate is then a function of the mass and the coefficient of restitution. For granular gases, where deviations from Gaussian are relevant, expressions including Sonine corrections are also derived for the velocity-correlation distribution and a comparison with a direct simulation Monte Carlo (DSMC) shows accurate agreement with theoretical results. We emphasize that these quantities can be easily obtained in simulations and most likely also in experiments: therefore they could be an efficient probe of the local environment and of the degree of inelasticity of the collisions.

DOI: 10.1103/PhysRevE.78.041305 PACS number(s): 45.70.−n, 05.20.Dd, 51.10.+y, 02.50.−r

I. INTRODUCTION

The dynamics of hard-core particles consists of successive binary collisions. For atomic systems, the equilibrium state can be reached, and is characterized by velocity distributions which are purely Gaussian. Conversely, in the presence of dissipation, e.g., for granular particles, no equilibrium exists, but when an external source of energy is present the system reaches a steady state whose properties can be compared to the equilibrium state of atomic systems [1]. At low to intermediate densities, spatial correlations are not responsible for non-Gaussian deviations [2].

The short-time dynamics is usually analyzed by means of the velocity autocorrelation function. This quantity provides an average of the scalar product of the velocity at time 0 with the velocity at time t. For thermal systems at low density, the correlation function is generally not known exactly (with the only exception being the velocity correlation for one-dimensional systems [3]). Nevertheless, the characteristic time of the velocity correlation function corresponds to the time needed for the system to lose memory of the initial configuration of the velocities. Some progress has been made recently by investigating the collision statistics: Visco *et al.* [4,5] showed that the free flight time distribution is not exponential, even in the low-density limit (such a behavior was observed in molecular simulation of hard spheres some years ago [6]). Deviations from the Poisson law of the number of collisions can be captured in the framework of the Boltzmann equation and agree with molecular simulation results.

We introduce a quantity here by focusing on collision events irrespective of the time when individual collisions occur. We consider the scalar product between the velocity before a given collision and the velocity after n collisions. Note that this quantity is distinct from the distribution of velocities for a hard sphere on collision, which characterizes the distribution of the relative velocity of colliding spheres, for which Lue [7] obtained exact results in three, four, and five dimensions. The information obtained is not only the average of the scalar product, but the full distribution of the scalar product between the velocity before and after a sequence of n collisions. When $n=1$, this corresponds to the probability of the scalar product between the precollisional and post-collisional velocities during a collision; it is worth noting that the first moment of the distribution does not correspond to the velocity correlation function at the mean collision time: indeed, the probability distribution is built for collisions occurring at different collision times, whereas the velocity correlation function corresponds to the scalar product of the velocities at a given time.

As the number of collisions increases, the correlations between velocities decrease and the distribution evolves progressively to the limit where the velocities are uncorrelated. The paper is organized as follows. In Sec. II, we obtain the probability distributions in the limit of an infinite number of collisions, i.e., when the velocities are completely uncorrelated, in any spatial dimension. In Sec. III, we derive the first-collision velocity distribution in all dimensions. The corrections induced by the non-Gaussian behavior of granular systems are examined in Sec. IV, and analytical results are compared to DSMC results. Velocity-correlation distributions at the second and higher collisions are obtained in Sec. V and the approach to the limit of uncorrelated velocities is analyzed.

The central quantity of this study, the velocity-correlation distribution $P_n(z)$ at the nth collision is defined as

$$P_n(z) = \langle \delta(z - \mathbf{v} \cdot \mathbf{v}_n^*) \rangle, \tag{1}$$

where the brackets denote a statistical average in a given steady state, $\mathbf{v}$ denotes the precollisional velocity of a tagged particle before the first collision, and $\mathbf{v}_n^*$ the postcollisional velocity of the same particle after the nth collision. We only consider the case of homogeneous systems.

II. VELOCITY-CORRELATION DISTRIBUTION IN THE INFINITE COLLISION LIMIT

We first consider the situation where the number of collisions is very large, i.e., the velocity before the first collision and the velocity after a large number of collisions has become uncorrelated. The probability distribution of the scalar product $P_\infty(z=\mathbf{v}\cdot\mathbf{v}^*_\infty)$ is then given by

$$P_\infty(z) = \int\int d\mathbf{v}d\mathbf{v}^*_\infty f(\mathbf{v})f(\mathbf{v}^*_\infty)\delta(z-\mathbf{v}\cdot\mathbf{v}^*_\infty). \quad (2)$$

Let us consider the generating function $\tilde{P}_\infty(k) = \int dk e^{ikz}P_\infty(z)$. One has

$$\tilde{P}^{(d)}_\infty(k) = \int\int d\mathbf{v}d\mathbf{v}^*_\infty f(\mathbf{v})f(\mathbf{v}^*_\infty)e^{ik\mathbf{v}\cdot\mathbf{v}^*_\infty}. \quad (3)$$

We assume that the velocity distribution can be factorized as $f(\mathbf{v})=\Pi_{\alpha=1}^d f(v_\alpha)$, where α is an index running over all Cartesian components of the velocity and d the space dimension. For thermal isotropic systems, the velocity distribution $f(v)$ is always Gaussian

$$f(v) = \sqrt{\frac{M}{2\pi T}}e^{-Mv^2/2T}, \quad (4)$$

where M and T are the mass and the temperature of the particle, respectively. For granular systems, velocity distributions are not purely Gaussian. For thermal velocities, their deviations from Gaussian can be well captured systematically by introducing perturbative Sonine expansions. We show in Sec. V how the velocity-correlation functions are perturbatively modified by the insertion of Sonine corrections. Here, however, for the sake of simplicity, we restrict ourselves to the approximation of Gaussian velocity distribution for granular gases, as done by many authors [8–10].

Since the Cartesian components of the velocity are then independent random variables, the generating function $\tilde{P}^{(d)}_\infty(k)$ is simply the product of the generating functions of each Cartesian component

$$\tilde{P}^{(d)}_\infty(k) = (\tilde{P}^{(1)}_\infty(k))^d, \quad (5)$$

where $\tilde{P}^{(1)}_\infty(k)$ is the generating function for the one-dimensional problem.

The distribution $P^{(1)}_\infty(z)$ can be obtained from Eq. (2), which gives

$$P^{(1)}_\infty(z) = \int \frac{dv}{|v|}f(z/v)f(v). \quad (6)$$

It is worth noting that $P^{(1)}_\infty$ is the Mellin convolution of the two velocity distributions as this distribution is that of the product of two independent random variables.

$P^{(1)}_\infty(z)$ can be explicitly obtained and is then equal to

$$P^{(1)}_\infty(z) = \frac{MK_0\left(\frac{|z|M}{T}\right)}{\pi T}, \quad (7)$$

where $K_0(z)$ is the modified Bessel function of second kind. The basic property of $P^{(1)}_\infty$ is that the distribution is symmetric because the velocities are uncorrelated. The behavior of $P^{(1)}_\infty$ is intriguing at small values of z, as one observes a logarithmic divergence at $z=0$. This means that there is an overpopulated density of very small scalar products even though the velocity distribution remains finite for very small velocities. For large velocities, $P^{(1)}_\infty$ decays as $\exp(-|z|M/T)/\sqrt{z}$ for large values of z, i.e., less rapidly than the original velocity distribution which has a Gaussian decay.

In two and more dimensions, the velocity-correlation distribution can be obtained by noting that the Fourier transform of Eq. (7) [or integrating Eq. (3)], leads to

$$\tilde{P}^{(1)}_\infty(k) = \frac{1}{\sqrt{1+k^2}}. \quad (8)$$

By inserting Eq. (8) in Eq. (5), the generating function $\tilde{P}^{(d)}_\infty(k)$ in d dimensions is then

$$\tilde{P}^{(d)}_\infty(k) = (1+k^2)^{-d/2}. \quad (9)$$

The inverse Fourier transform can be calculated in any dimension: in 2D, the Fourier transform has a Lorentz profile, which gives in real space

$$P^{(2)}_\infty(z) = \frac{M\exp(-|z|M/T)}{2T} \quad (10)$$

and, in three dimensions,

$$P^{(3)}_\infty(z) = z\frac{MK_1\left(\frac{|z|M}{T}\right)}{\pi T}. \quad (11)$$

In two and three dimensions, the probability distribution is no longer singular at the origin. However, there exists a nonanalytic behavior which is a cusp in 2D and a cusp in the derivative in 3D. For completeness, the solution in odd dimensions; $P^{(d)}_\infty(z)$ is given by

$$P^{(d)}_\infty(z) = \sqrt{\frac{2}{\pi}}|z|^{(d-1)/2}\frac{(d-2)!}{2^{(d-3)/2}[(d-3)/2]!}K[(d-1)/2,|z|], \quad (12)$$

where $K[(d-1)/2,|z|]$ is the modified Bessel function of second kind of order $(d-1)/2$.

III. FIRST-COLLISION VELOCITY-CORRELATION DISTRIBUTION

In order to have tractable expressions for the first-collision velocity-correlation distribution $P_1(z)$, we assume that "molecular chaos" is valid, i.e., that there are no correlations between the particles before collision. The joint velocity distribution of the tagged particle and the bath particles is simply the product of the individual velocity distributions. Moreover, it is necessary to account for the rate of collisions which depends on the relative velocity at the point of impact as well as all possible collisions by summing over the locations of the impact on the sphere. $P_1(z)$ is then given by

$$P_1(z) = C\int_S \int\int d\mathbf{n}d\mathbf{u}d\mathbf{v}|(\mathbf{v}-\mathbf{u})\cdot\mathbf{n}|f(\mathbf{v}) \times f_B(\mathbf{u})\delta(z-\mathbf{v}\cdot\mathbf{v}^*), \quad (13)$$

where $f(\mathbf{v})$ and $f_B(\mathbf{u})$ are, respectively, the velocity distributions of the tagged and bath particles. The integral with the subscript S corresponds to the integration over the unit sphere with the restriction $(\mathbf{u}-\mathbf{v})\cdot\mathbf{n}<0$, where $\mathbf{n}$ is a unit vector along the axis joining the two centers of particles (this imposes that the particles are approaching each other before colliding). C is the normalization constant such that $\int_{-\infty}^{\infty}dzP_1(z)=1$.

The postcollisional velocity $\mathbf{v}^*$ is given by the collision rule which is

$$\mathbf{v}^* = \mathbf{v} + m\frac{1+\alpha}{m+M}[(\mathbf{u}-\mathbf{v})\cdot\mathbf{n}]\mathbf{n}, \quad (14)$$

where M and m are, respectively, the mass of the tagged and of the bath particles. α is the normal restitution coefficient lying between 0 and 1. For convenience [3,11,12], we introduce α' such that

$$\frac{1+\alpha'}{2} = m\frac{1+\alpha}{M+m}. \quad (15)$$

A. One dimension

In one dimension, the integral over angles is replaced by counting the right and left collisions. Therefore, Eq. (13) becomes

$$P_1^{(1)}(z) = C\int\int dudv|u-v|f(v)f_B(u)\delta(z-vv^*). \quad (16)$$

For granular gases when $\alpha<1$, even if the velocity distributions of the tagged particle and of the bath particle are Gaussian [13,14] (or close to the Gaussian profile [15]), the granular temperatures of these two particle species are always different. Let us denote by γ the ratio between the bath and the tagged particle temperatures. The velocity distribution of the two species read

$$f(v) = \sqrt{\frac{M}{2\pi T}}e^{-Mv^2/2\gamma T} \quad (17)$$

and

$$f_B(v) = \sqrt{\frac{m}{2\pi T}}e^{-mv^2/2T}. \quad (18)$$

It is necessary to distinguish the case $z<0$, where the distribution $P_1^{(1)}(z)$ is given by

$$P_1^{(1)}(z) = \frac{4C}{(1+\alpha')^2}\int dv\left(1-\frac{z}{v^2}\right)f(v) \times f_B\left(\frac{v(1-\alpha')}{1+\alpha'}-\frac{2z}{(1+\alpha')v}\right), \quad (19)$$

from the case $z>0$, where $P_1^{(1)}(z)$ is equal to

$$P_1^{(1)}(z) = \frac{4C}{(1+\alpha')^2}\left[\int_0^{\sqrt{z}}dv - \int_{\sqrt{z}}^{+\infty}\right]\left(\frac{z}{v^2}-1\right)f(v) \times f_B\left(\frac{v(1-\alpha')}{1+\alpha'}-\frac{2z}{(1+\alpha')v}\right). \quad (20)$$

Explicit integration over the velocity can be performed and more details of the calculation are given in Appendix A. Let us introduce

$$a = \sqrt{\frac{M}{\gamma T}+\frac{m}{T}\left(\frac{1-\alpha'}{1+\alpha'}\right)^2}, \quad (21)$$

$$b = \sqrt{\frac{m}{T}\left(\frac{2}{1+\alpha'}\right)^2}, \quad (22)$$

$$c = \frac{2m}{T}\frac{1-\alpha'}{(1+\alpha')^2}. \quad (23)$$

The first-collision velocity-correlation distribution $P_1^{(1)}(z)$ then reads for $z<0$

$$P_1^{(1)}(z) = P_1^{(1)}(0)e^{(ab+c)z} \quad (24)$$

and for $z>0$

$$P_1^{(1)}(z) = P_1^{(1)}(0)e^{cz}\left[\frac{a-b}{a+b}e^{-abz}\,\mathrm{erf}\left(\frac{a-b}{\sqrt{2}}\sqrt{z}\right) + e^{abz}\,\mathrm{erfc}\left(\frac{a+b}{\sqrt{2}}\sqrt{z}\right)\right], \quad (25)$$

where $P_1^{(1)}(0)$ is given by

$$P_1^{(1)}(0) = \frac{(a+b)(a^2b^2-c^2)}{2ab\sqrt{a^2+b^2-2c}}. \quad (26)$$

Note that $P_1^{(1)}(z)$ is always asymmetric, contrary to an uncorrelated velocity distribution; this results from the existence of correlations between precollisional and postcollisional velocities of a particle. Secondly, $P_1^{(1)}(z)$ is finite when z goes to 0, which is not the case for $P_\infty^{(1)}(z)$.

To simplify the above expressions (24) and (25) and to allow us to discuss the physical results, we now need to specify the temperature ratio γ. For inelastic particles in a polydisperse granular bath, γ is in general a complicated function of parameters such as the bath composition, the heating mechanism and the coefficient of restitution. However, three interesting limiting cases provide a simple expression of the temperature ratio.

(i) Monodisperse systems, for which $\gamma=1$ (in a Gaussian approximation).

(ii) A mixture of granular gases in the limit of infinite dilution. Martin and Piasecki [13] showed that the velocity distribution of an inelastic tracer in an elastic bath remains Gaussian with a granular temperature of the tracer given by the relation $T_{\rm eff}=\gamma T$ (equipartition does not hold); this ratio γ is given by

$$\gamma=\frac{M}{m}\frac{1+\alpha'}{3-\alpha'}. \tag{27}$$

(iii) Thermalized systems of elastic particles ($\alpha=1$), for which $P_1^{(1)}(z)$ provides nontrivial information about the short-time dynamics, even for equilibrium systems.

In the first case ($M=m$ and $\gamma=1$), $\alpha'=\alpha$. This gives for the first-collision velocity-correlation distribution, for $z<0$

$$P_1^{(1)}(z)=\frac{M}{T}\frac{2+\sqrt{2(1+\alpha^2)}}{2(1+\alpha)\sqrt{1+\alpha^2}}e^{2/(1+\alpha)^2(\sqrt{2(1+\alpha^2)}+1-\alpha)Mz/T} \tag{28}$$

and, for $z>0$,

$$\begin{aligned}P_1^{(1)}(z)=&\frac{M}{T}\frac{e^{[2(1-\alpha)/(1+\alpha)^2](Mz/T)}}{2(1+\alpha)\sqrt{1+\alpha^2}}\Bigg[[2-\sqrt{2(1+\alpha^2)}]\\&\times e^{-2/(1+\alpha)^2[\sqrt{2(1+\alpha^2)}]Mz/T}\\&\times\text{erf}\left(\frac{\sqrt{2}-\sqrt{(1+\alpha^2)}}{1+\alpha}\sqrt{\frac{Mz}{T}}\right)\\&+[2+\sqrt{2(1+\alpha^2)}]e^{2/(1+\alpha)^2[\sqrt{2(1+\alpha^2)}]Mz/T}\\&\times\text{erfc}\left(\frac{\sqrt{2}+\sqrt{(1+\alpha^2)}}{1+\alpha}\sqrt{\frac{Mz}{T}}\right)\Bigg].\end{aligned} \tag{29}$$

The decay of $P_1^{(1)}(z)$ also depends on both the temperature and the coefficient of restitution α.

In the second case (granular tracer in a thermalized bath), substituting Eq. (27) in Eqs. (21) and (22), one obtains $a=b=\sqrt{\frac{m}{T}}\frac{2}{1+\alpha'}$, which gives a simple expression for $P_1^{(1)}(z)$. For $z<0$

$$P_1^{(1)}(z)=\frac{m}{T}\frac{3-\alpha'}{(1+\alpha')^{3/2}}e^{[(3-\alpha')/(1+\alpha')^2](2mz/T)} \tag{30}$$

and for $z>0$

$$\begin{aligned}P_1^{(1)}(z)=&\frac{m}{T}\frac{3-\alpha'}{(1+\alpha')^{3/2}}e^{(2m/T)[(3-\alpha')/(1+\alpha')^2]z}\\&\times\text{erfc}\left(\frac{2}{1+\alpha'}\sqrt{\frac{2mz}{T}}\right).\end{aligned} \tag{31}$$

In order to show that the local environment influences the first-collision velocity-correlation distribution, we reexpress $P_1^{(1)}(z)$ in terms of the temperature of the tracer γT. Substituting Eq. (27) in Eqs. (30) and (31), one obtains for $z>0$, $P_1^{(1)}(z)=\frac{M}{\gamma T}\frac{1}{\sqrt{1+\alpha'}}e^{[1/(1+\alpha')](2Mz/\gamma T)}$. A comparison with Eq. (28) shows that $P_1^{(1)}(z)$ is sensitive to the heating procedure, the temperature of the tracer particle being the same in both cases.

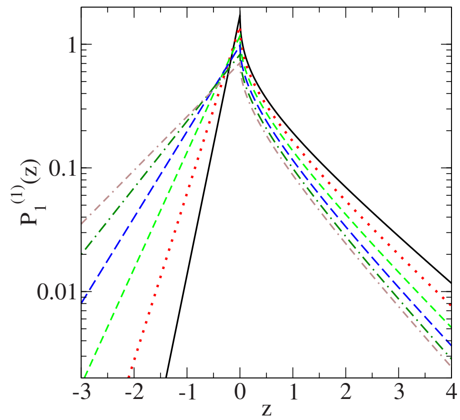

FIG. 1. (Color online) Log-linear plot of $P_1^{(1)}(z)$ versus z (M/T is set to 1) [Eqs. (28) and (29)]: Left, from top to bottom, the coefficient of restitution $\alpha=0,0.2,0.4,0.6,0.8,1$.

Finally, for elastic hard particles ($\alpha=1$), equipartition holds, $\gamma=1$, and therefore Eqs. (21)–(23) become $a=b=(M+m)/(2\sqrt{mT})$ and $c=(M^2-m^2)/(4mT)$, and $P_1^{(1)}(z)$ reads for $z<0$

$$P_1^{(1)}(z)=\frac{M}{2T}\sqrt{1+\frac{M}{m}}e^{[M(M+m)/2mT]z} \tag{32}$$

and for $z>0$

$$P_1^{(1)}(z)=\frac{M}{2T}\sqrt{1+\frac{M}{m}}e^{[M(M+m)/2mT]z}\,\text{erfc}\left((M+m)\sqrt{\frac{z}{2mT}}\right). \tag{33}$$

Figure 1 displays $P_1^{(1)}(z)$ as a function of z for different values of the coefficient of restitution $\alpha=0,0.2,0.4,0.6,0.8,1$ for a monodisperse system [Eqs. (28) and (29)]. For elastic hard particles, $P_1^{(1)}(z)$ is plotted in Fig. 2 as a function of z for different values of the mass ratio $m/M=1,1/2,1/5,1/10$.

Averaged quantities can be deduced from the first-collision distributions: The integral of $P_1^{(1)}(z)$ over $z<0$ cor-

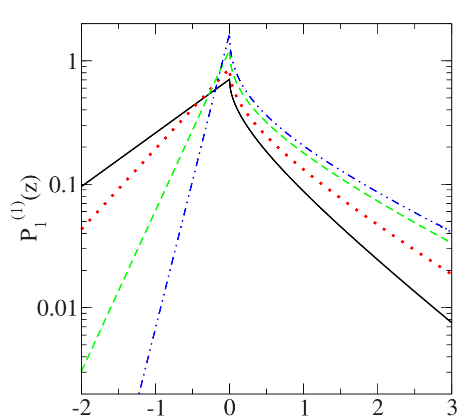

FIG. 2. (Color online) Log-linear plot of $P_1^{(1)}(z)$ versus z, for elastic hard spheres [Eqs. (32) and (33)]. The mass ratios are $\frac{m}{M}=1,\frac{1}{2},\frac{1}{5},\frac{1}{10}$ (on the left side, from top to bottom).

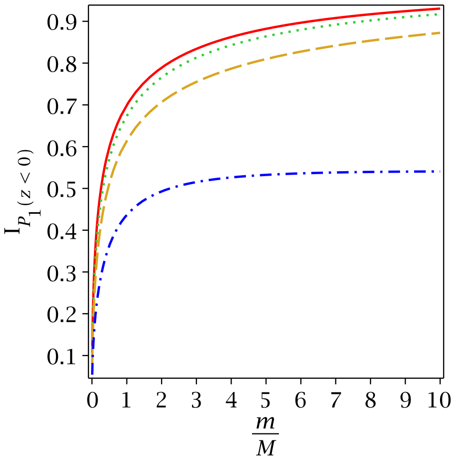

FIG. 3. (Color online) $I_{P_1^{(1)}(z<0)}$ versus mass ratio m/M for different values of the coefficient of restitution α: from top to bottom α=0.99,0.8,0.5,0.

responds to the fraction of events in which the particle velocity after collision is opposite to the precollisional velocity. Integrating Eq. (24) over all negative values of z leads to

$$I_{P_1^{(1)}(z<0)} = \frac{[M_2 + \sqrt{\gamma}(m+M)][M_2 - \sqrt{\gamma}(M - m\alpha)]}{(1+\alpha)M_2\sqrt{mM + \gamma m^2}} \quad (34)$$

with

$$M_2 = \sqrt{(1+\alpha)^2 mM + \gamma(M - m\alpha)^2}. \quad (35)$$

For elastic particles (i.e., $\alpha=1$), the fraction of collisions in which the post-collisional velocity has a direction opposite to that of the precollisional velocity becomes very simple because the equipartition property is satisfied ($\gamma=1$):

$$I_{P_1^{(1)}(z<0)} = \sqrt{\frac{m}{m+M}}. \quad (36)$$

Thus, for a monodisperse system, the probability of having a velocity inverted after a collision is higher than the probability of having a velocity whose direction is not changed by the collision [in one dimension (1D)].

For inelastic particles ($\alpha<1$), Fig. 3 shows that $I_{P_1^{(1)}(z<0)}$ increases with the mass ratio m/M for all values of α. For the sake of simplicity, γ is assumed to be equal to 1. Attention must be paid to the case $\alpha=0$: in this case, the limit of $I_{P_1^{(1)}(z<0)}$ when $m/M\to\infty$ is equal to $1/2$ whereas $I_{P_1^{(1)}(z<0)}$ tends to 1 when $m/M\to\infty$ if $\alpha>0$. This discontinuity is clearly apparent in Fig. 3.

B. Two dimensions

The first-collision velocity-correlation distribution can also be obtained analytically in two dimensions and above. Indeed the calculation can be performed following a method used in the one-dimensional case. Let us note that the scalar product of the precollisional and post-collisional velocities $\mathbf{v}\cdot\mathbf{v}^*$ can be expressed in an orthonormal basis associated with the collision as

$$\mathbf{v}\cdot\mathbf{v}^* = v_n v_n^* + v_t v_t^*, \quad (37)$$

where v_n and v_t denote the normal and tangential components of the velocity. The post-collisional quantities on the rhs of Eq. (37) can be eliminated by using Eq. (14):

$$\mathbf{v}\cdot\mathbf{v}^* = v_t^2 + \frac{1-\alpha'}{2}v_n^2 + \frac{1+\alpha'}{2}v_n u_n, \quad (38)$$

where u_n is the normal component of the velocity of the bath particle.

Since the normal and tangent components of the tracer particle are independent random variables, the integrals can be performed successively over u_n and v_n as in the one-dimensional case, provided that z is shifted to $z-v_t^2$. It is worth noting that the final integration over angular variables $(\mathbf{n})$ is trivial, since the integrand does not depend on $\mathbf{n}$.

For $z<0$, the decay of $P_1^{(2)}(z)$ remains exponential and is equal to

$$P_1^{(2)}(z) = P_1^{(1)}(0)\frac{e^{(ab+c)z}}{\sqrt{1+2(ab+c)\frac{\gamma T}{M}}}. \quad (39)$$

For $z>0$, $P_1^{(2)}(z)$ has two contributions

$$P_1^{(2)}(z) = \frac{P_1^{(1)}(0)e^{(ab+c)z}}{\sqrt{1+2(ab+c)\frac{\gamma T}{M}}}\operatorname{erfc}\left[\sqrt{z\left(\frac{M}{2\gamma T}+(ab+c)\right)}\right] + P_1^{(1)}(0)\sqrt{\frac{M}{2\pi\gamma T}}e^{cz}\int_0^z dy\frac{1}{\sqrt{y}}e^{-(M/2\gamma T+c)y} \times\left\{e^{ab(z-y)}\operatorname{erfc}\left[\frac{(a+b)\sqrt{(z-y)}}{\sqrt{2}}\right] + \frac{a-b}{a+b}e^{-ab(z-y)}\operatorname{erf}\left[\frac{(a-b)\sqrt{(z-y)}}{\sqrt{2}}\right]\right\}. \quad (40)$$

Note that $P_1^{(2)}(z)$ has an exponential decay when the scalar product of velocities is negative (i.e., $z<0$), with the same coefficient $(ab+c)$ as we obtained in one dimension. The integration over v_t only changes the normalization constant compared to the one-dimensional case. Conversely, for positive z, the shape of $P_1^{(2)}(z)$ is more complicated than in one dimension. As will be seen in the next section, the exponential decay of $P_1^{(2)}(z)$ is universal since this result is the same in any dimension and for different heating mechanisms (through the γ dependence). The fraction of events in which the scalar product between the precollisional and post-collisional velocities is negative is then given by

$$I_{P_1^{(2)}(z<0)} = \frac{(a+b)(ab-c)}{2ab\sqrt{a^2+b^2-2c}}\frac{1}{\sqrt{1+2(ab+c)\frac{\gamma T}{M}}}, \quad (41)$$

where a, b, and c are given by Eqs. (21)–(23).

For instance, for elastic hard particles, the fraction of events in which the scalar product is negative after a collision is given by

$$I_{P_1^{(2)}(z<0)} = \sqrt{\frac{m}{m+M}}\sqrt{\frac{m}{M+2m}}. \quad (42)$$

Therefore, for a monodisperse system $(m=M)$, $I_{P_1^{(2)}(z<0)} = 1/\sqrt{6} \simeq 0.40824\cdots$ in 2D whereas $I_{P_1^{(1)}(z<0)} = 1/\sqrt{2} \simeq 0.707\cdots$ in 1D. In other words, in 2D, most collisions do not change the scalar product sign, whereas the converse is observed in 1D.

C. Three dimensions

In three dimensions, the first-collision velocity-correlation distribution can be similarly derived. The scalar product between the precollisional and post-collisional velocities can be expressed as

$$\mathbf{v}\cdot\mathbf{v}^* = v_n v_n^* + v_t v_t^* + v_z v_z^* = \frac{1-\alpha'}{2}v_n^2 + \frac{1+\alpha'}{2}v_n u_n + v_t^2 + v_z^2, \quad (43)$$

where u_n is the normal component of the velocity of the bath particle. $P_1^{(3)}(z)$ is the probability distributions associated with the sum of two independent random variables. The first is the 1D collision term $\frac{1-\alpha'}{2}v_n^2 + \frac{1+\alpha'}{2}v_n u_n$ and the second is the sum $v_{1t}^2 + v_{1z}^2$, which is a χ_2^2-distributed variable and, as a result, an exponentially distributed variable

$$\chi_2^2(y) = \frac{M}{2\gamma T}e^{-My/2\gamma T}. \quad (44)$$

$P_1^{(3)}(z)$ can be expressed as the convolution of the two probability distributions of these variables. As the distributions are normalized, the distribution obtained via the convolution is normalized. For $z<0$,

$$P_1^{(3)}(z) = P_1^{(1)}(0)\frac{M}{2\gamma T}\int_0^{+\infty} dy e^{-My/2\gamma T}e^{(ab+c)(z-y)} = P_1^{(1)}(0)\frac{e^{(ab+c)z}}{1+2(ab+c)\frac{\gamma T}{M}} \quad (45)$$

and for $z>0$, $P_1^{(3)}(z)$ is the sum of several contributions

$$P_1^{(3)}(z) = P_1^{(1)}(0)\left[\frac{M}{\gamma T}\frac{e^{(ab+c)z}\,\mathrm{erfc}\left[\frac{(a+b)\sqrt{z}}{\sqrt{2}}\right]}{\frac{M}{\gamma T}+2(ab+c)} + \frac{M}{\gamma T}\frac{(b-a)e^{(-ab+c)z}\,\mathrm{erf}\left[\frac{(a-b)\sqrt{z}}{\sqrt{2}}\right]}{(a+b)\left(-\frac{M}{\gamma T}+2ab-2c\right)} + \frac{M}{\gamma T}\frac{4abe^{-Mz/2\gamma T}\sqrt{a^2+b^2-2c-\frac{M}{\gamma T}}\,\mathrm{erf}\left[\frac{\sqrt{z}\sqrt{a^2+b^2-2c-\frac{M}{\gamma T}}}{\sqrt{2}}\right]}{(a+b)\left(-\frac{M}{\gamma T}+2ab-2c\right)\left(\frac{M}{\gamma T}+2(ab+c)\right)}\right], \quad (46)$$

where a, b, and c are given by Eqs. (21)–(23) and γ is the temperature ratio.

As already noted, $P_1^{(3)}(z)$ has the same z dependence as in 1D and 2D when $z<0$. The influence of the dimension is in the amplitude factor which decreases when the dimension increases, the temperature and other microscopic parameters (masses, coefficient of restitution) being kept constant. From Eq. (45), the fraction of events with a negative scalar product of velocities can be exactly obtained; moreover, a general formula can be obtained in any dimension

$$I_{P_1^{(d)}(z<0)} = \frac{(a+b)(ab-c)}{2ab\sqrt{a^2+b^2-2c}}\left(1+2(ab+c)\frac{\gamma T}{M}\right)^{(1-d)/2}. \quad (47)$$

IV. INFLUENCE OF THE SONINE CORRECTIONS OF THE VELOCITY DISTRIBUTION ON $P_1^{(1)}(z)$

For granular gases, whose kinetic properties are well described by the Boltzmann equation, the velocity distribution is no longer a Gaussian. The deviations from Gaussian behavior can be captured by Sonine corrections. It is then possible to quantify the influence of these corrections on the distribution $P_1(z)$ (since the definition of the latter does not depend on the details of the velocity distribution function).

The nonlinear Boltzmann equation can be solved numerically by using a direct simulation Monte Carlo (DSMC) method [16,17]. We have performed DSMC simulations for monodisperse homogeneous systems excited through a stochastic thermostat. This allowed us to compare the distribution $P_1(z)$ obtained by simulation with the theoretical prediction calculated with a Sonine correction.

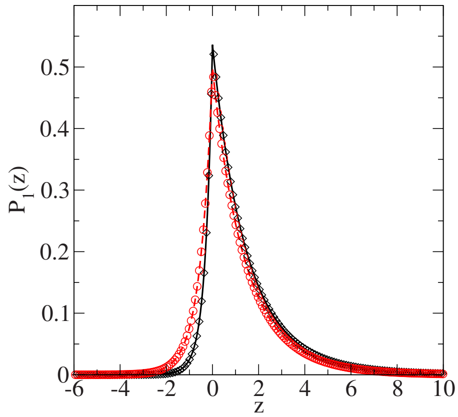

FIG. 4. (Color online) DSMC results (symbols) and theoretical predictions with the first Sonine correction (lines) for $P_1^{(2)}(z)$ versus $z=mv_1v_1'/T$ in 2D. Diamonds and circles correspond to the simulations for $\alpha=0.2,0.5$, respectively.

The calculation is similar to that of Eq. (19), but in the case studied here we no longer consider a tracer particle, so that $f=f_B$. Calculations were performed by considering only the first correction. This gives

$$f(\mathbf{v}) = \left(\frac{M}{2\pi T}\right)^{d/2} e^{-M\mathbf{v}^2/2T}\left[1 + a_2(\alpha) S_2\left(\frac{M\mathbf{v}^2}{2T}\right)\right], \quad (48)$$

where S_2 is the second Sonine polynomial expressed in the appropriate dimension. The value of $a_2(\alpha)$ is taken as equal to its usual approximation for the stochastic thermostat [17,18]. As the form of the perturbation introduced is simply a multiplicative polynomial, the expressions obtained for the 1D distribution $P_1^{(1)}(z)$ are analytical. As the result for $z>0$ is lengthy, we will only show that obtained for $z<0$, which is

$$P_1^{(1)}(z) = \frac{e^{(Mz/T)[2(1-\alpha+\sqrt{2}\sqrt{1+\alpha^2})/(1+\alpha)^2]}}{64\sqrt{2\pi}(1+\alpha+\alpha^2+\alpha^3)^3}\Bigg[Q(\alpha) + a_2(\alpha) \times\left(Q_0(\alpha) + \frac{Mz}{T}Q_1(\alpha) + \frac{M^2z^2}{T^2}Q_2(\alpha)\right)\Bigg], \quad (49)$$

where the $Q_i(\alpha)$'s are simple functions of α given in Appendix B.

Since the 2D case is closer to possible experimental systems, we have also included Sonine corrections to the velocity distribution for calculating the velocity-correlation distribution $P_1^{(2)}(z)$, but the lengthy expressions are not shown here. Figure 4 displays the analytical result [$P_1^{(2)}(z)$ with Sonine corrections] and the DSMC results for two values of the coefficient of restitution: $\alpha=0.2,0.5$. Even for the more inelastic case, the agreement between analytical results and DSMC is remarkable.

V. SECOND AND HIGHER-COLLISION VELOCITY-CORRELATION DISTRIBUTIONS

The collision statistics can be followed beyond the first-collision distribution. Formally, the second-collision velocity-correlation distribution $P_2(z)$ is given by the relation

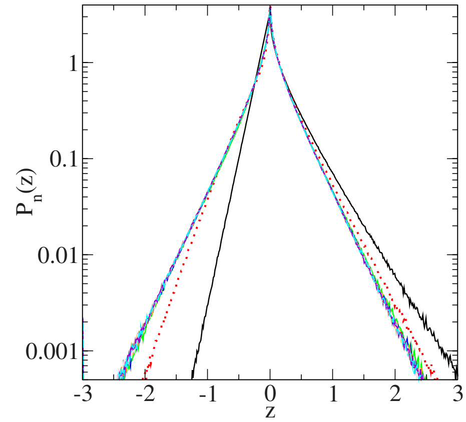

FIG. 5. (Color online) nth collision velocity-correlation distributions $P_n^{(1)}(z)$ versus z for various values of n: $n=1,2,\ldots,10$ ($D=1$).

$$P_2(z) = C_2\int_{S_1}\int_{S_2}\int\int d\mathbf{n}_1 d\mathbf{n}_2 d\mathbf{u}_1 d\mathbf{u}_2 d\mathbf{v}|(\mathbf{u}_1-\mathbf{v}_1)\cdot\mathbf{n}_1| \times|(\mathbf{u}_2-\mathbf{v}_1^*)\cdot\mathbf{n}_2| f(\mathbf{v}) f_B(\mathbf{u}_1) f_B(\mathbf{u}_2)\delta(z-\mathbf{v}\cdot\mathbf{v}_2^*), \quad (50)$$

where $\mathbf{v}_1$ denotes the precollisional velocity of the tagged particle for the first collision, $\mathbf{v}_1^*$ the velocity after the first collision and $\mathbf{v}_2^*$ the post-collisional velocity after the second collision. $\mathbf{u}_1$ and $\mathbf{u}_2$ correspond to the velocities of the bath particles for the first and second collisions, respectively. [Recall that $f(\mathbf{v})$ and $f_B(\mathbf{v})$ are the velocity distributions of the tagged and bath particles, respectively.] Obviously, $\mathbf{v}_2=\mathbf{v}_1^*$, and by using Eq. (14), the collision rule gives for the two collisions

$$\mathbf{v}_1^* = \mathbf{v}_1 + \frac{1+\alpha'}{2}[(\mathbf{u}_1-\mathbf{v}_1)\cdot\mathbf{n}_1]\mathbf{n}_1, \quad (51)$$

$$\mathbf{v}_2^* = \mathbf{v}_1^* + \frac{1+\alpha'}{2}[(\mathbf{u}_2-\mathbf{v}_2)\cdot\mathbf{n}_2]\mathbf{n}_2. \quad (52)$$

Finally, C_2 is the normalization constant ensuring that

$$\int_{-\infty}^{\infty} dz P_2^{(1)}(z) = 1. \quad (53)$$

In a similar way, it is possible to write down closed equations for $P_n(z)$. However, whereas tractable expressions have been obtained in any dimension for $P_1(z)$, the calculation increases drastically in complexity for obtaining the distribution at the second collision. In the restricted case where $\alpha'=1$ in one dimension, it is nonetheless possible to obtain the exact expression of $P_2^{(1)}(z)$ (details of the calculation are given in Appendix C). Thus, for $z<0$,

$$P_2^{(1)}(z) = C_2'\Bigg\{\left(\frac{e^{\sqrt{2}abz}}{a} + \frac{e^{b\sqrt{a^2+b^2}z}}{b}\right) + \frac{(1+b^2z)}{b} \times\int_0^\infty dv\frac{e^{-a^2v^2/2-b^2z^2/2v^2}}{v}\left[\mathrm{erfc}\left(\frac{bv}{\sqrt{2}}\right) + \mathrm{erf}\left(\frac{bz}{\sqrt{2}v}\right)\right]\Bigg\} \quad (54)$$

and for $z>0$,

$$P_2^{(1)}(z) = C_2'\Bigg\{\frac{\sqrt{2\pi}}{b^2}\left[\frac{e^{-\sqrt{2}abz}}{a}\,\mathrm{erf}\left(\frac{(\sqrt{2}a-2b)\sqrt{z}}{2}\right)\right] + \frac{e^{\sqrt{2}abz}}{a}\,\mathrm{erfc}\left(\frac{(\sqrt{2}a+2b)\sqrt{z}}{2}\right) - \frac{e^{-b\sqrt{a^2+b^2}z}}{b}\,\mathrm{erfc}\left(\frac{(-b+\sqrt{a^2+b^2})\sqrt{z}}{\sqrt{2}}\right) + \frac{e^{b\sqrt{a^2+b^2}z}}{b}\,\mathrm{erfc}\left(\frac{(b+\sqrt{a^2+b^2})\sqrt{z}}{\sqrt{2}}\right) + 2\frac{\sqrt{2\pi}(1+b^2z)}{b^3}\int_{\sqrt{z}}^{\infty} dv \frac{e^{-a^2v^2/2-b^2z^2/2v^2}}{v} \times\left[\mathrm{erfc}\left(\frac{bv}{\sqrt{2}}\right)+\mathrm{erf}\left(\frac{bz}{\sqrt{2}v}\right)\right]\Bigg\}, \quad (55)$$

where C_2' is determined from Eq. (53) and, with the help of Eqs. (21) and (22), $a=\sqrt{\frac{M}{\gamma T}}$ and $b=\sqrt{\frac{m}{T}}$. From Eqs. (54) and (55), one obtains the small-z expansion for $P_2^{(1)}(z)$:

$$P_2^{(1)}(z) \sim K_0\left(\sqrt{\frac{ab}{\gamma}}\frac{|z|}{T}\right). \quad (56)$$

Therefore, the second-collision velocity-correlation distribution shows a divergence at $z=0$, reminiscent of the divergence of $P_\infty^{(1)}(z)$, when the two velocities are completely uncorrelated. However, note that the coefficient of the modified Bessel function of the second kind $K_0(z)$ is ab instead of a^2 for $P_\infty^{(1)}(z)$. To continue the analysis of the velocity-correlation distributions in general, we have performed DSMC in various situations, and monitored several $P_n^{(1)}(z)$'s.

Figure 5 shows $P_n^{(1)}(z)$ as a function of z for $n=1, 2,\ldots,10$. Note that for $n\geqslant 3$, the distribution practically reaches the asymptotic value, namely, $P_\infty(z)$. A simple physical interpretation is that after three collisions the systems loses memory of its initial velocity configuration, and the correlation between the initial velocity and the velocity after n collisions vanishes when n is larger than 3. Similar plots are displayed in Figs. 6 and 7 for $P_n^{(2)}(z)$ and $P_n^{(3)}(z)$, respectively. Interestingly, the convergence to the asymptotic function $P_\infty(z)$ becomes slower when the space dimension increases.

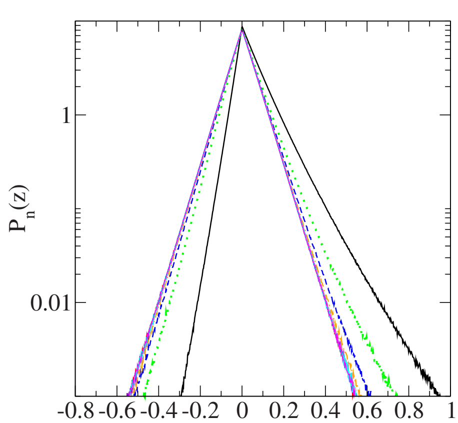

FIG. 6. (Color online) nth collision velocity-correlation distributions $P_n^{(2)}(z)$ versus z for various values of n: $n=1,2,\ldots,10$ ($D=2$).

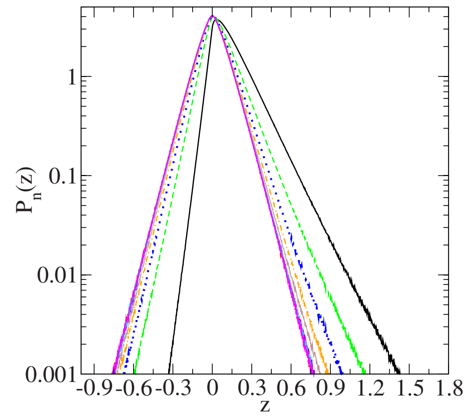

FIG. 7. (Color online) nth collision velocity-correlation distributions $P_n^{(3)}(z)$ versus z for various values of n: $n=1,2,\ldots,10$ ($D=3$).

VI. CONCLUSION

We have introduced velocity-correlation distributions that capture the early stages of the dynamics. These distributions are easily accessible in computer simulations. This should also be the case in experiments: provided that the framing rate is higher than the mean collision frequency, the probability that two collisions occur during a time step is small and the collision history could be monitored accurately. This would allow the measurement of the first-collision velocity-correlation distributions.

These nontrivial quantities have an interesting characteristic which is an exponential decay for negative scalar product of velocities, when the velocity distribution is Gaussian (corrections can be easily calculated for granular gases when the velocity distribution is no longer Gaussian). This exponential decay shows a very simple dependency on the system characteristics: particle mass, temperature, and dissipation. We therefore expect that these distributions could be efficient for probing the environment of a particle in granular gases. Since they give a direct access to a fundamental quantity related to one event, we believe they would be most appropriate to compare theory and experiments in granular systems.

ACKNOWLEDGMENTS

We thank Kristin Combs, Rhoda Hawkins, Jeffrey Olafsen, Julian Talbot, and Gilles Tarjus for suggestions and fruitful discussions.

APPENDIX A: 1D FIRST COLLISIONS

We have the following integrals for $z<0$:

$$\int_0^{+\infty} dv\left(1-\frac{z}{v^2}\right)\exp\left(-\frac{a^2v^2}{2}-\frac{b^2z^2}{2v^2}\right)=\frac{a+b}{ab}\sqrt{\frac{\pi}{2}}e^{abz} \tag{A1}$$

and, for $z>0$,

$$\int_0^{\sqrt{z}} dv\left(\frac{z}{v^2}-1\right)\exp\left(-\frac{a^2v^2}{2}-\frac{b^2z^2}{2v^2}\right) = \sqrt{\frac{\pi}{2}}\frac{1}{2ab}\left\{(a-b)e^{-abz}\left[\operatorname{erf}\left(\frac{a-b}{\sqrt{2}}\sqrt{z}\right)+1\right] + (a+b)e^{abz}\operatorname{erfc}\left(\frac{a+b}{\sqrt{2}}\sqrt{z}\right)\right\} \tag{A2}$$

and

$$\int_{\sqrt{z}}^{\infty} dv\left(1-\frac{z}{v^2}\right)\exp\left(\frac{a^2v^2}{2}-\frac{b^2z^2}{2v^2}\right) = \sqrt{\frac{\pi}{2}}\frac{1}{2ab}\left\{(a-b)e^{-abz}\left[\operatorname{erf}\left(\frac{a-b}{\sqrt{2}}\sqrt{z}\right)-1\right] + (a+b)e^{abz}\operatorname{erfc}\left(\frac{a+b}{\sqrt{2}}\sqrt{z}\right)\right\}, \tag{A3}$$

which gives for $z<0$

$$P_1^{(1)}(z)=\frac{4C}{(1+\alpha')^2}\frac{a+b}{ab}e^{(ab+c)z} \tag{A4}$$

and for $z>0$

$$P_1^{(1)}(z)=\frac{4C}{(1+\alpha')^2}\sqrt{\frac{\pi}{2}}e^{cz}\left\{\frac{a-b}{ab}e^{-abz}\left[\operatorname{erf}\left(\frac{a-b}{\sqrt{2}}\sqrt{z}\right)\right] + \frac{a+b}{ab}e^{abz}\operatorname{erfc}\left(\frac{a+b}{\sqrt{2}}\sqrt{z}\right)\right\}. \tag{A5}$$

The constant C can be obtained by calculating the normalization condition $\int dzP_1(z)=1$, which gives

$$C=\frac{(1+\alpha')^2}{4}\frac{a^2b^2-c^2}{\sqrt{2\pi(a^2+b^2-2c)}}. \tag{A6}$$

APPENDIX B: SONINE CORRECTION TO THE 1D CALCULATION

For $z<0$, one finds

$$P_1^{(1)}(z)=e^{[2(1-\alpha)/(1+\alpha)^2](Mz/T)}C\int_0^{\infty} du\left(1-\frac{z}{u^2}\right) \times\exp\left[-\frac{M}{T}\left(\frac{(1+\alpha^2)u^2}{(1+\alpha)^2}+\frac{2z^2}{u^2(1+\alpha)^2}\right)\right] \times\left\{1+a_2(\alpha)\left[S_2\left(\frac{Mu^2}{2T}\right) + S_2\left(\frac{Mu^2}{T}\frac{(2z/u^2-(1-\alpha))^2}{2(1+\alpha)^2}\right)\right]\right\}. \tag{B1}$$

After integration of Eq. (B1), one obtains

$$P_1^{(1)}(z)=\frac{P_1(0)}{Q(\alpha)+a_2(\alpha)Q_0(\alpha)}e^{(Mz/T)[2(1-\alpha+\sqrt{2}\sqrt{1+\alpha^2})/(1+\alpha)^2]} \times\left[Q(\alpha)+a_2(\alpha)\left(Q_0(\alpha)+\frac{Mz}{T}Q_1(\alpha) + \frac{M^2z^2}{T^2}Q_2(\alpha)\right)\right], \tag{B2}$$

where

$$Q(\alpha)=16(1+\alpha)^4(1+\alpha^2)^2(1+\alpha^2+\sqrt{2}\sqrt{1+\alpha^2}), \tag{B3}$$

$$Q_0(\alpha)=3(1+\alpha)^4[2+6\alpha^2+6\alpha^4+2\alpha^6 + \sqrt{2}\sqrt{1+\alpha^2}(1+6\alpha^2+\alpha^4)], \tag{B4}$$

$$Q_1(\alpha)=2\sqrt{2}(1+\alpha)^2(1+\alpha^2)^{3/2}(37-12\alpha+42\alpha^2 -20\alpha^3+17\alpha^4)+2(1+\alpha)^2(1+\alpha^2) \times(54-16\alpha+84\alpha^2-32\alpha^3+54\alpha^4-16\alpha^5), \tag{B5}$$

$$Q_2(\alpha)=8(1+\alpha^2)(3-2\alpha+3\alpha^2)[(7-6\alpha+3\alpha^2)(1+\alpha^2) + \sqrt{2}\sqrt{1+\alpha^2}(5-4\alpha+5\alpha^2-2\alpha^3)]. \tag{B6}$$

APPENDIX C: SECOND-COLLISION VELOCITY-CORRELATION DISTRIBUTION

In one dimension when $\alpha'=1$, the velocities of the tagged particle and the bath particle are exchanged during the collision. This drastically simplifies the expression of the second-collision velocity-collision distribution and the calculation becomes tractable. Indeed, if $\alpha'=1$, $P_2^{(1)}(z)$ becomes

$$P_2^{(1)}(z)=C_2\int dv\int du_1\int du_2|u_1-v||u_2-u_1|f_B(u_1) \times f_B(u_2)f(v)\delta(vu_2-z), \tag{C1}$$

where $f_B(u)$ denotes the bath velocity distribution and $f(v)$ the tagged particle velocity distribution.

We first integrate over the velocity of the bath particle 2, namely, the velocity of the colliding particle at the second collision. We drop the subscript of the velocity of the bath particle for the collision 1, and $P_2^{(1)}(z)$ reads

$$P_2^{(1)}(z)=C_2\int dv\int du|u-v|\left|\frac{z}{v^2}-u\right|f_B(u)f_B\left(\frac{z}{v^2}\right)f(v). \tag{C2}$$

Let us introduce the function $I(z,v)$:

$$I(z,v)=\int du|u-v||z-uv|e^{-b^2u^2/2}. \tag{C3}$$

When $z<v^2$, one has

$$I(z,v) = \frac{2v^2}{b^2} e^{-b^2 z^2/2v^2} - \frac{2z}{b^2} e^{-b^2 v^2/2} + \frac{\sqrt{2\pi}|v|(1+b^2 z)}{b^3} + \frac{\sqrt{2\pi}v(1+b^2 z)}{b^3}\left[\operatorname{erf}\left(\frac{bz}{\sqrt{2}v}\right) - \operatorname{erf}\left(\frac{bv}{\sqrt{2}}\right)\right] \quad (C4)$$

and when $z > v^2$

$$I(z,v) = -\frac{2v^2}{b^2} e^{-b^2 z^2/2v^2} + \frac{2z}{b^2} e^{-b^2 v^2/2} - \frac{\sqrt{2\pi}|v|(1+b^2 z)}{b^3} - \frac{\sqrt{2\pi}v(1+b^2 z)}{b^3}\left[\operatorname{erf}\left(\frac{bz}{\sqrt{2}v}\right) - \operatorname{erf}\left(\frac{bv}{\sqrt{2}}\right)\right]. \quad (C5)$$

Inserting Eq. (C4) in Eq. (C1) and integrating out the first two terms of the integrand leads to Eq. (54). For $z > 0$, by using the property of $I(v,z)$ [Eqs. (C4) and (C5)], for $z > 0$, $P_2^{(1)}(z)$ is expressed as

$$P_2^{(1)}(z) = C_2\left[\int_{\sqrt{z}}^{\infty} dv - \int_0^{\sqrt{z}} dv \left(\frac{e^{-a^2 v^2/2 - b^2 z^2/2v^2}}{v^2} I(v,z)\right)\right]. \quad (C6)$$

Integrating out the first terms of the right-hand side of Eq. (C6) leads to Eq. (55).

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