Collision of viscoelastic spheres: Compact expressions for the coefficient of normal restitution

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The coefficient of restitution of colliding viscoelastic spheres is known analytically as a complete series expansion in terms of the impact velocity where all (infinitely many) coefficients are known. While being analytically exact, this result is not suitable for applications in efficient event-driven molecular dynamics (eMD) or direct simulation Monte Carlo (DSMC) methods. Based on the analytic result, here we derive expressions for the coefficient of restitution that allow for application in efficient eMD and DSMC simulations of granular systems.

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I. INTRODUCTION AND DESCRIPTION OF THE SYSTEM

A. Introduction

Granular systems are frequently modeled as assemblies of dissipatively colliding spheres. Several review articles show that viscoelastic spheres are an important and widely used collision model for soft spheres (see Refs. [1–3]).

So far, the simulation of systems of viscoelastic spheres was restricted to force-based molecular dynamics (MD). To perform much more efficient event-driven molecular dynamics simulations (eMD) as well as direct simulation Monte Carlo (DSMC) methods, the coefficient of restitution is needed as a function of the impact velocity, material, and system parameters.

Although the exact solution for the coefficient of restitution for viscoelastic spheres is known [4], it is impractical for eMD and DSMC simulations since the solution is given as a complete but extremely slowly converging series. Thus, at present, eMD simulations of systems of viscoelastic spheres are impossible in general.

In this paper, we provide approximate expressions for the coefficient of restitution that allow for a direct application in eMD and DSMC simulations and, thus, for a substantial increase of the efficiency of simulations, provided the preconditions for the application of event-driven simulations are given.

B. System description

The collision of frictionless (smooth) viscoelastic spheres obeys Newton's equation of motion,

$$m_{\text{eff}}\ddot{\xi} = F(\dot{\xi},\xi), \tag{1}$$

with the effective mass $m_{\text{eff}} \equiv m_1 m_2/(m_1+m_2)$ and compression $\xi \equiv R_1 + R_2 - |\vec{r}_1 - \vec{r}_2|$, where $\vec{r}_1$ and $\vec{r}_2$ are the time-dependent positions of the spheres. $F(\ldots)$ is the normal component of the vectorial interaction force $F = \vec{F}\cdot\hat{e}$, with the unit vector $\hat{e} = (\vec{r}_1 - \vec{r}_2)/|\vec{r}_1 - \vec{r}_2|$. For nonadhesive viscoelastic spheres, it reads [5]

$$F = F^{el} + F^{\text{dis}} = \min\left(0, -\rho\xi^{3/2} - \frac{3}{2}A\rho\sqrt{\xi}\dot{\xi}\right), \tag{2}$$

with

$$\rho \equiv \frac{2Y\sqrt{R_{\text{eff}}}}{3(1-\nu^2)}, \tag{3}$$

and Y, ν, and R_{eff} standing for the Young modulus, the Poisson ratio, and the effective radius $R_{\text{eff}} \equiv R_1R_2/(R_1+R_2)$, respectively. The dissipative constant A is a function of the elastic and viscous material parameters [5]. The min(...) function ensures that the force is always repulsive.

The elastic part in Eq. (2), F^{el}, is the Hertz contact force [6], while its dissipative part, F^{dis}, was first motivated in Ref. [7] and then rigorously derived in Refs. [5] and [8], where only the approach in Ref. [5] leads to an analytic expression of the material parameter A.

While knowledge of the interaction force, Eq. (2), is sufficient to perform MD simulations, the coefficient of restitution is needed to perform much more efficient eMD and DSMC simulations, as well as for the kinetic theory of granular gases, e.g., Ref. [9]. By disregarding the dynamics of the collision process and idealizing the collision as an instantaneous event, the coefficient of restitution relates the postcollisional deformation rate $\dot{\xi}'$ to the precollisional deformation rate v,

$$\varepsilon \equiv -\dot{\xi}'/v. \tag{4}$$

Event-driven MD uses this concept for simulations of dilute granular systems, where the frequency of three-particle interactions is negligible compared with the frequency of binary collisions. Therefore, eMD is mainly important for dilute granular gases and, thus, our results may be significant for the simulation of dilute gases of viscoelastic spheres. Beyond its theoretically justified limit, in some applications eMD was also used successfully for moderately dense systems.

In general, the coefficient of restitution is not a constant but depends on the details of the interaction force and the impact velocity. It can be obtained by integrating Eq. (1) with the initial conditions $\xi(0) = 0$ and $\dot{\xi}(0) = v$, assuming that the spheres start contacting at $t = 0$. The coefficient of restitution is then obtained from

$$\varepsilon = -\dot{\xi}(t_c)/v, \tag{5}$$

where the duration of the collision, t_c, is determined by the condition

$$\ddot{\xi}(t_c) = 0, \quad t_c > 0, \tag{6}$$

that is, the collision terminates at time t_c when the interaction force vanishes.

Solving the set of Eqs. (5) and (6) is a complicated problem that was solved rigorously in Ref. [4]. The solution reads

$$\varepsilon = 1 + \sum_{k=0}^{\infty} h_k (\beta^{1/2} v^{1/10})^k \equiv 1 + \sum_{k=0}^{\infty} h_k v_*^k, \tag{7}$$

where we define the shorthand v_* with

$$\beta = \frac{3}{2} A \left(\frac{\rho}{m_{\mathrm{eff}}}\right)^{2/5}. \tag{8}$$

This solution is *exact* since all coefficients h_k are analytically known (see Ref. [4]). It is, moreover, *universal* since all material and particle properties are covered by β, that is, the h_k are pure numbers that are independent of the material and particle properties.

Although it is exact, there are two main problems with the solution, Eq. (7), that prohibit its application in efficient eMD or DSMC simulations: First, it converges extremely slowly. To obtain ε up to quadratic order in v we need 20 terms of the series expansion. Second, wherever we truncate the series at some order k_c, Eq. (7) diverges to $\varepsilon \to \pm\infty$, depending on the sign of h_k.

The divergence of the truncated series is a serious problem. For example consider the very accurate experimental data by Bridges *et al.* [10] for the coefficient of restitution of ice balls at very low temperature (where ice behaves viscoelastically) in which material and particle properties correspond to $\beta = 1.307\ (\mathrm{s/cm})^{1/5}$. Then from Fig. 1 we see that the series truncated at order $k_c = 20$ starts deviating at $v_* \approx 1$, corresponding to the impact velocity $v = v_*^{10}/\beta^5 \approx 0.262$ cm/s. That is, for typical impact velocities of $v \sim 1$ m/s we would need to go to an impractically high truncation order. Consequently, eMD becomes inefficient and one has to apply force-based MD to the simulation of granular gases of viscoelastic particles. By providing a convergent expression for the coefficient of restitution, the work presented here extends the applicability of eMD to granular systems of viscoelastic particles.

To illustrate the relevance of this problem, consider a granular gas of viscoelastic particles. Assume further that its initial granular temperature T corresponds to the scaled thermal velocity $v_* = 1.25$ (see Fig. 1). For the material parameters $\beta = 1.307\ (\mathrm{s/cm})^{1/5}$ this corresponds to the unscaled (physical) velocity $v \approx 2.5$ cm/s. At this velocity the coefficient of restitution is $\varepsilon \approx 0.278$; however, if we truncate the series after the tenth term ($k_c = 10$ in Fig. 1), we would obtain $\varepsilon \approx 1.85$. Therefore, if we would simulate a granular gas initialized at temperature T using the truncated series, almost all collisions would take place with $\varepsilon > 1$; thus, the gas would heat up. Using the correct expression, of course, the gas cools due to inelastic collisions. Thus, the truncation of the series, Eq. (7) (hereafter the tenth term), would cause a qualitatively incorrect result.

From an approximate expression for the coefficient of restitution for applications in efficient eMD and DSMC simulations, we suggest that (a) the approximative solution be close to the correct solution; (b) it can be computed efficiently; that is, it contains only a small number of universal coefficients that are independent of the material and particle properties; and (c) the representation must not reveal divergences, unlike the truncated series, Eq. (7), shown in Fig. 1.

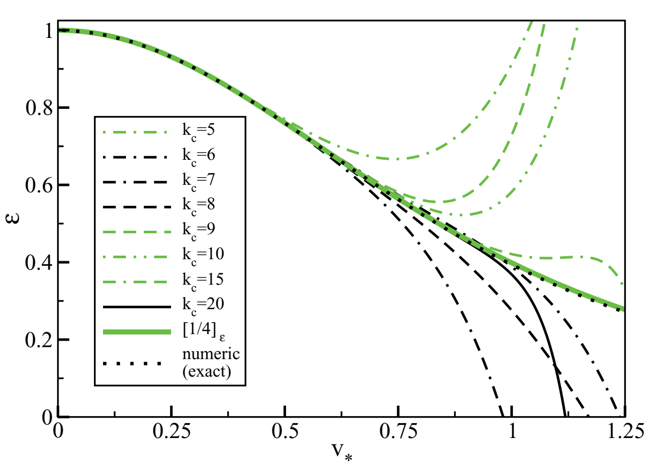

FIG. 1. (Color online) Coefficient of restitution, ε, over $v_* \equiv \beta^{1/2} v^{1/10}$. The analytic solution, Eq. (7), truncated at different order k_c leads to divergence. The dotted line shows ε as it follows from the numerical solution of Eqs. (5) and (6). It almost coincides with the thick green line showing the Padé approximant $[1/4]_\varepsilon$, Eq. (11), to the analytical solution, Eq. (7) (for explanation, see text).

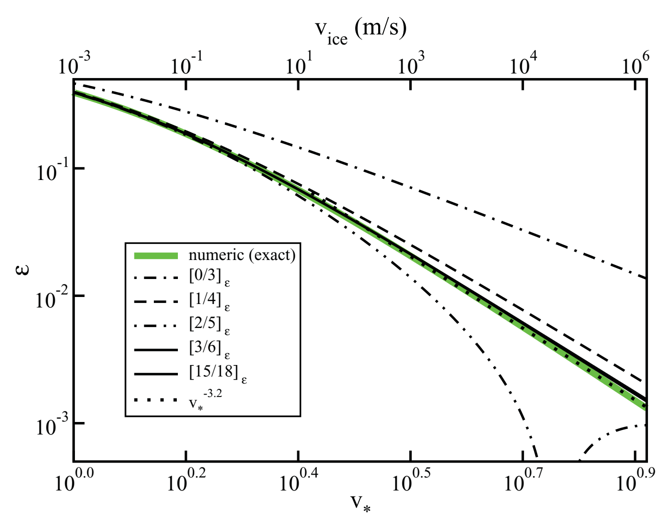

FIG. 2. (Color online) Coefficient of restitution, ε, for large v_* (bottom scale). The thick green line shows the numerical solution of Eq. (9) revealing the asymptotic behavior $\varepsilon = v_*^{-3.2}$ (dotted line). Additionally, various Padé approximants, Eq. (11), of the analytical solution, Eq. (7), are shown (for discussion, see text). The Padé approximants $[3/6]_\varepsilon$ and $[15/18]_\varepsilon$ (which are virtually identical) agree almost perfectly with the exact solution. The scale at the top displays the corresponding physical velocity for the case of ice spheres [$\beta = 1.307\ (\mathrm{s/cm})^{1/5}$] [10]. Note that the covered range of v_* corresponds to 9 orders of magnitude in the physical velocity, $v \propto v_*^{10}$, being the relevant velocity in simulations.

II. NUMERICAL SOLUTION

As described in Refs. [4] and [11], Eq. (1), with the interaction force Eq. (2) and the corresponding initial conditions, may be scaled to

$$\ddot{x} + x^{3/2} + v_*^2\,\dot{x}\sqrt{x} = 0, \quad x(0) = 0, \quad \dot{x}(0) = 1, \tag{9}$$

with the only free parameter $v_* \equiv \beta^{1/2} v^{1/10}$. Compression and time are scaled by $x \equiv \xi/[(\rho/m_{\rm eff})^{-2/5} v^{4/5}]$ and $\tau \equiv t/[(\rho/m_{\rm eff})^{-2/5} v^{-1/5}]$. From the numerical solution of Eq. (9) we determine $\varepsilon(v_*)$ via Eq. (5): $\varepsilon = -\dot{\xi}(t_c)/v = -\dot{x}(\tau_c)$, where τ_c is obtained from the condition $\ddot{x}(\tau_c) = 0$, $\tau_c > 0$. Apart from numerical errors, this solution is exact and may serve as a benchmark for our approximate solution, even for large values of v_*. Using the numerical solution, we find the asymptotic behavior

$$\lim_{v_*\to\infty} \varepsilon(v_*) = v_*^{-3.2} \tag{10}$$

for large v_*, in agreement with Ref. [4] (see Fig. 2).

III. PADÉ APPROXIMANTS

Using the analytical solution, Eq. (7), and the asymptotics, Eq. (10), we construct an approximative expression for $\varepsilon(v)$ that agrees with the analytical solution for the entire range of definition, $v \in (0,\infty)$, and is thus much more suitable for numerical simulations. The Padé approximant $[m/n]_\varepsilon(v_*)$ approximates the $m+n$ times differentiable function $\varepsilon(v_*)$ by a rational function

$$[m/n]_\varepsilon(v_*) = \frac{\sum_{i=0}^{m} a_i v_*^i}{\sum_{i=0}^{n} b_i v_*^i} \tag{11}$$

in a way that the Maclaurin series of the approximant and of the approximated function match up to order $m+n$:

$$\begin{aligned} \varepsilon(0) &= [m/n]_\varepsilon(0),\\ \varepsilon'(0) &= [m/n]'_\varepsilon(0),\\ &\vdots\\ \varepsilon^{(m+n)}(0) &= [m/n]_\varepsilon^{(m+n)}(0). \end{aligned} \tag{12}$$

TABLE I. Coefficients of the Padé approximants $[m/m+3]_\varepsilon$ for $m \in \{0,1,2,3\}$. $[2/5]_\varepsilon$ reveals a pole at $v_* \approx 5.6801$.

m	n	a_i	b_i	
0	3	$a_0 = 1.0$	$b_0 = 1$	$b_2 = 1.15345$
			$b_1 = 0$	$b_3 = 0$
1	4	$a_0 = 1.0$	$b_0 = 1.0$	$b_3 = 0.577977$
		$a_1 = 0.501086$	$b_1 = 0.501086$	$b_4 = 0.532178$
			$b_2 = 1.15345$	
2	5	$a_0 = 1.0$	$b_0 = 1.0$	$b_3 = 0.638466$
		$a_1 = 0.553528$	$b_1 = 0.553528$	$b_4 = 0.384023$
		$a_2 = -0.128445$	$b_2 = 1.025$	$b_5 = 0.027908$
3	6	$a_0 = 1.0$	$b_0 = 1.0$	$b_4 = 1.19449$
		$a_1 = 1.07232$	$b_1 = 1.07232$	$b_5 = 0.467273$
		$a_2 = 0.574198$	$b_2 = 1.72765$	$b_6 = 0.235585$
		$a_3 = 0.141552$	$b_3 = 1.37842$	

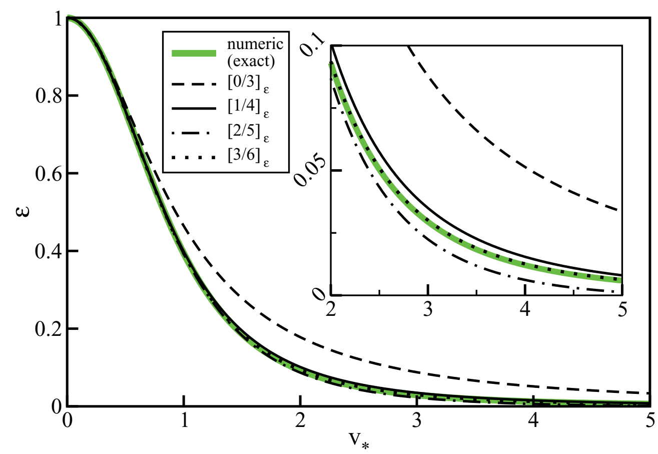

FIG. 3. (Color online) Coefficient of restitution, ε, over v_*. The first four Padé approximants are shown together with the numerical (exact) solution. The inset shows a magnification. The order $[3/6]_\varepsilon$ (dotted line) coincides almost perfectly with the exact solution in the entire range of definition.

Asymptotically, the Padé approximant behaves like a power law, $\lim_{v_*\to\infty}[m/n]_\varepsilon \sim v_*^{m-n}$. These properties allow us to represent the function $\varepsilon(v_*)$ similar to a Taylor expansion for small arguments and asymptotically as a power law, and, thus, convergent if $m < n$ (see Ref. [12]).

Since $\varepsilon \sim v_*^\alpha$ with $\alpha \approx -3$ [see Eq. (10) and Fig. 2], we chose a Padé approximation $[m/m+3]_\varepsilon$. To find an accurate yet compact approximant to Eq. (7), we start at $m = 0$ and increase the order until sufficient agreement with the exact solution is achieved. The result is shown in Fig. 2: $[0/3]_\varepsilon$ is certainly not acceptable; $[1/4]_\varepsilon$ offers a good tradeoff between simplicity and accuracy. $[2/5]_\varepsilon$ reveals a pole at $v_* \approx 5.68$; therefore, it is suitable only for small impact velocity $v_* \lesssim 10^{0.3}$. For ice spheres as described in Ref. [10], this implies $v \lesssim 2.6$ m/s. The next order, $[3/6]_\varepsilon$, offers almost perfect agreement with the benchmark. We checked all orders up to $[25/28]_\varepsilon$ and could not find any significant improvement as compared to $[3/6]_\varepsilon$. As an example, $[15/18]_\varepsilon$ is shown in Fig. 2.

Table I displays the coefficients a_i and b_i for the relevant Padé approximants $[m/m+3]_\varepsilon$ for $m \in \{0,1,2,3\}$ and Fig. 3 shows these Padé approximants together with the exact (numerical) solution. Again, $[1/4]_\varepsilon$ and $[3/6]_\varepsilon$ turn out to be good compromises between accuracy and simplicity.

IV. CONCLUSION

The universal exact solution, Eq. (7), for the coefficient of restitution of smooth viscoelastic spheres cannot be applied directly in eMD and DSMC simulations since the series diverges for any finite truncation order. We have shown that the Padé approximations of order $[1/4]_\varepsilon$ and $[3/6]_\varepsilon$ are suitable for representing the coefficient of restitution over the entire range of impact velocities, including its asymptotic behavior up to an excellent accuracy, and we provided the constants of this approximation. Similar to the full solution, Eq. (7), the Padé expansion is universal, that is, the constants a_i and b_i are universal. They depend on neither material properties (Young

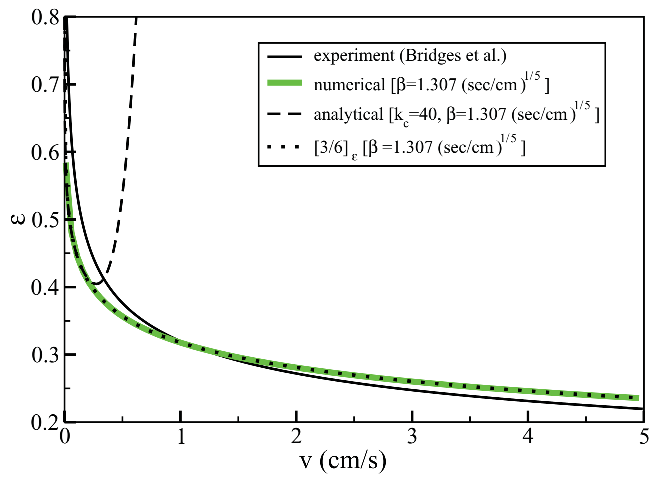

FIG. 4. (Color online) Coefficient of restitution, ε, as a function of the impact velocity v. The Padé approximant $[3/6]_\varepsilon$ (dotted line) agrees almost perfectly with the numerical integration of Newton's equation, Eqs. (1)–(6), in the entire range of impact velocity v (physical units), while the analytical solution, Eq. (7), truncated at order as large as $k_c = 40$, diverges at $v \approx 0.3$ cm/s. For the material constant, $\beta = 1.307\ (\mathrm{s/cm})^{1/5}$, we used the experimental values by Bridges *et al.* [10] for the collision of ice spheres at low temperature.

modulus, Poisson ratio, and dissipative constant) nor particle properties (radii and masses). All nonuniversal parameters enter exclusively via β, Eq. (8), which in turn enters the argument of the Padé expansion via $v_* = \beta^{1/2} v^{1/10}$, with v being the impact velocity in physical units (cm/s). Thus, the presented Padé approximation can be conveniently applied in numerical simulations.

The precision of the approximant can be assessed in Fig. 4, which shows the Padé approximation together with the numerical integration of Newton's equation, Eq. (1), in combination with Eqs. (2)–(6) , and with the divergent analytical solution, Eq. (7), truncated at an order as large as $k_c = 40$. We see that over the entire range of definition, the Padé approximation coincides almost perfectly with the numerical solution and with the truncated analytical solution up to $v \approx 0.3$ cm/s, where the latter starts to diverge. For the material constant, $\beta = 1.307\ (\mathrm{s/cm})^{1/5}$, we used the experimental values from Bridges *et al.* [10] for the collision of ice spheres at low temperature. The corresponding data also are shown in the plot. While the agreement among the exact analytical result, the numerical integration, and the Padé approximant is remarkable, the experimental data deviate slightly. This deviation is not surprising because in addition to viscoelasticity, described by the force in Eq. (2), other forces may contribute, such as surface forces, plastic deformation, and adhesion, among others.

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