Controlling the temperature of one-dimensional systems composed of elastic and inelastic particles

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We have studied systems composed of either elastic or inelastic particles constrained to move in one dimension and confined on a line by using molecular dynamics (MD) simulation techniques. We have tested several ways of modeling a boundary that exchanges energy with the system. Furthermore, we have studied one-dimensional granular systems composed of soft particles under cooling and found that the decay in temperature follows a power law $T \propto t^{-\alpha}$ similar to the case of rigid particles, but now, the value of α depends on the density and degree of inelasticity in the system. For systems composed of inelastic particles thermostated by one of the boundaries we find that the ''extraordinary'' state reported by Y. Du, H. Li, and L. P. Kadanoff [Phys. Rev. Lett. **74**, 1268 (1995)] is an artifact introduced by method of providing energy to the system. [S1063-651X(98)05202-7]

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I. INTRODUCTION

Granular material flows appear in nature (sand dunes, planetary rings, powders) and are of great technological importance (handling and transport of, e.g., seeds and pharmaceuticals). In the dry state, granular materials interact mainly by repulsive forces and there is energy dissipation during collisions due to the excitation of internal modes. Thus, in the absence of an energy source the granular medium cools, and the motion of the grains eventually stops. One-dimensional models of granular media have been studied in the hope that the origin of phenomena that appear in models for two or three dimensions can be enlightened by results from more ''simple'' one-dimensional models. The dynamics of particles in one dimension, nevertheless, has the peculiarity that their motion is confined between two neighbors, and therefore the transport of physical quantities across the system is very inefficient.

The present investigation was motivated by the work of Du *et al.* [1] where they report the appearance of an ''extraordinary'' state in thermostated systems composed of model granular particles in one dimension. In such a state, the majority of the particles form a clump in the side of the simulation box opposite to the thermostat, and they move at a very low speed. The rest of the particles move at a much higher speed between the thermostat and the clump.

The first part of this investigation is devoted to analyzing the thermostating devices used in Ref. [1]. We have tested whether these thermostating devices are able to produce true equilibrium states at a desired temperature. With this purpose, we have studied systems composed of rigid and soft particles constrained to move in one dimension. We found that the thermostating devices used in Ref. [1] either failed in setting the system at the target temperature (which is the assumed temperature of the boundary), or produced a wrong distribution of energies in the systems. Therefore, we propose alternative methods that successfully produce equilibrium states at a desired temperature in one-dimensional systems, and test another method due to Ciccotti *et al.* [2–4].

In the second part of the paper, we elucidate whether the appearance of the ''extraordinary'' state is a universal behavior for systems composed of inelastic particles (granular particles) constrained to move in one dimension, or it is an artifact of the model. We found that the appearance of the ''extraordinary'' state depends on how the energy is pumped into the system.

Additionally, we compare the behavior of soft and rigid inelastic particles under cooling, i.e., when there is no thermostating device coupled to the system. It has been established [5–7] that the cooling granular medium is not spatially uniform but it shows clusters and voids. In the case of inelastic particles in one dimension and in absence of any thermostating device, it is possible to show [5,8] that the temperature of the system will decrease following a power law, i.e., t^{-2}; this is referred to as the cooling problem in granular materials. We verify this result for rigid particles, but find that for soft particles, although the dependence of temperature on time is a power law $T \propto t^{-\alpha}$, the value of α depends on the density and the degree of inelasticity in the system. McNamara and Young have numerically verified the cooling problem in one and two dimensions [5,9].

The outline of the paper is the following: Sec. II describes the system composed of rigid particles, Sec. III presents the system composed of soft particles and describes how inelastic collisions can be introduced. The thermostating devices studied in this paper are described in detail in Sec. IV. In Sec. V, we present and discuss the results from the simulations. A summary and the conclusions of the investigation are collected in Sec. VI.

II. RIGID PARTICLES

We consider a system of N point particles of equal mass m, which are constrained to move in one dimension and confined in a box. The interaction between particles occurs through collisions only. If the collisions are elastic, in the particular case of one dimension, a collision simply means

an exchange of momenta between the colliding particles. Moreover, it should be noticed that the particles are points make the properties of the system independent of the density of particles in the box. The walls confining the system are hard walls of infinite mass. In some of the simulations the particles are allowed to exchange energy with one of the walls, which, thus, acts as a thermostat. This is described in detail in Sec. IV.

Inelasticity is introduced into the system in the same way as in previous simulations [1,5]. Let i and j denote the indexes of two colliding particles. The velocities after collision, v_i' and v_j', are related to the velocities before collision, v_i and v_j, as

$$v_i' = \epsilon v_i + (1-\epsilon) v_j , \tag{1}$$

$$v_j' = (1-\epsilon) v_i + \epsilon v_j , \tag{2}$$

where $\epsilon = (1-r)/2$ and r is the restitution coefficient. The parameter r is the ratio of the relative velocities right after and just before a collision and provides a measure of how inelastic the collisions are. The case $r=1$ the collisions are elastic, and the case $r=0$ the collisions are completely inelastic. This model is identical to the one chosen in Ref. [1], where the simulation results indicate a breakdown of hydrodynamics for inelastic particles in one dimension.

The temperature of the system is defined as [10]

$$T = \frac{1}{N} \sum_{i=1}^{N} v_i^2 , \tag{3}$$

where N is the number of particles. The temperature as defined above is used in all simulations.

For this model, all the results are reduced with the mass of the particle, m, the length of the simulation box, L, and the time between collisions τ_{coll}. Thus, for instance, the units for energy are $mL^2 \tau_{\text{coll}}^{-2}$.

We have studied systems of $N=100$ particles. The simulation program for the rigid particles is simple, and we will describe our program in general terms. The program tracks the collisions, advances the position, and changes the velocities. Finding the next collision is easy for a one-dimensional system: a particle i can only collide with two particles, namely, $i-1$ and $i+1$ (and we only have to check with one of them). The computational effort is, therefore, clearly $O(N)$ where N is the number of particles.

III. SOFT PARTICLES

Our soft particle models are disks of equal mass m constrained to move in one dimension and confined in a box. The interaction between particles is purely repulsive and the shape of the potential is the Weeks-Chandler-Andersen (WCA) potential [11]:

$$u(x_{ij}) = \begin{cases} 4\epsilon \left[\left(\dfrac{\sigma}{x_{ij}} \right)^{12} - \left(\dfrac{\sigma}{x_{ij}} \right)^{6} \right] + \epsilon & \text{for} \quad x_{ij} \leqslant 2^{1/6}\sigma \qquad (4) \\ 0 \quad \text{for} \quad x_{ij} > 2^{1/6}\sigma , & \qquad (5) \end{cases}$$

where x_{ij} is the distance between the centers of the disks. The potential parameters σ, ϵ and the mass m of the particles are the units of length, energy, and mass, respectively. All the quantities obtained for this model are presented in reduced units. The reduced temperature is defined as $k_B T/\epsilon$ (k_B is Boltzmann's constant) and the reduced time as $\sigma(m/\epsilon)^{1/2}$.

Inelasticity can be brought into the system by introducing dissipative forces during collision. In the present model, contrary to rigid particles, collisions have finite duration. We have chosen to let the particles experience dissipative forces whenever the distance between them is less than $2^{1/6}\sigma$, i.e., during the whole period of time of the collision. The shape of the dissipative force is

$$F_{\text{dis}} = \gamma D^{1/2} \frac{dD}{dt} , \tag{6}$$

where D is a so-called deformation parameter defined as

$$D = 2^{1/6}\sigma - x_{ij} , \quad x_{ij} \leqslant 2^{1/6}\sigma , \tag{7}$$

$$D = 0 , \quad x_{ij} > 2^{1/6}\sigma \tag{8}$$

and γ is related with the degree of dissipative friction in the system. Hence, the dissipative forces depend on the degree of deformation of the grains and the relative velocities between the colliding particles, v_{ij}:

$$F_{\text{dis}} = \gamma D^{1/2} \frac{dD}{dt} \tag{9}$$

$$= -\gamma D^{1/2} v_{ij} . \tag{10}$$

The force F_{dis} represents the dissipation that arises from frontal friction between two granular particles. This specific form of the dissipative force was recently proposed independently by Morgado *et al.* [12] and Brilliantov *et al.* [13]. To the best of our knowledge, this is the first time it has been implemented in a MD simulation.

Actually, the loss of kinetic energy due to tangential collisions should also be taken into account, but because we are considering the relative motion in one dimension only, tangential collisions will not be considered here.

The equations of motion are solved using the leap-frog algorithm [14]. Since dissipative forces depend on the relative velocity of a pair of particles, for our one-dimensional system the resolution of the equations of motion involves solving a set of linear equations, where the velocities at time $t+h/2$ (h is the length of the time step) are the unknown quantities. The matrix of this set of equations is presented in Appendix A. This matrix is tridiagonal, and therefore, the resolution of the system is a fast procedure from a computational point of view [15]. The use of this model of dissipative forces in a system of two or three dimensions will be far more expensive computationally since it will entail an iterative process to compute the forces.

The length of the time step was set to 0.002 reduced units of time and systems of $N=100$ and 1000 particles were considered.

IV. THERMOSTATING

As written previously, without any energy supply, the motion of inelastic particles will eventually stop. In order to investigate steady states of the flow of granular materials, one needs to pump energy into the system, i.e., we have to introduce a thermostating device. We have chosen to supply energy into the system from the left boundary (thermal wall), which should basically act as a wall held at constant temperature $T_{\rm wall}$. The right boundary is an insulating wall modeled as a hard wall of infinite mass (reflecting wall). Thus, in our one-dimensional systems, only the left-most particle will exchange energy with the thermal wall. In this section we describe a number of ways of doing this. In Sec. V we will reveal how the different implementations work.

Gaussian wall: When a particle hits a wall (the left-most particle–particle 1), it is sent back with a random velocity drawn from a Gaussian distribution. The distribution is a Maxwell-Boltzmann (MB) distribution, corresponding to a temperature $T_{\rm wall}$. This type of thermostat was used in Ref. [1].

Stochastic wall: The original idea of a stochastic boundary is due to Lebowitz *et al.* [16] and used intensively by Ciccotti *et al.* [2–4]. In their work, after a particle hits the stochastic wall it comes off with a distribution corresponding to $T_{\rm wall}$. This is done by sampling the value of the velocity component in the direction normal to the wall from the probability density:

$$P(v_n)=\frac{mv_n}{k_BT_{\rm wall}}\exp\left(-\frac{mv_n^2}{2k_BT_{\rm wall}}\right) \tag{11}$$

where k_B is Boltzmann's constant, $T_{\rm wall}$ the temperature of the thermal wall, m the mass, and v_n the component of the velocity normal to the wall (we set k_B and m to 1 in our simulations). The rest of the components are sampled from a MB distribution at the temperature of the thermal wall. Notice that for a one-dimensional system, the distribution of the velocities of the particles emitted by the Gaussian wall is different than in the present case due to the factor v_n in Eq. (11). This is discussed in the next section.

Constant velocity wall: After the collision with the wall, the left-most particle is always returned with the same velocity, $\sqrt{T_{\rm wall}}$. It has been used in previous studies [1,17].

Frequency: This type of thermostat does not involve a collision with a wall. Instead, the velocity of the left-most particle is changed with a certain frequency. The velocity is drawn from a MB distribution with temperature $T_{\rm wall}$. This way of thermostating the system has, to the best of our knowledge, never been used before.

Wall particle coupled to a Nosé-Hoover (NH) thermostat: We substitute the left hard wall by a particle tethered to the point $x_0=0$ by a harmonic potential $U_{\rm wall}=\frac{1}{2}k_{\rm wall}(x-x_0)^2$. The value of $k_{\rm wall}$ is set to 100 reduced units. The dynamics of this particle is coupled to a Nosé-Hoover thermostat [18]. Moreover, the wall particle interacts with the left-most particle of the system through a WCA potential with the same parameters as for the rest of the particles in the system. There is no dissipation of energy during the collision of the left-most particle and the wall particle. The equations of motion for the wall particle are

$$\dot{x}=\frac{p}{m}, \tag{12}$$

$$\dot{p}_x=f_x-\zeta p_x, \tag{13}$$

$$\dot{\zeta}=\frac{1}{\tau^2}\left(\frac{p_x^2}{mk_BT}-1\right), \tag{14}$$

where ζ and τ are, respectively, the friction parameter and the relaxation time of the thermostat. The relaxation time of the thermostat was set to 0.15 reduced units.

The system composed of rigid particles was thermostated with the first four devices. The system composed of soft particles were thermostated with all of them.

V. RESULTS

A. Elastic particles

We have performed simulations of one-dimensional systems containing rigid and soft particles. The results of our simulations will be discussed in this section. To begin with, we analyzed the final states obtained with the thermostating devices described above. Our goal is to obtain equilibrium states at a temperature $T_{\rm wall}$.

Figure 1 shows the temperature as a function of time for a system composed of rigid point particles undergoing elastic collisions when the different thermostats described in the previous section are coupled to the system. The target temperature of the thermostats is $T_{\rm wall}=1.0$ in all the cases. The velocities of the starting configuration were drawn from an MB distribution with $T=1.0$. Apparently, the only thermostat that fails to maintain the temperature of the system is the Gaussian wall used in Ref. [1], which sets the temperature of the system below the target temperature [see Fig. 1(a)]. However, the constant velocity thermostat [Fig. 1(b)] for one-dimensional systems composed of rigid particles produces configurations where the velocities of the particles take the values $\pm\sqrt{T_{\rm wall}}$ only, and therefore, these configurations are not equilibrium configurations. This is due to the fact that in such a one-dimensional system the collisions between particles involve exchange of momenta only, since there is no scattering. This introduces an extra peculiarity in the system since equilibrium states can never be reached with the thermostating devices used in this work if the initial configuration includes particles whose velocity is 0. In summary, given an initial configuration where all the velocity of the particles are non-negligible only the stochastic wall [Fig. 1(d)] and the frequency thermostat [Fig. 1(c)] are able to generate equilibrium states at $T_{\rm wall}$.

We have also performed simulations with hard disks instead of point particles at low (0.01) and high density (0.83) and there is no qualitative difference.

The same analysis for the one-dimensional system composed of soft particles (undergoing elastic collisions) yields similar results. In Table I, we summarize the temperatures of the final states obtained for both rigid and soft particles. The results for soft particles are for a density $\rho=0.83$; ρ defined as N/L ($N=100$ and L is the length of the box), the target temperature of the thermostats is 1.0, and the temperature of the system was averaged over 5×10^6 time steps after equili-

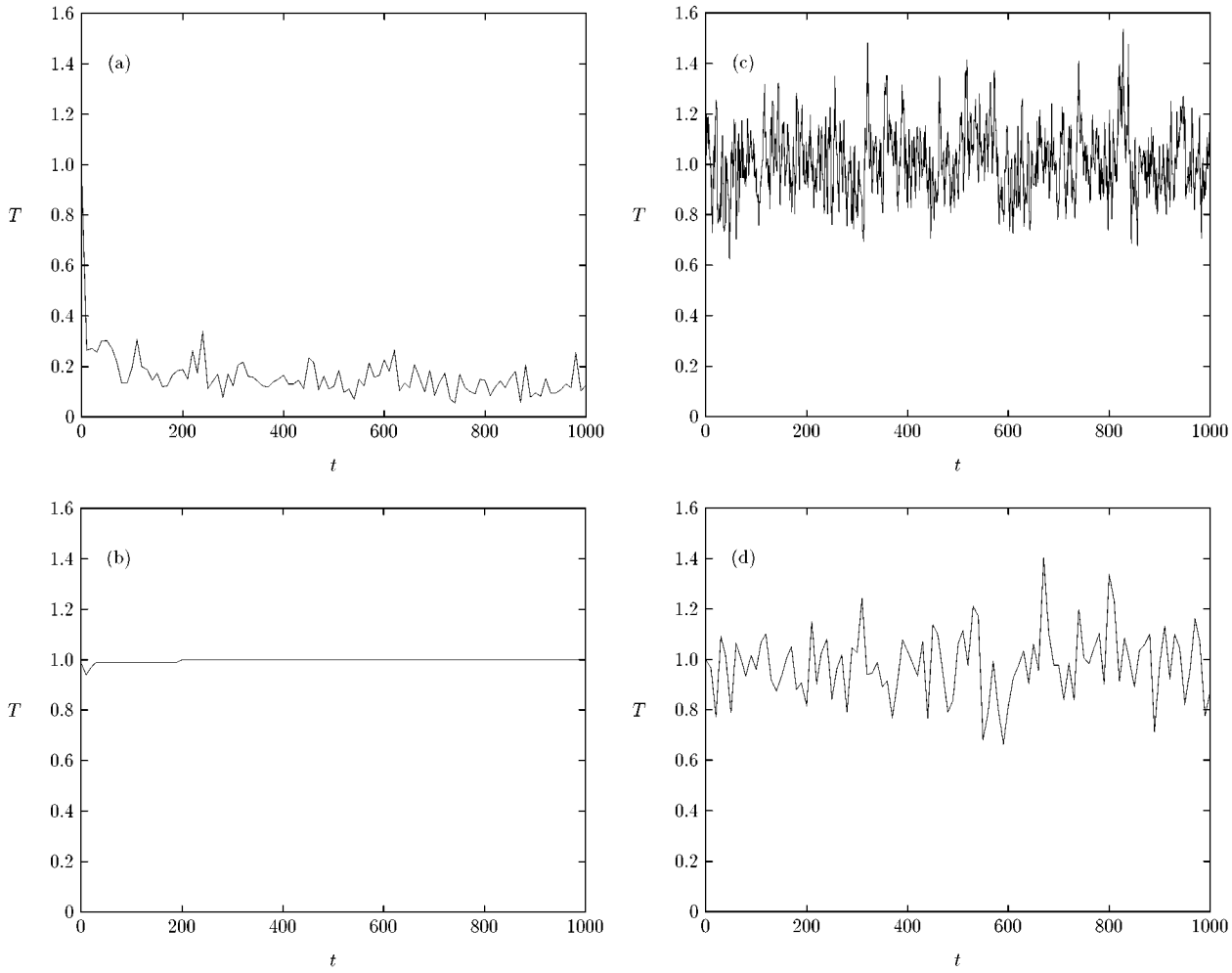

FIG. 1. The temperature as a function of time. Both quantities are in reduced units. System of point rigid particles and elastic collisions is shown. The number of particles is 100, and the length of the system is 1. The target temperature of the thermostats is 1.0. (a) Gaussian wall. (b) Constant velocity wall. (c) Frequency. (d) Stochastic wall.

bration for the soft particles. As in the case of rigid particles, the Gaussian wall coupled to the system composed of soft particles does not perform well as a thermostat. Furthermore, the constant velocity thermostat and the frequency thermostat at high frequency also fail to set the temperature of the system to the target temperature. All three devices set the temperature of the soft particle system below the target temperature. Moreover for the system composed of soft particles, the final states obtained with these thermostats do not fulfill equipartition, i.e., the kinetic energy is not equally distributed among the particles in the systems. This is illustrated in Fig. 2, where we show the mean kinetic energy (temperature) for each particle in the system for a final state reached with the Gaussian wall. The kinetic energy of the left-most particle is significantly lower than the average temperature of the system ($T=0.62$). This indicates that this is not an equilibrium state but a nonequilibrium steady state.

TABLE I. Equilibrium temperatures.

Thermostat	Hard particles	Soft particles
Gaussian wall	0.15 ± 0.05	0.62 ± 0.02
Stochastic wall	1.00 ± 0.14	0.98 ± 0.02
Constant	1.00 ± 0.03	0.507 ± 0.005
Frequency	1.00 ± 0.13	1.01 ± 0.01 [a]
Frequency	1.02 ± 0.09	0.49 ± 0.02 [b]
Wall particle+NH		0.99 ± 0.01

[a]The velocity of particle 1 is taken from an MB distribution every 100th time step (soft particles) or with frequency 1/0.0243 (rigid particles).

[b]The velocity of particle 1 is taken from a MB distribution every time step (soft particles) or with frequency 1/2.4299 (rigid particles).

The explanation of why the Gaussian wall proposed in Ref. [1] and the constant velocity thermostat does not produce equilibrium states at the target temperature is as follows. The principle behind a thermal wall is to change the distribution of velocities of the particles arriving at the wall to the distribution corresponding to the temperature of the wall [16]. Let us assume a three-dimensional system, and denote as $\vec{n}$ the unit vector normal to a wall boundary. Then the probability that a particle with velocity $\vec{v}$ arrives at the wall (or, in general, crosses a planar surface) is

$$\vec{v}\cdot\vec{n}f(v_x,v_y,v_z)dv_xdv_ydv_z, \tag{15}$$

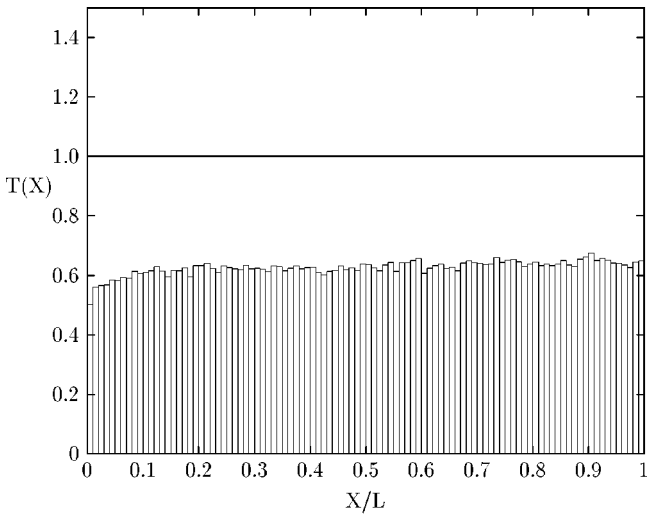

FIG. 2. Mean kinetic energy (in reduced units) for each particle of the soft particles system at $\rho=0.83$ when the Gaussian wall thermostat is applied.

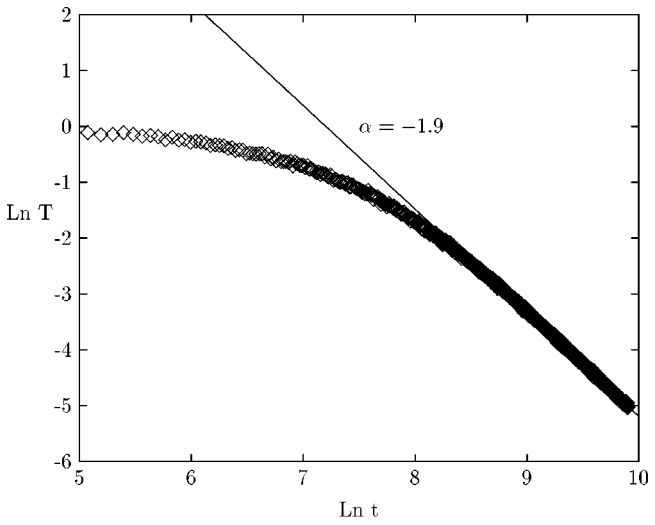

FIG. 3. ln$T$ plotted versus ln$t$. The temperature T and the time t are in reduced units. Results for a system of soft particles undergoing inelastic collisions and no thermostating device coupled to the system. The system is composed of $N=1000$ particles. $\rho=0.83$ and $\gamma=0.001$. $\diamond$: simulation results; straight line: least square fit.

where $f(v_x,v_y,v_z)$ is the MB distribution of velocities at the temperature of the fluid. At equilibrium, the probability that a particle with velocity $\vec{v}$ leaves the wall will have the same shape. For our one-dimensional system this probability is

$$v_x f(v_x) dv_x . \tag{16}$$

This is obviously not the case for the Gaussian wall or the constant velocity wall. Furthermore, the distribution of velocities of the particles arriving at these boundaries will be different from that of the particles emitted by these boundaries, and therefore, equilibrium will never be reached.

The fact that the frequency thermostat works so well for the system composed of rigid particles is easy to understand. Due to the one-dimensional nature of the system, the distribution of velocities remains unchanged when there is no thermostating device coupled to it. This is so because, in the collisions, the particles simply exchange momentum. With the frequency thermostat, a random number generator will ensure that particle 1 has the kinetic energy corresponding to the desired temperature. Thus, particle 1 simply provides velocities to the rest of the system sampled from the correct distribution function. In the case of the frequency thermostat, the frequency at which particle 1 gets a new velocity from the MB distribution is totally uncorrelated with the previous velocity of the particle. In the case of a system composed of soft particles, energy should be distributed among all the potential and kinetic energy of the particles. If the velocity of particle 1 is not changed too rapidly by the random number generator, particle 1 will be in equilibrium with the rest of the system because energy will have time to be redistributed among all the degrees of freedom in the system. Equipartition will then be fulfilled, and the system will reach the desired temperature, i.e., the temperature of particle 1. When the velocity of particle 1 is exchanged at too high frequency the system has not time enough to relax (redistribute the energy). Indeed, our results show nonequipartition of the energy in the system when the frequency is high.

The system thermostated with the wall particle coupled to a Nosé-Hoover thermostat works as one should expect, since it is a well-defined system, where the equations of motion can be derived from an extended Hamiltonian [18].

B. Inelastic particles

The main purpose of the present investigation is to study the behavior of one-dimensional systems where particles undergo inelastic collisions, since these are models for granular materials.

We start looking at the system under cooling (i.e., there is no thermostating device coupled to the systems). In Fig. 3, the typical behavior of the temperature as a function of time for a system composed of $N=1000$ soft particles is shown. After a transient, whose length depends on the density of the system, the temperature decays following a power law $t^{-\alpha}$. For rigid particles, we found similar behavior and a value of the exponent $\alpha=2$ (within the statistical uncertainty) that agrees with theoretical predictions [5,8] and previous simulations [5]. For the system composed of soft particles, the value of the exponent seems to depend on the density and the degree of inelasticity in the system. The values of the exponent α obtained for different densities and degrees of inelasticity are collected in Table II. At sufficiently high density and weak inelasticity the value of the exponent α agrees with the theoretical predictions [5,8] for rigid particles. This is interesting in the case of Haff's theory [8] since it was developed for very dense granular systems, where the interparticle distances are significantly smaller than the diameter of

TABLE II. Values of the exponent in the cooling law $T \propto t^{-\alpha}$.

Density	Inelasticity	α
0.2	Weak	1.16
0.2	Strong	1.39
0.83	Weak	1.90
0.83	Strong	1.59

the particles. On the other hand, the theory developed by McNamara *et al.* [5] was based in the fact that in one-dimensional granular systems composed of point rigid particles under cooling, a bimodal velocity distribution raises. They predict that the temperature will decay as

$$T=\frac{U_0^2}{(1+2\epsilon\rho t U_0)^2}, \tag{17}$$

where U_0 is the mean value of the velocity modulus at $t=0$, ϵ is the friction parameter introduced in Eqs. (1) and (2), and ρ is the density. Nevertheless, we do not find any trace of a bimodal velocity distribution as the one-dimensional system composed of soft particles cools down.

Finally, we analyze the behavior of one-dimensional systems with inelastic collisions and a thermostat coupled to the system. As mentioned, for one-dimensional systems of particles undergoing inelastic collisions an ''extraordinary'' state was found in Ref. [1]. In such an ''extraordinary'' state, the majority of the particles get clamped in a small region of space moving with very low velocities, and few remaining particles travel between one of the boundaries and the group of clamped particles at a much higher speed. In the present investigation, nevertheless, we find that the thermostating devices used in Ref. [1] failed to produce equilibrium states for elastic particles. Therefore, we have carried out simulations where our one-dimensional systems are coupled to thermostats that we have shown perform well in equilibrium, namely, the stochastic wall and a wall particle coupled to a NH thermostat.

We have repeated the simulations performed in Ref. [1] for rigid point particles but now coupling the system to a stochastic wall (the left-side wall) and we have reproduced their main findings. In other words, we observe that the ''extraordinary'' state also appears when a correct thermostating device is used. The appearance of the ''extraordinary'' state is illustrated in Fig. 4(b) for a system composed of $N=100$ particles. This figure shows the position of the center of mass, $\langle x\rangle=(1/N)\Sigma_{i=1}^{N}x_i$, as function of time. The position of the center of mass of the system moves to the right side of the box and remains there as steady state is reached. For the sake of completeness we also show results without a thermostat in Fig. 4(a); the value of $\langle x\rangle$ stays around zero, which shows that the particles are uniformly distributed. This is indeed what we would except with only $N=100$ particles (for $\epsilon=0.005$ clustering does not occur for a number of particles less than or equal to $N_{\min}=599$ [5]). In Ref. [1] it is found that the particles in the clump get squeezed into a smaller space and move with slower speeds, for a fixed number of particles and decreasing ϵ. We, on the contrary, find that when the initial distribution of velocities is Maxwellian the formation of the clump disappears. This is illustrated in Fig. 4(c), where one can see that for $\epsilon=10^{-7}$, the position of the center of mass fluctuates about the center of the simulation box. Furthermore, the density profile shows that, at steady state, the particles remain homogeneously distributed in the simulation box in agreement with the predictions of the hydrodynamic equations. Nevertheless, we have also started the simulations with all the particles uniformly distributed, and with only the leftmost particle having nonzero velocity. In this case, the position of the center of mass oscillates with a greater amplitude and a long period (about 10^6 collision times), and the distribution of particles is not uniform but the system is more dense on the right side, but we do not see the formation of a clear clump. Furthermore, the velocities of the particles are smaller than in the previous

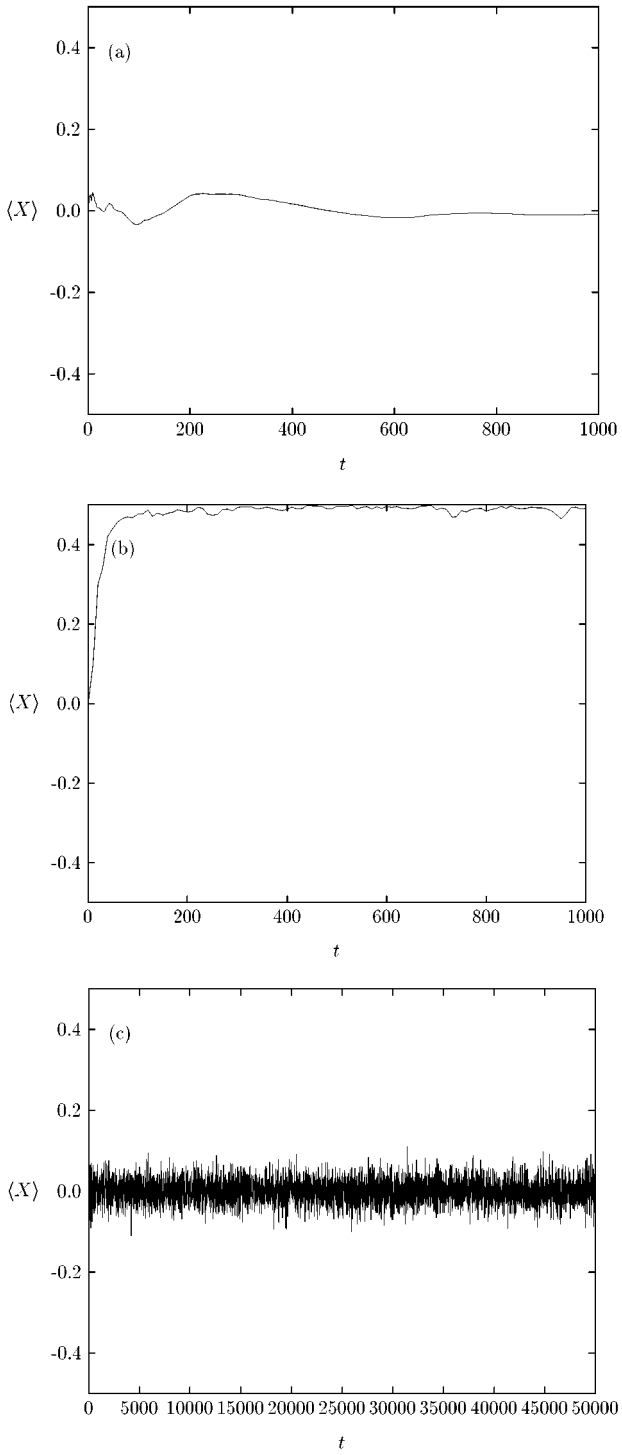

FIG. 4. The center of mass position versus time. X and t are in reduced units. Results for a system composed of rigid point particles undergoing inelastic collisions. The length of the system is 1, and the ''box'' is the interval from -0.5 to 0.5. (a) $\epsilon=0.005$, reflecting walls (b) $\epsilon=0.005$, stochastic wall (c) $\epsilon=10^{-7}$, stochastic wall.

case. Thus, for $\epsilon \to 0$, we observe a dependence of the final steady state on the initial conditions of the simulations. We assume then that the observations from Ref. [1] quoted above correspond to our second initial conditions. However, even in this case we do not observe that the particles, when $\epsilon \to 0$, get squeezed into a smaller space than for greater values of ϵ.

In order to investigate the origin of the ''extraordinary'' state, we have simulated a similar system composed of soft particles. This allows us to use as a thermal boundary a wall particle coupled to a NH thermostat, which is the most realistic way, among those described in Sec. IV, of modeling a wall held at constant temperature. Moreover, in this case, the exchange of energy between the wall and the left-most particle takes place during a finite time interval, instead of instantaneously.

Figure 5 shows the steady state profiles of density and temperature for the soft particle system at $\rho = 0.2$ for different degrees of inelasticity in the collisions (we have chosen three values of the friction coefficient $\gamma = 0.001$, 0.01, and 0.1). The density is normalized as $\rho_{\rm nor}(x) = \rho(x)/\rho$ and the X coordinated as x/L. The results are for a system coupled either to the wall particle coupled to a NH thermostat or to the stochastic wall. At the lowest inelasticity ($\gamma = 0.001$), the steady states produced by the two thermostats are equal. Density and temperature can be considered constant across the system, and the average value of temperature is about 0.9 in both cases [see Figs. 5(a) and 5(d)]. In the figures, the quasi straight lines in the middle of the density and temperature profiles are the arithmetic mean of those, and one can see that they form a symmetry axis about which the density and temperature profiles are mirror images.

For $\gamma = 0.01$, the steady state density and temperature profiles obtained with the two thermostats also show similar fashion [Figs. 5(b) and 5(e)]. Now there is no symmetry as we observed at $\gamma = 0.001$. Moreover, the average temperatures of the two steady states are different, $T = 0.427(6)$ when the system is coupled to the stochastic wall, and $T = 0.28(1)$ when it is coupled to the wall particle coupled to the NH thermostat. The shape of the temperature profiles can be assumed as exponentials within the left-hand half of the box, i.e., in the side closest to the thermostat. This is illustrated in Fig. 6 where the $\ln T$ is plotted versus x/L. The straight lines are the least square fits to the simulation data. The exponential decay of temperature is what one could expect from a hydrodynamic approach.

Finally, we show the results for $\gamma = 0.1$. Here, the final steady states obtained with the two thermostats are clearly different. The steady state obtained with the wall particle coupled to the NH thermostat corresponds to a state with an average temperature of $O(10^{-4})$, this means that the particles have practically stopped moving. The density profile indicates that the particles are homogeneously distributed in the simulation box [see Fig. 5(c)]. The steady state obtained with the stochastic wall is very different. The density profile indicates the appearance of a clump of particles in the right-side of the box and mean kinetic energy of these particles is practically zero [see Fig. 5(f)]. Although the velocities of the rest of the particles close to the thermal wall are very low, they are several orders of magnitude higher than the particles in the clump. This steady state is very much like the ''extraordinary'' state described in Ref. [1].

The differences between the steady states created with the two different thermostating devices [Figs. 5(c) and 5(f)] should emerge from differences in the way that the two thermal boundaries pump energy into the system. The stochastic wall can be interpreted as a boundary that destroys the arriving particles and emits new ones with a velocity drawn for an MB distribution for the target temperature. Thus, the value of the velocity of the outcoming particle is totally independent of the value of the incoming velocity, and therefore the increase in kinetic energy of a particle hitting a stochastic wall can be arbitrarily large. On the other hand, when the left boundary is a wall particle coupled to the NH thermostat, the left-most fluid particle will also increase its kinetic energy by the interaction with the wall particle. Nevertheless, the magnitude of the velocity of the particle after hitting the wall particle will depend on its incoming velocity and therefore the amount of kinetic energy that the left-most particle can load in this way is limited. Furthermore, we have measured in our simulations for soft particles the amount of energy that a particle loads, in a time step, from a stochastic boundary and found that it is several orders of magnitude greater than from a wall particle coupled to a NH thermostat.

When our one-dimensional inelastic models are coupled to a thermostat in the left-side boundary of the simulation box, as the inelasticity of the model increases (the value of ϵ or γ increases), a temperature gradient appears in the system and the density profiles indicate that the more energetic particles on the left side of the box press the particles on the right side of the box to the right-side boundary. We believe that the origin of this ''extraordinary'' state is due to the great amount of energy that the stochastic wall pumps into the system in the limit of (relatively) high inelasticity, where the temperature of the particles (due to inelastic collisions) is well below the temperature of the boundary. Thus, the particles emitted by the stochastic wall have significantly more kinetic energy than the rest of the particles in the system and press them against the other side of the box, where due to their low kinetic energy remain together and form a clump. In the same limit of (relatively) high inelasticity, but when the thermal boundary of the system is a wall particle coupled to a NH thermostat, the thermostat will simply not be able to maintain the temperature of the system, and the motion of particles will eventually stop.

VI. CONCLUSION

We have tested several models used in the literature for modeling a thermal boundary in one-dimensional systems. The results of our simulations indicate that only the stochastic wall, the frequency thermostat, and the wall particle coupled to a NH thermostat are able to generate equilibrium states at the desired temperature of the boundary.

We have studied the cooling of one-dimensional models for granular systems, modeled as rigid and soft particles. For rigid particles we found that the cooling of the system follows the power law, $T \propto t^{-2}$, which agrees with theoretical predictions [5,8], and previous simulations [5]. For soft particles we found a similar power law, $T \propto t^{-\alpha}$, but now, the value of the exponent, α, depends on density and the degree

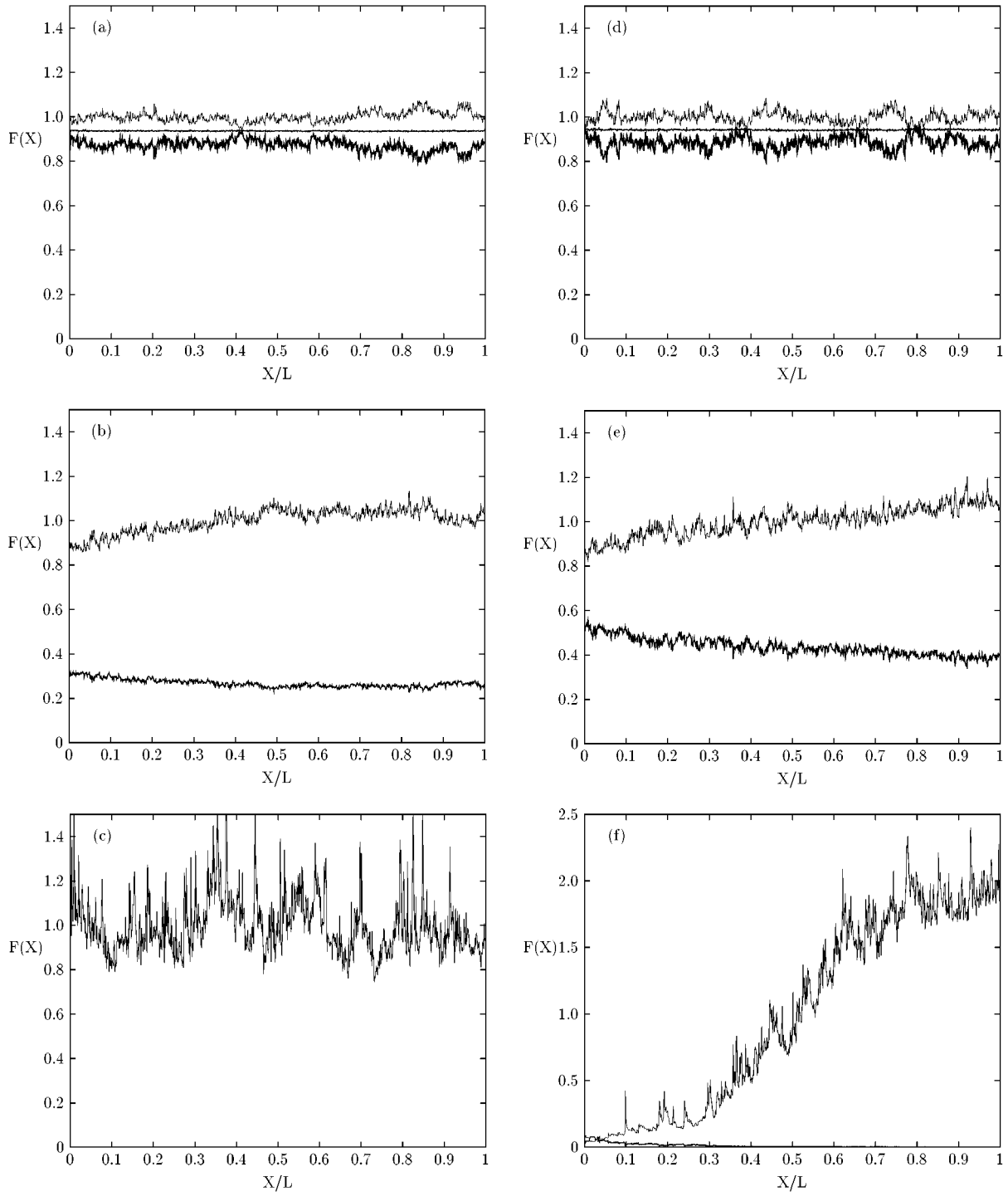

FIG. 5. Temperature (in reduced units) and density profiles. Density is expressed as $\rho(X)/\rho$ where $\rho(X)$ is the local density and $\rho = N/L$, L being the length of the box. Results for a system of soft particles undergoing inelastic collisions. The system is composed of $N = 1000$ particles at a density $\rho = 0.2$. Thin lines: density profiles. Thick lines: temperature profiles. (a) System thermostated with a wall particle coupled to a NH thermostat and $\gamma = 0.001$, (b) $\gamma = 0.01$, (c) $\gamma = 0.1$, (d) system thermostated with a stochastic wall and $\gamma = 0.001$, (e) $\gamma = 0.01$, (f) $\gamma = 0.1$.

of inelasticity in the system. In the limit of high density and low inelasticity the value of the exponent for soft particles seems to tend to the value for rigid particles.

Finally, we have investigated the appearance of the ''extraordinary'' state in one-dimensional granular systems thermostated at the boundaries, described in Ref. [1]. We believe that the origin of such a state is in the way that the thermal boundaries chosen in Ref. [1] or the stochastic boundary used by Ciccotti *et al.* [2–4] work. The interaction with any of these boundaries can be interpreted as an exchange of incoming particles and outgoing particles whose velocity is set to a value totally independent of the incoming velocity. In other words, the kinetic energy of the particles after leaving the boundary can be arbitrarily high in comparison with the mean kinetic energy of the rest of the particles in the fluid. This is the case when the particles undergo inelastic colli-

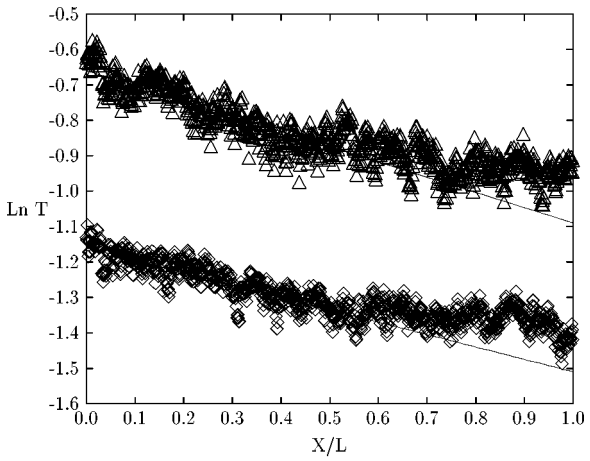

FIG. 6. ln$T$ plotted vs X/L. The temperature is in reduced units. Soft particles undergoing inelastic collisions for $\rho=0.2$ and $\gamma=0.01$. $\diamond$: System thermostated with a wall particle coupled to a NH thermostat. $\triangle$: System thermostated with a stochastic wall, straight lines: least square fits.

sions if the energy dissipated during the collisions is high enough. Hence in this case, the particles emitted by the boundary press the majority of the particles in the system against the opposite boundary forming a clump. If, on the other hand, the interaction with a thermal boundary is such that the particle hitting the boundary can only load a limited amount of kinetic energy, in the limit of high inelasticity the system will simply cool down until all motion stops.

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APPENDIX: INELASTIC COLLISIONS FOR SOFT PARTICLES

The equations for the time evolution of velocities for our (one-dimensional) system of soft particles undergoing inelastic collisions are

$$\begin{aligned}
\dot{v}_1 &= a_1 + \gamma D_{12}^{1/2} v_{12}, \\
\dot{v}_2 &= a_2 - \gamma D_{12}^{1/2} v_{12} + \gamma D_{23}^{1/2} v_{23}, \\
\dot{v}_3 &= a_3 - \gamma D_{23}^{1/2} v_{23} + \gamma D_{34}^{1/2} v_{34}, \\
&\cdots
\end{aligned} \tag{A1}$$

where a_i are the accelerations coming from the conservative forces, and the second term in the right-hand side is the accelerations coming from the dissipative forces due to collisions ($v_{ij}=v_i-v_j$ and γ and D are defined in Sec. III). These equations conserve the momentum of the center of mass but kinetic energy is dissipated.

In the leap-frog algorithm scheme, the velocity of the system at time $t+h/2$ (h is the length of the time step) is calculated as

$$v(t+h/2)=v(t-h/2)+ha(t) \tag{A2}$$

and the velocity at time t is approximated as

$$v(t)=\tfrac{1}{2}[v(t+h/2)+v(t-h/2)]. \tag{A3}$$

Writing Eq. (A1) in the leap-frog scheme:

$$\begin{aligned}
v_1(t+h/2) &= v_1(t-h/2)+h[a_1(t)+\gamma'_{12}(t)v_{12}(t)], \\
v_2(t+h/2) &= v_2(t-h/2)+h[a_2(t)-\gamma'_{12}(t)v_{12}(t) \\
&\quad +\gamma'_{23}(t)v_{23}(t)], \\
v_3(t+h/2) &= v_3(t-h/2)+h[a_3(t)-\gamma'_{23}(t)v_{23}(t) \\
&\quad +\gamma'_{34}(t)v_{34}(t)], \\
&\cdots
\end{aligned} \tag{A4}$$

where for the sake of compactness we rename the product $\gamma D_{ij}^{1/2}(t)$ as $\gamma'_{ij}(t)$. Substituting the value of $v_{ij}(t)$ for the expression given in Eq. (A3), we obtain a set of linear equations where the unknown quantities are $v_i(t+h/2)$. The matrix of this set of equations is

$$\begin{pmatrix}
1+\frac{h}{2}\gamma'_{12}(t) & -\frac{h}{2}\gamma'_{12}(t) & 0 & \cdots \\
-\frac{h}{2}\gamma'_{12}(t) & 1+\frac{h}{2}\gamma'_{12}(t)+\frac{h}{2}\gamma'_{23}(t) & -\frac{h}{2}\gamma'_{23}(t) & \cdots \\
0 & -\frac{h}{2}\gamma'_{23}(t) & 1+\frac{h}{2}\gamma'_{23}(t)+\frac{h}{2}\gamma'_{34}(t) & -\frac{h}{2}\gamma'_{34}(t) \\
 & & \cdots & 1-\frac{h}{2}\gamma'_{n-1,n}(t)
\end{pmatrix}$$

and the right-hand side term is

$$\begin{pmatrix} v_1\left(t-\frac{h}{2}\right)\left[1-\frac{h}{2}\gamma'_{12}(t)\right]+ha_1(t)+v_2\left(t-\frac{h}{2}\right)\left[\frac{h}{2}\gamma'_{12}(t)\right] \\ v_1\left(t-\frac{h}{2}\right)\left[\frac{h}{2}\gamma'_{12}(t)\right]+v_2\left(t-\frac{h}{2}\right)\left[1-\frac{h}{2}\gamma'_{12}(t)-\frac{h}{2}\gamma'_{23}(t)\right]+ha_2(t)+v_3\left(t-\frac{h}{2}\right)\left[\frac{h}{2}\gamma'_{23}(t)\right] \\ \cdots \end{pmatrix}.$$

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