PHYSICAL REVIEW E **89**, 053202 (2014)

Granular chain between asymmetric boundaries and the quasiequilibrium state

Edgar Ávalos*
Department of Physics, Chung Yuan Christian University, Chungli, Taiwan 32063, Republic of China

Surajit Sen†
Department of Physics, State University of New York, Buffalo, New York 14260-1500, USA
(Received 23 February 2014; published 13 May 2014)

Some 30 years have passed since we learned that any velocity perturbation develops into a propagating solitary wave in a granular chain, and over a decade has passed since we learned that these solitary waves break and reform upon collision, leaving behind small secondary solitary waves. The production of the latter eventually precipitates the quasiequilibrium state characterized by large energy fluctuations in dissipation-free granular systems. Here we present dynamical simulations on the effects of soft boundaries on solitary wave interaction in granular chains held between fixed walls. We show that at short time scales, a gradient in the distribution of kinetic energy between the boundaries is indeed sustained. At long times, however, such a gradient gets obliterated and there is no measurable difference between the average kinetic energies of the particles adjacent to walls. Our findings suggest that (i) the quasiequilibrium state can effectively erase small gradients of the average kinetic energies of the particles adjacent to walls in a system, (ii) Boltzmann distribution of grain speeds is realized in the system of interest, and (iii) time and space averages yield the same result, thus suggesting that the system is ergodic.

DOI: 10.1103/PhysRevE.89.053202 PACS number(s): 46.40.Cd, 43.25.+y, 45.70.−n

I. INTRODUCTION

Nesterenko provided experimental evidence and theoretical arguments to show that a velocity perturbation results in a traveling solitary wave (SW), i.e., a nondispersive bundle of energy, in a one-dimensional (1D) granular chain [1,2]. His work was reconfirmed and elaborated upon by many theoretical and experimental works (for some representative studies, see [3–10]). These studies have highlighted the effects of the highly nonlinear potential between two grains in gentle contact, the so called Hertz law [11].

When these SWs collide with one another or with walls, they break and reform. Earlier work has suggested that energy-conservation conditions require the formation of low-energy (hence low-amplitude) SWs in the vicinity of the collision region. We called these waves secondary solitary waves (SSWs); they were first reported in numerical studies in Ref. [12] and later experimentally confirmed by Job *et al.* [13]. SSWs include all waves resulting from the collision of primary SWs, as well as waves arising from collisions of their by-products. Progressive breakdown of SWs would mean that eventually all energy would disappear. Hence, energy conservation requires that colliding SWs could also result in the effective increase in the energy of one of the SWs. This effect is indeed seen [14–17]. The balance of the breakdown and growth processes eventually leads the chain to the so-called quasiequilibrium (QEQ) state [17,18].

At first glance, the QEQ state may seem no different than the equilibrium state. However, it turns out that while the velocity distribution in this state is a Gaussian, the equipartition theorem does not hold [18]. Further, in some cases the system's evolution appears to have no memory of the initial conditions, whereas in others they do [17]. In addition, when one investigates the fluctuations in kinetic energy (K) of the Hertzian system in the QEQ state, one finds that the fluctuations are typically larger than those for a corresponding harmonic system [2]. These systems are also known to sustain metastable special regions such as breathers [19–21] and hot and cold spots for extended times [17], where the kinetic energy can be localized along well-defined regions along the chain. The conclusion is that this state is not the same as the equilibrium state as seen in a harmonic chain. Therefore, this state was named the *QEQ* state to distinguish it from the ordinary equilibrium state [14,18].

Job *et al.* established that it is possible to increase the energy content of the SSWs by softening the walls [13]. Since an increase in the amplitude of the SSWs would imply higher kinetic energy of these SWs, which are slowly produced in the vicinity of the collision region, it seems reasonable to expect slightly hotter temperatures near a soft wall even for small granular chains. Moreover, because soft materials propagate energy at a slower speed, one would expect the soft wall to remain slightly "hotter" for measurably long times, at least in dynamical simulations. Here we address whether our expectation is realized in a model system where the softness can be widely varied [22].

While the interaction of SWs with boundaries in confined granular chains with both walls made of the same material has been extensively investigated [2,17], little is known for systems placed between asymmetric boundaries. The aim of the present work is to investigate the short- and long-time behavior of a chain at zero dissipation between asymmetric boundaries. This paper is organized as follows. Section II outlines the model and numerical details. Results for the case of walls of different softnesses are presented in Sec. III. In Sec. IV we discuss our findings.

*e.avaloscycu@gmail.com
†sen@buffalo.edu

II. MODEL AND NUMERICAL DETAILS

We consider an alignment of N identical elastic spheres, each of mass m and radius R, placed in such a way that they are barely in contact with each other. There is no grain-grain interaction when there is no contact [1]. The alignment is held between walls of variable softness. The interaction potential is given as

$$V(x_{i+1}-x_i) = a[2R-(x_{i+1}-x_i)]^n \equiv a\delta_{i,i+1}^n \geqslant 0, \quad (1)$$

where x_i is the displacement of grain i from the original position (i.e., grains are at a distance of $2R$ between the centers initially), $2R \geqslant x_{i+1}-x_i \geqslant 0$, and $\delta_{i,i+1}$ is the overlap between the grains. Since the grains do not interact when the grain-grain contact is broken, for $2R < x_{i+1}-x_i$ or $\delta_{i,i+1} < 0$, $V(x_{i+1}-x_i) = 0$. More details on the properties of $V(\delta_{i,i+1})$ are discussed in some detail in Ref. [7]

According to the Hertz law, for spheres in contact, $n = 5/2$ [11]. Hence, the one-sided interaction potential is fully nonlinear in nature, i.e., there is no $n = 2$ term. This means that there is no acoustic propagation from grain to grain [1,23]. The equation of motion of each grain (except for the two boundary grains) is given by

$$m\frac{d^2x_i}{dt^2} = an\left[\delta_{i,i-1}^{n-1} - \delta_{i,i+1}^{n-1}\right], \quad n \geqslant 2, \quad (2)$$

where i runs from 1 to N. The calculations are done via a velocity-Verlet algorithm [24] and the outcomes are presented using dimensionless quantities. In our simulations, we assume, as reference, that spheres are made of Ti alloy (TiAlV), where Al and V are added to stabilize the corresponding Ti phases, with grain radius 5 mm, $\rho = 4.42$ mg/mm^3, $D = 0.012\,06$ mm^2/N. This value of D holds also for the reference value of the walls. To change the value of softness, a factor f_D was placed before the value of a. The integration time step dt was set to 10^{-6} μs. To initiate the dynamics, we start a δ function velocity perturbation at one end of the chain that develops into a propagating SW in the system within about 10 grain diameters from the edge [25]. The SW velocity depends on the magnitude of the initial perturbation, $V_0 = 0.01$ [1,2].

III. ASYMMETRIC BOUNDARIES

Here we consider an array of $N = 31$ beads of equal size and softness, located between a hard wall and a soft wall. During the early stages of the dynamics, a SW propagates along the chain initiating a series of collisions against the walls and against other waves. As is shown in Fig. 1, the time to form reflected SWs increases with wall softness. The various collision processes lead to the formation of SSWs of various energy contents, which in turn collide with each other and with the walls. Figure 1 shows the trajectories of the main SW and other lower-energy SWs for increasingly larger values of wall softness. The gray scale in the figures indicates the energy content of the SWs. Note that SW's velocity reverses its direction when it bounces from the wall, and this is indicated by a gap in the light gray color. The emergence of SSWs can be seen at late times in the gray scale plots in Figs. 1(a)–1(d). It may be possible to actually observe the stickiness of the SWs in the vicinity of soft walls at early times. However, since all real granular systems are dissipative, the late time effects discussed below may not be easily seen in granular systems in the laboratory. However, seeing the simulated behavior is not expected to be a problem in the circuit realizations of these systems [22].

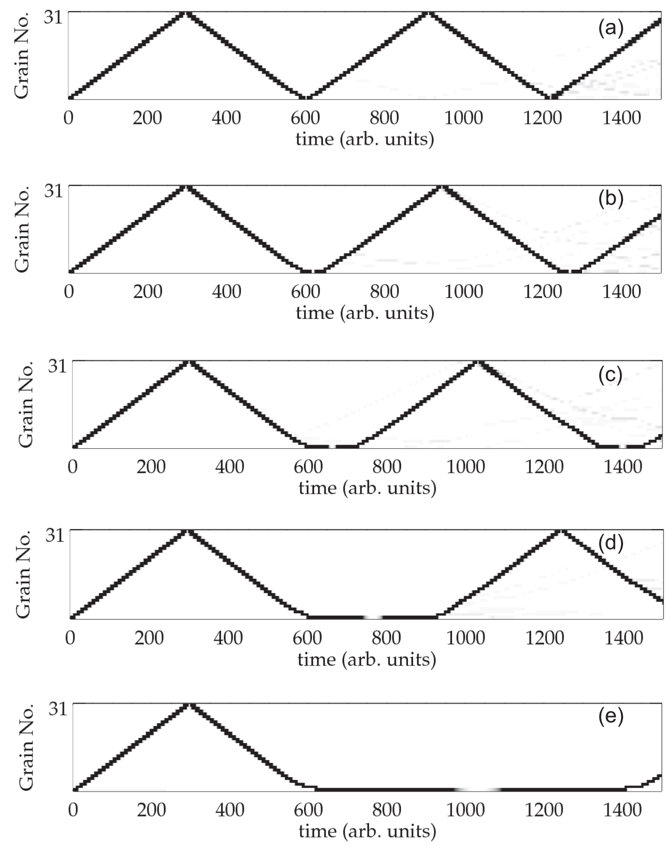

FIG. 1. Lengthening of collision time for increasingly softer walls. In each case, the soft wall becomes softer by a factor f_D. From top to bottom, $1/f_D = 1$, 10, 100, 1000, and 10 000.

A notable feature in Fig. 1 is the lengthening of the time of formation of reflected SWs as the wall increases in softness. This suggests that the particle adjacent to the soft wall possesses an average kinetic energy that is likely to be larger than the particle adjacent to the opposite wall. This is indeed correct, but as we shall see, only for early times. We show that for long times, the average kinetic energy at the ending particles adjacent to the walls is indistinguishable.

Another characteristic of SWs colliding with soft materials is that the resulting SSWs created from the collision are more energetic [13]. Figure 2 shows snapshots around the time of the first collision at the soft and hard walls. Note that SSWs near the soft wall can be better appreciated on this scale, whereas near the hard wall SSWs are too small to be seen in the same scale of energy. Next, we show that the presence of SSWs of higher energy at the soft wall does not imply larger average kinetic energy across extended time scales.

Landscape of energy. Since our goal is to investigate the role of wall softness in the time evolution of a granular chain, it would not be useful to be too worried about the softnesses of readily available materials. For this reason, we will use widely varying values of softening, and for now we will set

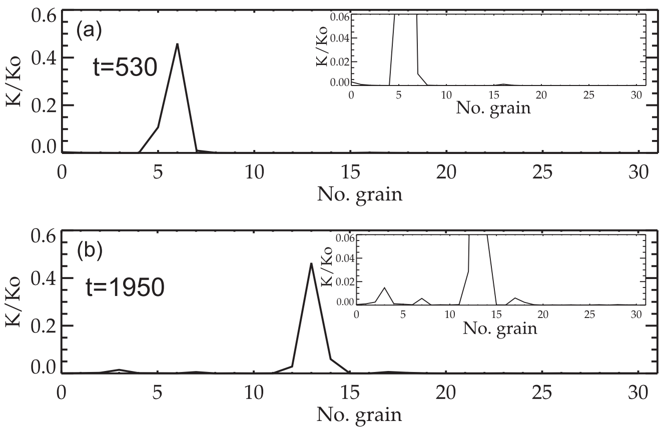

FIG. 2. Kinetic energy around collision times at (a) hard wall and (b) soft wall. The y axis in the insets has been amplified 10 times to show the finest detail of SSW formation. Values are normalized with the magnitude of the initial impulse, K_0, and the snapshot time is indicated.

the softening factor $f_D = 0.0001$ at one end of the chain and $f_D = 1$ at the other end, keeping in mind that circuit realizations of such systems are likely possible [22]. After a few round trips of the original pulse in the chain, the spatiotemporal energy distribution of the system reveals a roughly gray color with significant energy fluctuations in the gray scale plots, as shown in Fig. 3. The top figure represents the system's state in an intermediate stage of the simulation. As expected, the reflection of the SW from the soft wall takes longer times. However, in the long term, the asymmetric interaction with the walls does not result in a robust asymmetric distribution of average kinetic energy, even though the difference in wall softnesses is notable.

To measure how the energy of the particles adjacent to walls of different softnesses affects the distribution of kinetic energy over time, we look at the values of kinetic energy at both ending particles at each time step. We say that at a particular time step the wall is hot if its kinetic energy is larger than some appropriate minimum value. Considering the maximum energy value normalized to 1, we choose $1/100$ as the minimum value for the wall to be considered hot. Then, we add all the time periods in which the soft and hard walls are hot, and we divide the result by the total measurement time T. This quotient is written as $\Sigma T_{K>0}$ and it is a measure of the fraction

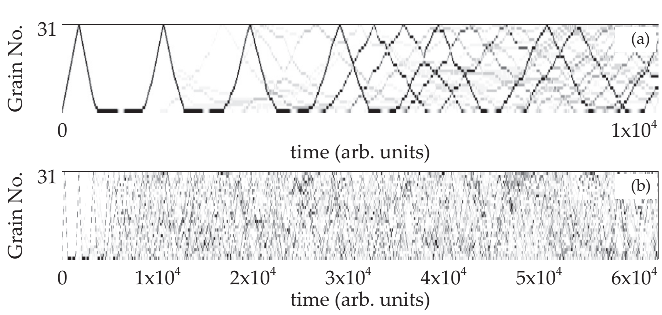

FIG. 3. Energy landscape of a chain between asymmetric boundaries. (a) Short-time simulation, (b) long-time simulation.

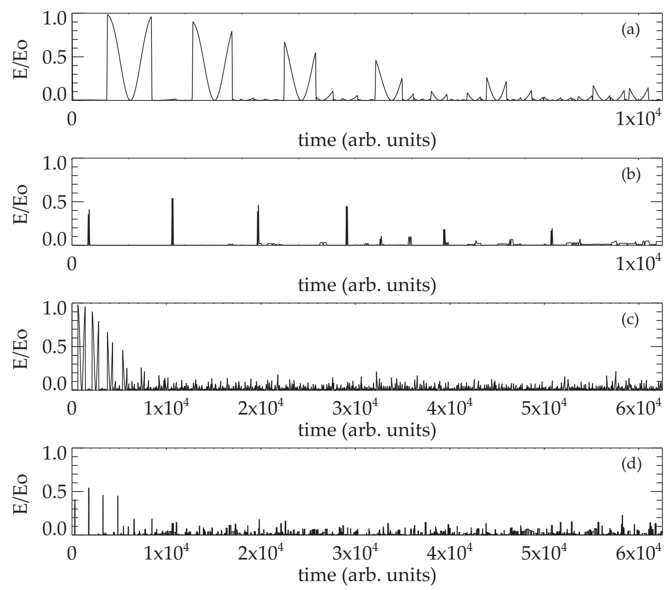

FIG. 4. Normalized energy of the first and last bead in the chain. These figures correspond to the case shown in Fig. 3. Parts (a) and (b) are the energies of grains $i = 1$ and 31, respectively, during the first 10 000 time steps. Parts (c) and (d) are the energies of the grains $i = 1$ and 31, respectively, at long times. Energy is normalized with the value of the initial impulse.

of time in which the energy content of the walls is significant during a time window T. We write this dimensionless quantity as follows:

$$\Sigma T_{K>0} = n_T/T, \tag{3}$$

where n_T is the number of time units in which the wall has an energy larger than $1/100$ in a time window of length T.

In this case, the total fraction of time in which the soft and hard walls are hot is $\Sigma T_{K>0} = 0.476$ and 0.438, respectively. We have employed the last 30 000 time steps in Fig. 3(b) as a time window. This constitutes a difference of less than 9% between the two walls. It should be noted here that the presence of precompression in the chain tends to raise the speed of energy propagation between the ends and does not help to sustain any kinetic energy differences between the walls.

The energy landscape shown in Fig. 3 accounts for the energy of the entire chain. In contrast, focusing on the energy of individual beads at each end of the chain allows us to compare side by side the effect on those grains immediately adjacent to the walls. To do this, we plot the time evolution of the energy at each end of the chain. Figure 4 shows the energy of the first and last beads in the chain. Similar to what is shown in the energy landscape in Fig. 3 at early times, Fig. 4 shows that the grain adjacent to the soft end holds energy for longer times than the grain at the other end does. Nonetheless, this effect diminishes when looking at long times, as illustrated in panels (c) and (d). Panels (c) and (d) in Fig. 4 represent the time evolution of energies of the ending grains within the QEQ region [18]. However, the effect of the soft wall is not appreciable in this figure even when looking at the energy per grain averaged over long times, as shown in Fig. 5. The energy scale is normalized with the energy of the initial impulse,

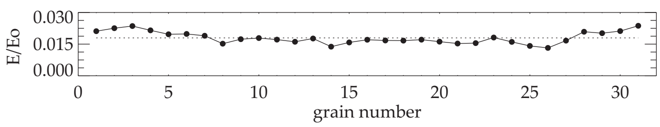

FIG. 5. Averaged kinetic energy per grain vs grain number. Kinetic energy is averaged in a time window corresponding to the time interval of Fig. 3 at late times (last 10 000 time steps). The dashed line indicates total average value.

$1/2V_0^2$. Note that the average kinetic energy in the whole chain is $0.01796 \times 31 = 0.556$, which is the value predicted by the virial theorem.

Dynamical and statistical analysis. Another way to assess the effect of breaking the symmetry on the distribution of kinetic energy is by looking at the statistical evidence along with making a simple dynamical analysis. Figure 6 shows phase portraits of individual grains that are symmetrically located along the chain. Panel (a) is for grain numbers 1 and 31. When looking at dynamical features, it is necessary to focus on long-time stages because the primary interest is the QEQ state. Therefore, this figure corresponds to approximately 15 000 time steps after QEQ has been established. Axes x and y, respectively, show the relative position and its time derivative (velocity) for these two grains. The most notable feature in this figure is that the grain adjacent to the soft wall has a wider range of motion than the grain adjacent to the hard wall, which indicates that grain no. 1 has access to larger energies.

Figure 6(b) shows the phase portrait of grain no. 13 and no. 19. These grains are located near the center of the chain at equal distances from the walls. Note that both grains have similar ranges of motion, which indicate that these two grains have access to a similar range of energies.

Panel (c) in this figure shows phase portraits for grain no. 1 and no. 31 of a reference system in which both walls are of equal softness. The reference system lacks the asymmetric interaction with the boundaries, and therefore it does not exhibit an unbalanced distribution of energy. If we look closely at the ending grains in the asymmetric case shown in panel (a) and the reference case in panel (c), one can state that the role of the soft wall is certainly related to the energy gain of grain no. 1.

Velocity distribution. For a gas in equilibrium, the constituent particles acquire energies according to a Boltzmann weighting. In a particulate chain with symmetric boundaries,

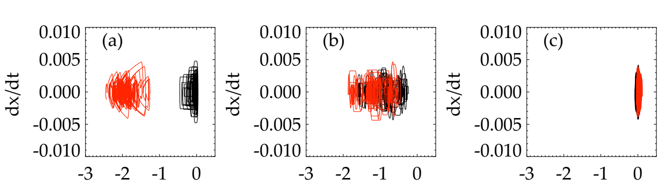

FIG. 6. (Color online) Phase-portrait of grains no. (a) 1 (red or gray) and 31 (black), (b) 13 (red or gray) and 19 (black), for the case of one hard wall and one soft wall. Panel (c) is the phase portrait of a reference system in which both walls are of equal softness. Grains no. 1 (red or gray) and no. 31 (black) are shown.

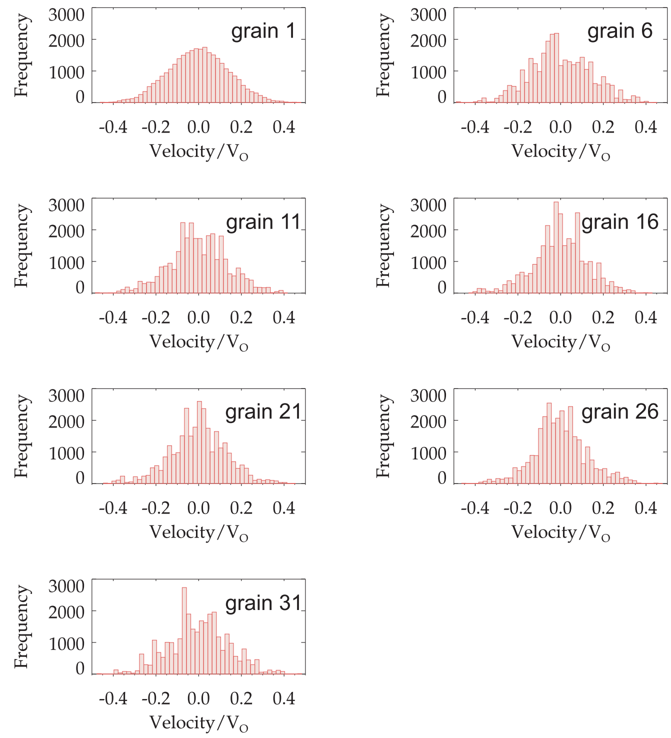

FIG. 7. (Color online) Velocity distribution binning per grain.

once the QEQ state has been reached, the grains in the chain obey the normal Gaussian distribution [26]. For the asymmetric chain, we pay special attention to the end grains, because those are in direct contact with the soft and hard walls. Figure 7 shows velocity distributions for grains no. 1, 6, 11, 16, 21, 26, and 31. The vertical axis represents the count per bin. These distributions are made using approximately 30 000 time units after the QEQ state has been reached. Although the soft wall smooths out the velocity distribution of energy at the soft end, velocity distributions turn out to be symmetric for all the grains. In other words, the soft wall has no appreciable effect on the velocity distribution at the boundary grains.

Figure 8 shows time averages, $\langle V^2\rangle_T/V_0^2$, for all the grains and the ensemble averages, $\langle V^2\rangle_S/V_0^2$, corresponding to the last 30 000 time units (see Fig. 3). The total average in

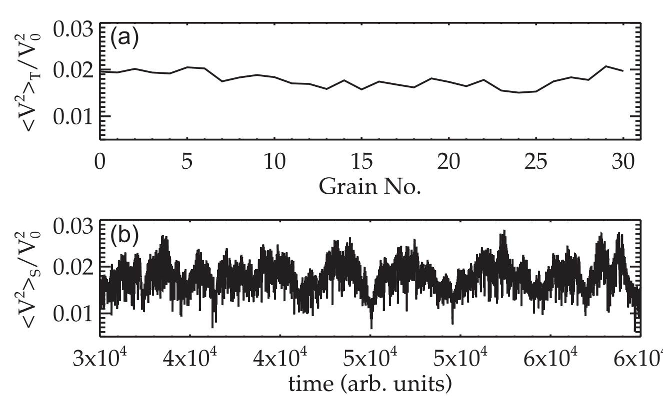

FIG. 8. (a) Time averages of the entire system and (b) ensemble averages over 30 000 time units.

both cases is 0.01789, which is in agreement with the value predicted by the virial theorem for every grain in the chain. Thus, the system appears to be ergodic.

IV. CONCLUSION

In this work, we have studied the time evolution of a velocity perturbation initiated at time $t = 0$ in a granular chain using dynamical simulations. The chain is held between fixed boundaries—one of these is a soft wall whereas the other is a rigid wall [1,2].

Let us first talk about a granular chain that is held between rigid walls. It is well known that any velocity perturbation results in a SW in these systems. These SWs break and reform when they collide with the walls and with one another. These processes give birth to SSWs, which are SWs that are born out of the first SW-wall collision and subsequent collisions and are of much lower energy content than the original SW. The continuous interaction between the SSWs of all energy contents typically leads to an equilibrium-like phase, the QEQ phase, with normal Gaussian distribution of velocities (or equivalently, Boltzmann distribution of energies, large fluctuations, and loss of memory of initial conditions [18]). When one of the walls is softer than the other, the SWs break and form SSWs of higher energy content than when the wall is rigid. This gives rise to higher kinetic energies near the vicinity of the soft wall [13]. The question we have addressed is whether this kinetic energy gradient is sustainable in this QEQ state, which is possible for strongly nonlinear systems. Our studies suggest that at short and even intermediate times, there is a kinetic energy gradient that may be seen if the soft wall is sufficiently soft. However, at large times, this gradient is erased. We find that the system behaves like an ergodic system and appears to have no memory of the initial conditions, thus suggesting that the QEQ state is a robust state.

ACKNOWLEDGMENT

S.S. thanks US Army Research Office for partial support of this research.

[1] V. F. Nesterenko, J. Appl. Mech. Tech. Phys. **24**, 733 (1983); A. N. Lazaridi and V. F. Nesterenko, *ibid.* **26**, 405 (1985); V. F. Nesterenko, J. Phys. IV **4**, C8-729 (1994); A. Chatterjee, Phys. Rev. E **59**, 5912 (1999); for a comprehensive review of the dynamics of granular chains, see V. Nesterenko, *Dynamics of Hetereogeneous Materials* (Springer, New York, 2001), Chap. 1.

[2] S. Sen, J. Hong, J. Bang, E. Avalos, and R. Doney, Phys. Rep. **462**, 21 (2008).

[3] C. Coste, E. Falcon, and S. Fauve, Phys. Rev. E **56**, 6104 (1997).

[4] R. S. Sinkovits and S. Sen, Phys. Rev. Lett. **74**, 2686 (1995); S. Sen and R. S. Sinkovits, Phys. Rev. E **54**, 6857 (1996).

[5] S. Sen, M. Manciu, and J. D. Wright, Phys. Rev. E **57**, 2386 (1998).

[6] A. Rosas and K. Lindenberg, Phys. Rev. E **68**, 041304 (2003); **69**, 037601 (2004); U. Harbola, A. Rosas, A. H. Romero, M. Esposito, and K. Lindenberg, *ibid.* **80**, 051302 (2009); U. Harbola, A. Rosas, M. Esposito, and K. Lindenberg, *ibid.* **80**, 031303 (2009).

[7] J. Y. Ji and J. Hong, Phys. Lett. A **260**, 60 (1999); J. Hong, J. Y. Ji, and H. Kim, Phys. Rev. Lett. **82**, 3058 (1999); J. Hong and A. Xu, Phys. Rev. E **63**, 061310 (2001).

[8] E. Hascoët and H. J. Herrmann, Eur. Phys. J. B **14**, 183 (2000).

[9] C. Daraio, V. F. Nesterenko, E. B. Herbold, and S. Jin, Phys. Rev. E **72**, 016603 (2005).

[10] F. Santibanez, R. Munoz, A. Caussarieu, S. Job, and F. Melo, Phys. Rev. E **84**, 026604 (2011).

[11] H. Hertz, J. Reine Angew. Math. **92**, 156 (1881).

[12] M. Manciu, S. Sen, and A. J. Hurd, Phys. Rev. E **63**, 016614 (2000); F. S. Manciu and S. Sen, *ibid.* **66**, 016616 (2002).

[13] S. Job, F. Melo, A. Sokolow, and S. Sen, Phys. Rev. Lett. **94**, 178002 (2005).

[14] E. Avalos, R. Doney, and S. Sen, Chin. J. Phys. **45**, 666 (2007).

[15] E. Avalos and S. Sen, Phys. Rev. E **79**, 046607 (2009).

[16] W. Zhen-Ying, W. Shun-Jin, Z. Xiu-Ming, and L. Lei, Chin. Phys. Lett. **24**, 2887 (2007).

[17] E. Ávalos, D. Sun, R. L. Doney, and S. Sen, Phys. Rev. E **84**, 046610 (2011).

[18] S. Sen, T. R. Krishna Mohan, and J. M. M. Pfannes, Physica A **342**, 336 (2004); S. Sen, J. M. M. Pfannes, and T. R. Krishna Mohan, J. Kor. Phys. Soc. **46**, 571 (2005); T. R. Krishna Mohan and S. Sen, Pramana J. Phys. **64**, 423 (2005).

[19] See, for example, A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).

[20] G. James, P. G. Kevrekidis, and J. Cuevas, Physica D **251**, 39 (2013).

[21] N. Boechler, G. Theocharis, S. Job, P. G. Kevrekidis, M. A. Porter, and C. Daraio, Phys. Rev. Lett. **104**, 244302 (2010).

[22] It may not be possible to vary softness widely in a granular system, but circuit realizations of such systems may help to realize a broad range of parameter values; see, for example, L. Sellami, R. W. Newcomb, and S. Sen, Mod. Phys. Lett. B **27**, 1350093 (2013).

[23] V. Vitelli and M. van Hecke, Europhys. News **43**, 36 (2012).

[24] M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids* (Clarendon, Oxford, 1987).

[25] A. Sokolow, E. Bittle, and S. Sen, Europhys. Lett. **77**, 24002 (2007); S. Job, F. Melo, A. Sokolow, and S. Sen, Gran. Matter **13**, 10 (2007).

[26] B. Doney, Ph.D. dissertation, State University of New York, 2007.