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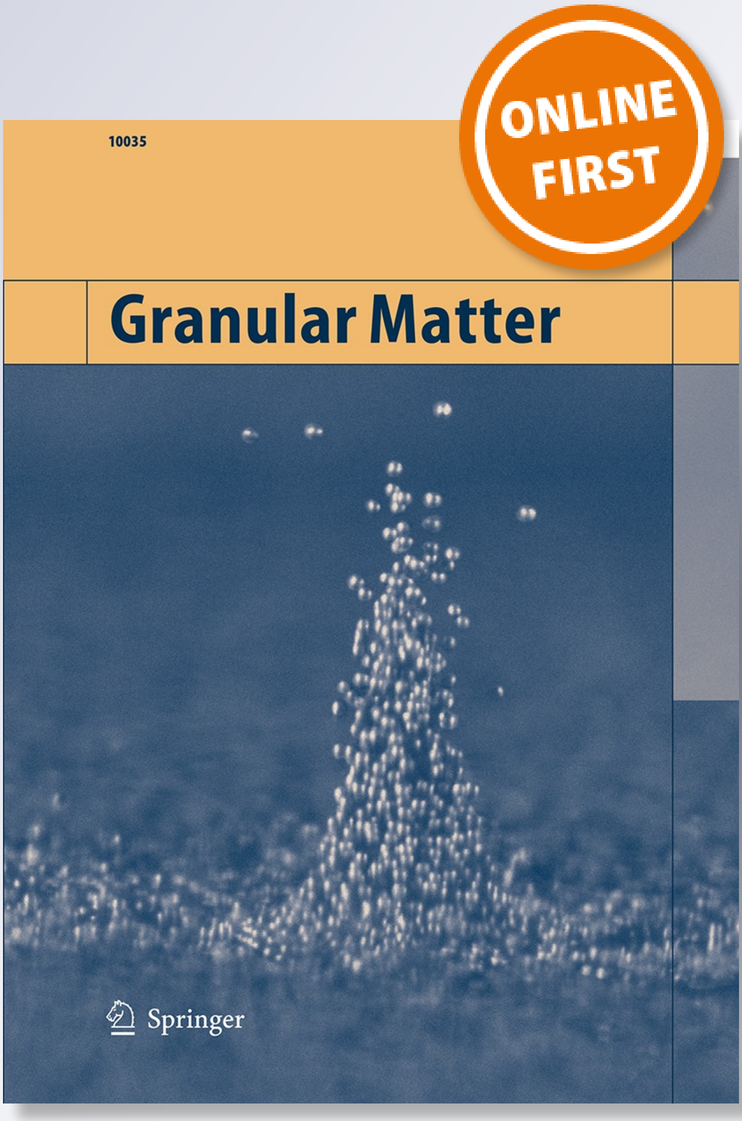
Granular Matter

ISSN 1434-5021

Granular Matter
DOI 10.1007/s10035-013-0400-5



Springer

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DOI 10.1007/s10035-013-0400-5

ORIGINAL PAPER

Nonlinear grain–grain forces and the width of the solitary wave in granular chains: a numerical study

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Received: 5 July 2012 / Accepted: 5 February 2013

Abstract Any impulse results in the formation of a solitary wave of time averaged width W in a granular chain. If the grain–grain interaction potential $V \sim \delta^n$, where δ is the distance by which the grains approach each other, then it is well established that $n \geq 2$. Here we present dynamical simulation based results which suggest that $W - 1 \propto (n-2)^{-\alpha}$ where $\alpha = 0.3283$ or $\approx$1/3. While in qualitative agreement, the result is quantitatively different from the formula for W proposed earlier by Nesterenko.

Keywords Solitary waves · Granular chain · Nonlinear forces · Hertz law

1 Introduction and motivation

In 1881, Hertz showed that when two elastic spheres are gently pressed against one another, they repel according to a nonlinear potential [1]. More than a century later, starting in 1983, Nesterenko carried out experimental and theoretical studies to show that an alignment of grains that are barely in contact, i.e., without the grains being precompressed, converts any impulse or δ function velocity perturbation to an edge grain into a propagating non-dispersive energy bundle or a solitary wave [2–5]. Existence of solitary waves in any system presents the possibility of enhanced energy transport through them and hence may be of interest from both scientific and engineering vantage points. These solitary waves have since been studied widely [6–19]. It has been established that the solitary wave that is found in the granular chain is distinct from the other well known solitary waves in known solitary wave bearing systems [20,21].

Nesterenko constructed an approximate stationary state solution to the dynamical equation which describes the solitary wave as one period of an otherwise continuous periodic solution. This solution is in the continuum limit of the space variable. The very definition of a period means that the solution has well defined limits. Thus Nesterenko's work naturally lend itself to measuring the width of the solitary wave [4,5].

In 2001, Sen and Manciu carried out numerical simulations and also developed an improved solution to the problem of solitary wave propagation in a granular chain [14]. These studies showed that the energy contained in the solitary wave in the stationary state approaches zero at the edges. Their study implies that estimating the width of the solitary wave ultimately depends upon the accuracy to which measurements can be made. Nevertheless, experimental measurements are always accuracy limited and both Nesterenko's and Sen and Manciu's works are in reasonable agreement with the experimentally measured results and with each other [20].

In a recent study, however, it has been suggested that it may be experimentally feasible to change the nonlinearity of the potential between the two grains in contact when the contact interfaces are not elliptical [22–25]. Such modifications have been shown to lead to Hertz-like potentials with different nonlinearities. Studies show that this means that the width of the solitary wave may be different when the nonlinear grain–grain potential changes [4,26]. When the potential is steeper than the Hertz law, the solitary wave will have a narrower width than in the chain of spherical grains. When the potential is softer, more like harmonic, the width will become quite large in keeping with the fact that in the harmonic limit there is no solitary wave and hence the width diverges. One

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Published online: 17 February 2013

then faces the following intriguing possibility—can we make granular assemblies where the propagating energy pulse can be squeezed or dilated? Here we try to understand to what degree the width of the solitary wave will be influenced by the nonlinearity in the potential. We show that the width depends on nonlinearity according to a power law. While in qualitative agreement with Nesterenko's original prediction regarding how width will vary with nonlinearity, the result presented below is quantitatively different.

This paper is organized as follows. In Sect. 2 we present the details of the model and the calculations. The results are presented in Sect. 3. We conclude with a summary and a discussion on the possible implications of this study.

2 Model details

We consider an alignment of N identical elastic grains, placed at positions x_i, each of mass m and of width (i.e., diameter for the special case of purely spherical grains) $2R$, 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]. We assume that the alignment is very long and held between perfectly reflecting walls. Wall effects will not enter into our discussions in this work. We will be concerned with solitary waves in their stationary states and hence far from boundaries, which means that in our system, the number of grains N will be quite large, typically with $N = 500$.

The interaction potential [1] is given as

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

where $a = \frac{2}{5D}\left(\sqrt{\frac{R}{2}}\right)$, $D = \frac{3}{2}\left(\frac{1-\sigma^2}{Y}\right)$, where Y, σ represent the Young's modulus and the Poisson's ratio, respectively, x_i is the position of grain i as measured from some appropriate origin and $\delta_{i,i+1}$ is defined as the overlap between the grains. Observe that the grains do not interact when the grain–grain contact is broken and when $x_i - x_{i+1} = 2R$.

For grains with circular or elliptical contacts, as per Hertz law, $n = 5/2$ [1]. Hence, the interaction potential is fully nonlinear in nature, i.e., there is no $n = 2$ term and hence there is no chance of any oscillatory dynamics of any of the grains when they are in contact. In turn, this means that there is no acoustic propagation from grain to grain as emphasized extensively in the literature [5,9,10]. It may be noted that one can formally show that for the majority of grain–grain contact potentials $n > 2$ [27]. To illustrate the effects of n in influencing the dynamics of the system, we will use various n values below. In this context we observe that various values of n can be realized by using grain–grain contacts that are non-elliptical as discussed in Ref. [25]. Further, a well known case of $n = 7$ has been experimentally realized in a chain of rings by several authors [22–24]. The value of a [Eq. (1)] also depends on the geometry of the grain–grain contact as shown in Refs. [25,28]. However, this aspect is not very important for our purposes because we are interested in the average width of the solitary waves that form in our systems and such widths are expressed simply in terms of $2R$. Thus, the details of the constants used in the simulations with a given n only play the role of modifying the energetics of the system and has no effect on the width of the solitary wave, which is what we are most interested in now. This realization simplifies the task at hand. The equation of motion of each grain (except for the two boundary grains) is given by

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

where i runs from 1 to N.

The calculations have been done via a velocity Verlet algorithm [29]. We set $m = 2.314 \times 10^{-2}$ kg, $a = 1.65836 \times 10^6$ J/m$^{5/2}$ and the total energy E_{tot} imparted via a δ function velocity perturbation to the edge grain where the total energy is set to 0.115715 J in all of our studies [30]. These numbers are consistent with those of quartz type materials. It is important to note that the amplitude associated with the initiated velocity perturbation must be $\ll 2R$ and is not important in the sense that it has no effect on the geometrical properties of solitary wave produced. It should be mentioned, however, that smaller amplitudes produce less energetic solitary waves than higher amplitudes and as is well known, the velocity of the solitary wave is dictated by its energy content [5,10]. The integration time step dt was set to 10^{-5} µs Reflecting boundary conditions are used at the walls.

In his pioneering studies [5], Nesterenko reported both experiments and theory. In the theoretical analyses, he assumed that the physical problem was well approximated by a weak impulse perturbation that is initiated at one end of a sufficiently long, weakly precompressed granular chain. He replaced Eq. (2) under weak precompression by a continuum equation that is expected to be approximately valid in the long wavelength approximation. The perturbation across time and space develops into a solitary wave as described in detail in Ref. [31]. In real time and space, the propagating energy pulse exhibits successive contractions and expansions in spatial extent much, like the way in which a caterpillar moves. However, the time averaged width, also the steady state width of the solitary wave assumes that the width is fixed in space and time and that the spatial and temporal coordinates are related by the velocity of the solitary wave. Nesterenko's stationary state solution to the continuum limit of Eq. (2), with some approximations, yields an equation that can be solved by a periodic function. Nesterenko showed that a single period of this solution (without the remaining periodic pieces) serves as a good approximation to the solution of the original equations of motion [2–5]. The total width of this wave then yields a width of the solitary wave. Nesterenko has shown that this width (defined by a single period), written as a function of n is given by

$$W = \frac{2\pi R}{n-2}\sqrt{\frac{n(n-1)}{6}}. \qquad (3)$$

For $n = 5/2$, this yields $W \approx 10R$, which is consistent with the measurements that have been done. Observe that as $n \to \infty$, that is when each grain acts like a hard sphere, $W \approx 2.56R$ or slightly more than a grain in width, not bad for a continuum theory that is not supposed to be reliable in this limit. An important point to note is that Nesterenko's solution has compact support, and hence the edges are well defined. It is, however, long known that an improved version of this solution that was developed by Sen and Manciu [14] does not have compact support. Therefore in an infinite system, the solitary wave would have a finite half width at half maximum but would be infinite in extent, as would be the case for instance for a solitary wave whose velocity distribution in space is described by an appropriate hyperbolic function. In reality, we cannot really say whether a solitary wave has compact support or not because our measurements are limited by precision. Same is the case for numerical studies where the extent of a solitary wave is eventually controlled by how small of a number is too small to be meaningful.

3 Results

In what follows, we will focus on the time averaged width $\langle W \rangle$, where $\langle \cdots \rangle$ implies a time average. Given the absence of compact support in the Sen and Manciu solution [14], we have used an indirect approach to measure the width of the solitary wave for a given n. Our main objective, however, is to find how W varies as a function of n. Based on Nesterenko's result and physical considerations in Eq. (3), we expect $W \to 1$ as $n \to \infty$ (ballistic limit where each grain is a hard sphere). Thus W varies between 1 and ∞, the latter being the case when $n \to 2$ and the interaction becomes quadratically dependent on δ and a solitary wave solution to the linear equations is no longer admissible.

It is important to note that in the absence of an exact solution to the equations of motion [(characterized by Eq. (2)], the definition of W is always going to be model dependent whether one is doing theory and/or simulations and will be experimental accuracy dependent in experiments. However, as we shall see, because Nesterenko's W and our W satisfy the same limits, and W only depends on n as shown by Nesterenko and others, it turns out that the behavior of W (in terms of grain diameter) as a function of n is not sensitive to precisely how W is defined as long as the same conditions are applied to find W.

Our goal now is to develop a relation between the steepness of the potential with increasing overlap δ in Eq. (1)

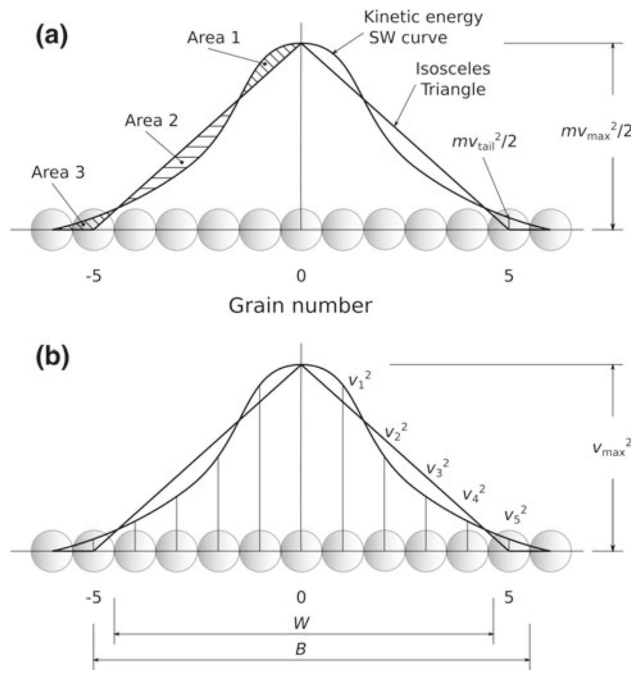

Fig. 1 Panels **a** and **b** are almost identical and show different aspects of the solitary wave in its stationary state. These two panels are meant to help understand Eq. (4) in the paper. In **a** the distribution of kinetic energy in a solitary wave with its center at a grain center is shown and its geometrical features are elucidated. The areas 1, 2 and 3 are defined in **a**. In **b**, we show the velocity squared for each grain explicitly and B and W are explicitly shown as well. Note that B exceeds W by a single grain diameter and the origin of this difference lies in the shape of the solitary wave in the stationary state. See the discussion around Eq. (4) in the text for further details

and the width of the solitary wave W. As we shall see, our results will reveal that W is independent of all quantities except n, which is in agreement with Nesterenko's results [2,5]. In the stationary state, the energy in the solitary wave is also the total energy E_{tot}. To measure the edges of the solitary wave from the simulation based data, we define the ratio of the grain–grain overlaps at the tail versus at the center, $\delta_{tail}/\delta_{max} < 10^{-8}$ as the equivalent of zero. This choice allows us to define the extremeties of the solitary wave for our analyses. The same criterion is used to define W regardless of the value of n.

Figure 1a, b represent the kinetic energy versus in the solitary wave as a function of space. We note that the grain with the highest kinetic energy, has velocity v_{max}. We now draw an isosceles triangle with the grain with velocity v_{max} at the center and with a base B being such that we satisfy the condition that the sum of the areas of the black regions equals that of the shaded region in Fig. 1a. Given the kinetic energy distribution in space of the solitary wave (Fig. 1a, b), our numerical analyses show that for the stated area condition to be satisfied, $B \geq 2$. This area condition suggests we describe the total kinetic energy of the solitary wave, $\langle KE \rangle$ as

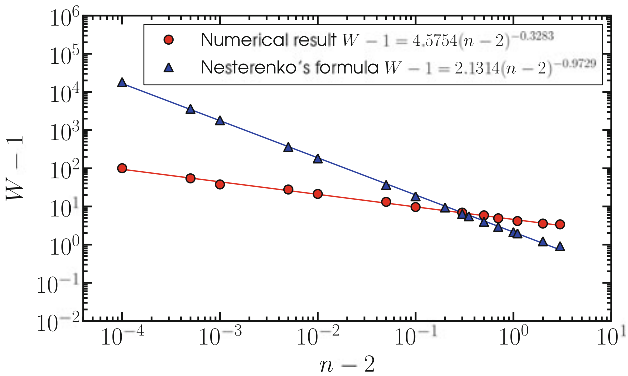

Fig. 2 (Color online) Plot of $W-1$ versus $n-2$ showing Nesterenko's continuum theory based formula expressed as a power law fit and those resulting from the present dynamical calculations based on Eqs. (2) and (4)

$$\langle KE\rangle = \frac{1}{2}B\left[\frac{1}{2}mv_{max}^2\right] \equiv \frac{1}{4}(W+1)mv_{max}^2, \tag{4}$$

where the identity above represents the total kinetic energy contained in the solitary wave whose width W is chosen to be such that $W+1 \equiv B$. Observe that the smallest B is 2 and this means the smallest $W = 1$ as we have already argued above. We further elaborate on this argument below.

Now, according to virial theorem of mechanics [32], the kinetic energy of the solitary wave is $\langle KE\rangle = \frac{n}{n+2}E_{tot}$, where $\langle\cdots\rangle$ represents a time average and E_{tot} is the total energy which must equal $\frac{1}{2}mv_0^2$, where v_0 is the velocity associated with the initial perturbation imparted to the system. Thus, we can write

$$W = \frac{4n}{n+2}\left(\frac{E_{tot}}{mv_{max}^2}\right) - 1 = \frac{2n}{n+2}\left(\frac{v_0^2}{v_{max}^2}\right) - 1. \tag{5}$$

Equation (5) above allows us to use the simulational data to infer v_{max} for each of our simulations for fixed n and obtain W. Our results suggest that $W \to 1$ as $n \to \infty$. It is interesting to note here that if we vary the initial velocity perturbation to the edge grain, the amount of energy being transmitted through the chain will vary as a function of the kinetic energy imparted in the perturbation. If we express this energy in terms of the momentary compression A suffered by the edge grain when a gentle impulse is initiated at one end of the chain, then based on Eq. (1), $E \sim A^n$. As shown in Eq. (9) in Sen and Manciu [14], $v_{max}^2 \sim A^n$. This means that W is independent of A as it should be. Unfortunately, however, the existing solution does not allow us to do further analysis. By obtaining v_{max} from our dynamical simulations, we are now able to readily obtain W. The plot in Fig. 2 suggests

$$W - 1 \propto (n-2)^{-\alpha}. \tag{6}$$

where $\alpha = 0.3283$ or $\approx 1/3$. This behavior differs quantitatively from Nesterenko's width formula [Eq. (3)] based behavior although the qualitative behavior of W versus n and the asymptotic behavior are the same for both.

4 Conclusion

The extent of the solitary wave characterized by its width W is known to depend on the index of the nonlinear law n. Nesterenko had proposed the only known relationship between W and n based on his solution to a continuum equation that is closely related to the actual dynamical equations obeyed by the grains. Here we show that while an analytical formula improving Nesterenko's formula is not at hand, simulations based on the actual dynamical equations without any long wavelength or continuum approximations suggest that W behaves quantitatively differently than proposed by Nesterenko. However, there is broad qualitative agreement between Nesterenko's formula and the numerical results presented here.

The solitary wave becomes one grain diameter wide as $n \to \infty$ and diverges at $n \to 2$. Now that we have developed an understanding of how n can be changed by changing the geometry of the grain–grain interfaces, it is possible to control n as needed [25,30]. Hence, using our proposed relationship between W and n it may some day be possible to design granular alignments with novel capabilities to focus and defocus the energy of propagating solitary waves.

Acknowledgments This work has been partially supported by the US Army Research Office through a STIR Grant. We thank Yoichi Takato for his role in redoing the figures. Sourish Chakravarty's help with the figures is also gratefully acknowledged.

References

1. Hertz, H.: Über die behrührung fester elastischer körper. J für die reine U. angew. math. **92**, 156–171 (1882)
2. Nesterenko, V.F.: The propagation of nonlinear pressure pulses in granular mediums. Prikl. Mekh. Tekh. Fiz. **5**, 136–148 (1983)
3. Lazaridi, A.N., Nesterenko, V.F.: The detection of isolated waves of a new type in a one-dimensional granular medium. Prikl. Mekh. Tekh. Fiz. **3**, 115–118 (1985)
4. Nesterenko, V.F.: Solitary waves in discrete media with anomalous compressibility and similar to "sonic vacuum". J. de Physique IV, Colloq C8, suppl. au J. de Physique III, 4, C8-729–C8-734 (1994), see Eq. (12)
5. Nesterenko, V.F.: Dynamics of Heterogeneous Materials. Springer, New York (2001)
6. Sinkovits, R.S., Sen, S.: Nonlinear dynamics in granular columns. Phys. Rev. Lett. **74**, 2686–2689 (1995)
7. Sen, S., Sinkovits, R.S.: Sound propagation in impure granular columns. Phys. Rev. E **56**, 6857–6865 (1996)
8. Coste, C., Falcon, E., Fauve, S.: Solitary waves in a chain of beads under Hertz contact. Phys. Rev. E **56**, 6104–6117 (1997)
9. Coste, C., Gilles, B.: On the validity of the Hertz contact law for granular material acoustics. Eur. Phys. J. B **7**, 155–168 (1999)

10. Sen, S., Manciu, M., Wright, J.D.: Soliton-like pulses in perturbed and driven Hertzian chains and their possible applications in detecting buried impurities. Phys. Rev. E **57**, 2386–2397 (1998)
11. Manciu, M., Sen, S., Hurd, A.J.: The propagation and backscattering of soliton-like pulses in a chain of quartz beads and related problems: I. Propagation. Physica A **274**, 588–606 (1999)
12. Hascoët, E., Herrmann, H.J., Loreto, V.: Shock propagation in a granular chain. Phys. Rev. E **59**, 3202–3206 (1999)
13. Hascoët, E., Herrmann, H.J.: Shocks in non-loaded bead chains with impurities. Eur. Phys. J. B **14**, 183–190 (2000)
14. Sen, S., Manciu, M.: Solitary wave dynamics in generalized Hertz chains: an improved solution of the equation of motion. Phys. Rev. E **64**, 056605 (2001)
15. Wu, D.T.: Conservation principles in soliton impulse propagation through granular chains. Physica A **315**, 194–202 (2002)
16. Rosas, A., Lindenberg, K.: Pulse propagation in chains with nonlinear interactions. Phys. Rev. E **69**, 016615 (2004)
17. Rosas, A., Lindenberg, K.: Pulse velocity in a granular chain. Phys. Rev. E **69**, 037601 (2004)
18. Melo, F., Job, S., Santibanez, F., Tapia, F.: Experimental evidence of shock mitigation in a Hertzian tapered granular chain. Phys. Rev. E **73**, 041305 (2006)
19. Job, S., Melo, F., Sokolow, A., Sen, S.: How Hertzian solitary waves interact with boundaries in a 1D granular medium. Phys. Rev. Lett. **94**, 178002 (2005)
20. Sen, S., Hong, J., Bang, J., Avalos, E., Doney, R.L.: Solitary waves in the granular chain. Phys. Rep. **462**, 21–66 (2008)
21. Lindenberg, K., Harbola, U., Romero, A.H., Rosas, A.: Pulse propagation in granular chains. AIP Conf. Proc. **1339**, 97–110 (2011)
22. Herbold, E., Nesterenko, V.F.: Solitary and shock waves in discrete strongly nonlinear double power-law materials. Appl. Phys. Lett. **90**, 261902 (2007)
23. Pinto, I.L.D., Rosas, A., Romero, A.H., Lindenberg, K.: Pulse propagation in a chain of o-rings with and without compression. Phys. Rev. E **82**, 031308 (2010)
24. Spadoni, A., Daraio, C., Hurst, W., Brown, M.: Nonlinear phononic crystals based on chains of disks of alternating toroidal structures. Appl. Phys. Lett. **98**, 161901 (2011)
25. Sun, D., Daraio, C., Sen, S.: Nonlinear repulsive force law between two solids with axial symmetry. Phys. Rev. E **83**, 066605 (2011)
26. Sen, S., Manciu, M.: Discrete Hertzian systems and solitons. Physica A **268**, 644–649 (1998)
27. Ji, J.Y., Hong, J.: Existence criteria of solitary waves in a chain of grains. Phys. Lett. A **260**, 60–61 (1999)
28. Goldsmith, W.: Impact—The Theory and Physical Behaviour of Colliding Solids. Edwards Arnold, London (1960)
29. Allen, M.P., Tildesley, D.J.: Computer Simulation of Liquids. Clarendon, Oxford (1987)
30. Sun, D.: The contact force in generalized Hertz type systems and solitary waves. Ph.D. thesis, SUNY Buffalo, Buffalo, New York (2009)
31. Bittle, E.G., Sokolow, A., Sen, S.: Formation of solitary wave trains in granular alignments. Europhys. Lett. **77**, 24002-1-4 (2007)
32. Goldstein, H., Poole, C., Safko, J.: Classical Mechanics, 3rd edn. Addison-Wesley, Reading (2000)