Maturing process of solitary wave train in a step-down chain*

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In a step-down chain a solitary wave (SW) evolves into an SW train (SWT), but the formation of well-defined SWT takes time and space and little is known of the process from immature into mature SWT. We therefore perform a detailed numerical study of this process by analysing the local velocity amplitude and peak overlap of immature ordered SWs. The first SW continuously increases to maximal velocity amplitude and peak overlap until it is matured, but for following SWs there exist a minimal and maximal value of local velocity amplitude and, a minimal and maximal value of local peak overlap, clarifying the details of the energy propagation along the stepped chain. The immature and mature SWTs show the same dependence of the phase velocity on the SWs sequence. These provide guidelines for when or where the attention should be paid in the study of SWT.

Keywords: granular systems, solitary wave, molecular dynamics simulation

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1. Introduction

Granular materials exhibit a strongly nonlinear behaviour affecting the propagation of energy and have been attracting significant interest because of their ubiquity and known applications, but it is difficult to understand their intrinsic dynamic properties due to the strong nonlinearity of forces between spheres and the complex distributions. A one-dimensional granular chain not only is a simple starting point of studying higher dimensional granular materials but also gives rich phenomena.[1−28] As reported in the pioneering work of Nesterenko,[1] the propagation of an elastic impulse in a granular chain possesses soliton-like feature and experimental results[11] have confirmed the existence of such solitary waves (SWs). The problem of mechanical energy propagation in an alignment of grains has attracted increasing attention in recent years.[2,5−7,9,11,19,20,22] In the absence of external loading, i.e., the grains barely touch one another, the sound wave cannot be sustained in such a chain, which is named sonic vacuum. While in such a sonic vacuum, any pulse no matter how small can propagate as an SW. The SW in a granular alignment of spheres is a highly symmetric object with a well-defined center and propagates as a non-dispersive energy bundle.[21,29]

The behaviour of pulse passing through the contact of two sonic vacua (stepped chain) is interesting and important for understanding the dynamics of more complicated granular systems. Much unique wave dynamics has been found when SWs are far away from the interface, for example, Nesterenko *et al.*[3] observed that when the SW passes through the interface from the region of heavy grains to that of light ones, one SW disintegrates into the solitary wave train (SWT) and no backscattered SW is generated. The SWT is a sequence of SWs ordered by decreasing amplitudes approximately exponentially. Using numerical calculation Vergara[22] observed the primary multipulse structure and the secondary multipulse structure, whose origin is not completely clear to us. Job *et al.*[19,20] studied numerically and experimentally the condition of formation of the SWT and proposed the quasi-particle model to describe the energy of each wave. The evolution from an SW into the SWT is not immediate, i.e., the SWT formation takes time and

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space. How long and how far away from the interface it takes to form the mature SWT? Are there differences between the immature and mature SWTs in the properties, for example, the dependence of the phase velocity (velocity amplitude, maximal overlap) on the SWs sequence? If it depends, we should be careful of studying the properties of SWT. However, to date, little is known of the formation processes of the SWT near the interface, these would be very important to understand how the SWT carries information. So in this article, we focus on the early/immature or just the mature stage in the life of SWT.

2. Computation method

We modeled the stepped chain by joining two chains of spherical particles of different radii. In the chains there were M particles, in which N had radius R_1 and L had radius R_2 with $R_1 > R_2$. All particles were made of the same material and both ends of the chain were free to move. The particles repelled one another when they were squeezed by the nonlinear Hertz force: $F(\delta_{i,i+1}) = k_{i,i+1}\delta_{i,i+1}^{3/2}$, where the overlap between two adjacent partilces $\delta_{i,i+1} = R_i + R_{i+1} - (x_{i+1} - x_i)$ and x_i was the position of particle i. In the present case the governing parameter of equation of motion was the ratio of radius. The system's parameters were chosen as $N = 30$, $L = 170$, $R_1 = 2.0$, $R_2 = 1.0$. An impulse defined by an initial velocity at time $t = 0$ was initiated at the first heavy particle, leading to the formation of an SW in the heavy (large) particles region. The fifth order Gear predictor–corrector method was used to integrate the particle equation of motion and time step was 1.25×10^{-5}.

3. Discussion and simulation results

In Fig. 1(a), we present the velocity of particle (32, 38, 44) versus the elapsed time (t). Note that the number of the last heavy/big particle is 30 and the number of the first light/small particle is 31. One sees clearly that the velocity of a particle decreases in the oscillatory way with time and forms many visible peaks with progressively decreasing amplitudes, indicating that one SW is splitting into multiple SWs after passing through the interface of the stepped chain even though such SWs do not separate into individual SWs. So these multiple SWs are being at the early stage of the SWT reported in many papers. The wave splitting is also clearly observed from Fig. 1(b), which shows the positions of the local velocity amplitudes for the six leading SWs as functions of their respective time of flight. As can be seen from Fig. 1(b), the slope of p-th SW is larger than that of $(p+1)$-th SW and the further quantitative analysis yields the relation between the phase velocity of the immature SWs and their sequence: $v_{im}(p) \sim \exp(-0.067p)$. Figure 1(c) shows the local velocity amplitude of the leading six SWs as a function of the particle number during their respective time of flight. The local velocity amplitude of the first SW first increases with particle number and reaches its maximum value ($V_{\max}$), indicating that the first SW is increased continuously in its kinetic energy and then arrives at its maximum kinetic energy, after that this wave propagates as a well defined and separated single SW along the chain with a constant kinetic energy and in the meantime it is far away from the interface (39 particles away from the interface, see Fig. 3 below). While the local velocity amplitude of the second SW first decreases with particle number, then passing through some particles the local velocity amplitude arrives at its minimum ($V_{\min}$), then it increases and finally reaches its $V_{\max}$ and forms a single well-defined SW, so for the second wave there exist a maximal amplitude and a minimal velocity amplitudes $V_{\max}$ and $V_{\min}$. The third, fourth, fifth, and sixth SWs do exhibit the similar behaviour as the second SW does. This obvious difference between the first SW and the following SWs results from the fact that the interaction at interface sustains for a very long time and thus except the first SW the following SWs propagate under the compression and the local compression changes with the time to transfer the energy until the formation of well-defined SWs. Note that the SW is typically considered as a propagating, non-dispersive energy bundle. The appearance of the minimum of velocity amplitude in those SWs except the first SW shows that (i) at the early time or near the interface, when or where these waves do not separate into the individual SWs, the p-th SW gains kinetic energy from the $(p+1)$-th wave and imparts more kinetic energy to the $(p-1)$-th wave; (ii) after some time (Δt) and passage of some particles the $(p-1)$-th wave is well separated from the p-th wave and matures into a single SW in time and space, the p-th wave thus gains the kinetic energy from the $(p+1)$-th without imparting the kinetic energy to the

$(p-1)$-th wave. Therefore, as shown in Fig. 1(c) the particle number, where the p-th SW arrives at its minimum and maximum of velocity amplitude, extends with the sequence of SWs.

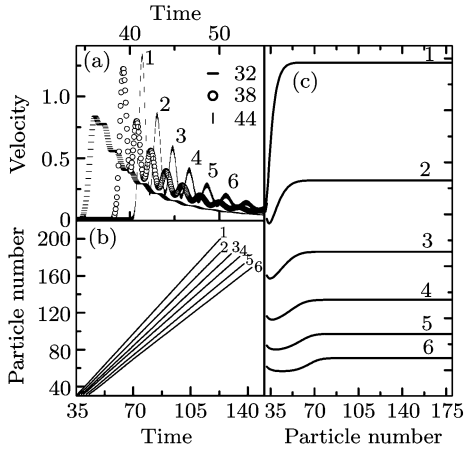


Fig. 1. (a) Velocity of particle 32, 38, 44 versus time. (b) Particle number of velocity maxima as a function of their respective time of flight for the first, second, third, fourth, fifth, sixth waves. (c) The velocity amplitude of these leading six waves as a function of particle number.

An SW in a chain carries kinetic and potential energies. The above results tell us the information of the kinetic energy in terms of the local velocity amplitude. We now turn our attention to the information of the potential energy by analysing the local compression degree in the chain. The local overlap of particle i in the chain is defined by $\delta_i = (\delta_{i-1,i} + \delta_{i,i+1})/2$, which represents the local compression degree at particle i. In Fig. 2(a), we display the evolution of the local overlap at particles 32, 38, 44. Similar to the particle velocity of these three particles shown in Fig. 1(a), the local overlap decreases in the oscillatory way with time and forms many visible peaks with progressively decreasing height, suggesting that the SW is splitting into multiple SWs after passing through the interface of the stepped chain and the multiple SWs are at the early stage of the SWT. Figure 2(b) shows the position of the local peak overlap for the six leading SWs as functions of their respective time of flight, indicating that the slope of p-th SW is larger than that of $(p+1)$-th SW and producing the relation of the phase velocity of these immature SWs: $v_{\mathrm{i}m}(p) \sim \exp(-0.067p)$, in good agreement with the result obtained from Fig. 1(b). Figure 2(c) shows the local peak overlaps of the leading six SWs as functions of the particle number during their respective time of flight. The local peak overlaps related to these SWs behave in the same manner as their velocity amplitudes, respectively. (i) The local peak overlap of the first SW continuously increases with particle number until it reaches its maximum value ($\delta_{\max}$), i.e., the first SW arrives at its maximum potential energy and then the first SW propagates as a well defined and separated SW along the chain with a fixed potential energy. (ii) For the following SWs there exist a maximal and a minimal peak overlaps, $\delta_{\max}$ and $\delta_{\min}$. At an early time or near the interface, when or where these waves do not separate into the individual SWs, the p-th SW gains potential energy from the $(p+1)$-th wave and imparts more energy to the $(p-1)$-th wave; after some time (Δt) and passage of some particles the $(p-1)$-th wave is separated from the p-th wave and matures into a single SW in time and space, the p-th wave thus gains the potential energy from the $(p+1)$-th without imparting it to the $(p-1)$-th wave. Therefore as shown in Fig. 2(c) the particle number, where the p-th SW arrives at its local minimum or maximum of peak overlap, increases with the sequence of SWs. It should be pointed out that the kinetic energy transferring between neighbouring SWs happens through the potential energy and the transferring of it takes place through the kinetic energy and a detailed comparison of Figs. 1(a) and 2(a) indicates that the appearance of overlap peak is later than that of velocity peak.

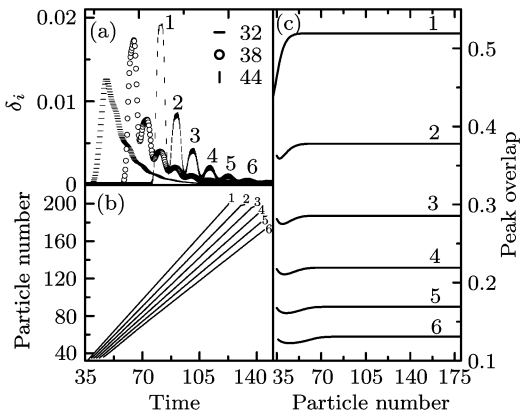


Fig. 2. (a) Overlap (δ) of particle 32, 38, 44 versus time; (b) Particle number of peak overlap as a function of their respective time of flight for the first, second, third, fourth, fifth, sixth waves; (c) The peak overlap of these leading six waves as a function of particle number.

Based on the obtained evolution of local velocity and local overlap in the stepped chain, each single SW formation of the SWT takes different time and space. Figure 3(a) shows the time Δt taken for different SWs in the stepped chain to arrive at their minimal and maximal velocity amplitudes or at their minimal and maximal peak overlaps. From this figure, we can see that, (i) Δt for each SW to reach

its minimal velocity amplitude (i.e., the minimal kinetic energy) increases approximately exponentially with the sequence of SWs, whereas Δt for each SW to reach its minimal peak overlap (i.e., the minimal potential energy) increases approximately linearly with the sequence of SWs. (ii) Δt for each SW to reach its maximal velocity amplitude (i.e., the maximal kinetic energy) is increased approximately linearly with the sequence number of SWs, whereas Δt for each SW to reach its maximal peak overlap (i.e., the maximal potential energy) is increased approximately exponentially with the sequence number of SWs. There exists an obvious difference in the dependence of Δt on the sequence of SWs between local velocity and local overlap. This figure also clearly indicates that the mature time of the first SW defined from the local velocity information is almost identical with that defined from the local overlap. The mature time of the following SWs needed, based on the maximal local velocity, is longer than that obtained from the maximal local overlap; however the difference becomes very small for the sixth SW.

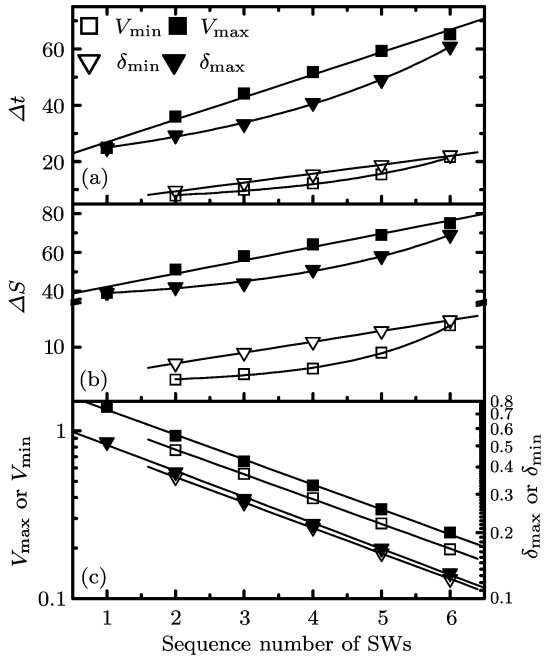


Fig. 3. (a) The time Δt taken for different SWs to arrive at their minimal and maximal velocity-amplitudes or peak-overlaps as a function of the sequence of SWs. (b) The space ΔS (defined by particle numbers away from the interface) taken for different SWs to arrive at their minimal and maximal velocity-amplitudes or peak-overlaps as a function of the sequence of SWs. (c) The maximal ($V_{\max}$) and minimal ($V_{\min}$) velocity-amplitudes or the maximal ($\delta_{\max}$) and minimal ($\delta_{\min}$) peak overlaps of the leading six SWs as functions of the sequence number of SWs. Lines are guides to the eyes in panels (a) and (b) and correspond to the exponential fits in panel (c).

How does the mature space of these SWs in the SWT depend on their sequence? Figure 3(b) presents the mature space ΔS of the SWs defined by the particle numbers that SW has passed when it reaches its maximal local velocity amplitude or the maximal local peak overlap and the SW is referred to as a matured SW. In this figure, the space for SWs to arrive at their minimal local velocity amplitude, as well as the minimal and maximal local peak overlaps, is also plotted against the sequence of the SWs formation. We can see that the mature space of the SWs exhibits the same dependence on the formation sequence as the mature time: the mature space of the SWs seems to enlarge linearly with the sequence of SWs according to the data related to local velocity, but it seems to enlarge exponentially with the sequence according to the data pertaining to local overlap. Similarly, the mature space of the first SW obtained from the local velocity information is identical with that obtained from the local overlap. The mature space of the next SWs defined from the local velocity is farther than that obtained from the local overlap, but the difference becomes very small for the sixth SW.

Job *et al.*[19,20] have performed a detailed study of the SWT far away from the interface of the stepped chain. So the SWs studied should be matured. They found that the force amplitude of the p-th single SW in the SWT behaves like $F_{\max}(p) \sim \exp(-\alpha p)$, the exponential coefficient α was demonstrated to depend only on the mass ratio. The phase velocity of SW is $v(p) \sim F_{\max}^{1/6}(p) \sim V_{\max}^{1/5}(p)$.[2] Therefore the velocity amplitude of the p-th single matured SW decreases exponentially with the sequence of SWs, i.e., $V_{\max}(p) \sim \exp(-\beta p)$ and $\beta = 5\alpha/6$. We obtained a relationship between $V_{\max}$ and the sequence of SWs in the SWT, displayed by solid squares in Fig. 3(c), which confirms the exponential dependence reported by Job *et al.*, with a fitting parameter $\beta = 0.340$. From this figure, it is found that the observed minimal velocity amplitude $V_{\min}$, the maximal and minimal peak overlaps behave with the same dependence on the sequence of the SWs as the maximal velocity amplitude $V_{\max}$, and the fitting parameter $\beta = 0.342$ for $V_{\min}$, the fitting parameters are 0.272 and 0.269 for $\delta_{\max}$ and $\delta_{\min}$, respectively. We thus obtain $\alpha = 0.408$ and $\delta_{\max}(\delta_{\min}) \sim \exp(-2\alpha p/3)$. In addition, the phase velocity of SWs should exhibit the dependence on the sequence number of SWs as $v(p) \sim \exp(-\alpha p/6) = \exp(-0.068p)$. Compared with the exponential dependence of the maximal velocity amplitude, the depen-

dence of the phase velocity of SWs on their sequence is strongly weakened. So the phase velocity of SWs exhibits an approximately weakly linearly decreasing dependence on their sequence in the range of limited SWs, which results in the similar sequence-number dependence of mature time and space. Here the obtained relation of mature SWs, $v(p) \sim \exp(-0.068p)$, is in good agreement with the relation of immature SWs, $v_{im}(p) \sim \exp(-0.067p)$. This indicates that the phase velocity of immature and mature SWs shows the same SWs-sequence dependence.

4. Conclusion

We have performed a numerical study of the early stage of the SWT in stepped chain. Right after passing through the interface of the stepped chain an SW is splitting into multiple SWs ordered by progressively decreasing amplitude. It takes time and space for these ordered SWs to be well separated/matured. The evolution of local velocity shows that both mature time and mature space of ordered SWs seems to depend approximately linearly on their formation sequence, whereas the evolution of local overlap suggests that both mature time and mature space of ordered SWs depend approximately exponentially on their formation sequence. In the maturing process, the first SW continuously increases in both local velocity amplitude $V_{\max}$ and local peak overlap $\delta_{\max}$ until it is matured, but for the SWs followed there exist a minimal $V_{\min}$ and a maximal $V_{\max}$ and, a minimal $\delta_{\min}$ and maximal $\delta_{\max}$. The immature and mature SWs show the same dependence of the phase velocity on the SWs sequence. These results provide guidelines for when or where the care should be taken in the study of multiple SWs or SWT. We have not observed in experiments that the existence of minimal value of local velocity amplitude and local peak overlap for those SWs that follows the first SW.

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