Interaction of solitary waves in confined granular alignments and the quasi-equilibrium state

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Abstract

We consider a chain of elastic beads, in which the individual grains repel upon contact according to the non-linear Hertz potential. We further assume that the chain is under zero loading, i.e., the grains barely touch one another. We show via careful numerical solution of the equations of motion that an impulse propagates as a solitary wave and that the collision of identical solitary waves propagating in opposite directions along the chain spawns a hierarchy of multiple weak solitary waves. We mention that the generated baby waves eventually must lead to a "volatile" equilibrium-like state, which we refer to as the quasi-equilibrium state.

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I. INTRODUCTION

The interaction of mechanical perturbations propagating in granular media exhibits striking nonlinear phenomena. When a mechanical pulse is initiated in a one-dimensional alignment of elastic grains, it propagates as a solitary wave [1]. Solitary waves are tight bundles of energy which can travel without dispersion in space or in time [2].

We assume that our beads are elastic objects. In a non-dissipative system, the solitary waves are expected to last forever. We consider such non-dissipative systems in this study. However when a mechanical perturbation travels from one grain to the next one, the geometry of the contact surfaces between adjacent grains change and as per Hertz law, leads to a non-linear interaction between them. When grains get compressed, mechanical energy flows from one to the next. Hertz showed that the potential energy cost associated with the grain deformation is initially softer than harmonic. However, with increasing compression, the potential energy cost rises sharply. The grain-grain contact is hence abruptly broken. These systems support ballistic-like propagation of energy. The softness of the repulsive potential determines the spatial extent of the propagating energy bundle or the solitary wave. These solitary waves travel in speeds that are proportional to their amplitudes, with those carrying higher energy and involving larger amplitude compressions traveling faster than those with smaller amplitudes and causing less compression.

In 1985 Nesterenko reported for the first time experimental evidence of solitary waves supported by granular alignments [3] and extensive experimental work has been done by C. Coste *et al.* [4] and by S. Job, *et al.* [5]. Since then there has been special interest in the propagation of solitary waves and the interaction between them.

In general it turns out that in a granular alignment under the influence of external forces [6, 7], the interaction between grains has both linear and non-linear components [2, 8]. When the beads in the linear array are not pre-compressed, the underlying interaction is purely non-linear and as a result the linear force is absent and hence sound propagation becomes impossible. These systems have hence been referred to by Nesterenko as *sonic vacuum* systems.

During the last few years there has been increasing interest in the investigation of the properties of propagating waves in uncompressed discrete media. This interest is driven mainly by the existence of a new kind of solitary wave in these systems and by the ways in which these solitary waves interact with one another and with the system boundaries. These phenomena include the formation of secondary solitary waves [9] and the establishment of an equilibrium-like state due to the interactive nature of the solitary waves [10, 11]. Regarding the formation of secondary solitary waves, most extensive efforts have been made to study the properties of these waves in different conditions as for instance, in granular chains with parity differences in the number of grains [12], or with non-uniform distribution of bead-size [13] or with different boundaries [5]. Furthermore, a second line of research deals with a novel collective state in which particle velocities satisfy a Gaussian distribution but the energy is not equi-partitioned in the system [14].

In this paper we briefly review the problem of the interaction of solitary waves in granular arrays with either themselves or with boundaries and introduce the basic features of the newly discovered quasi-equilibrium state. In both cases the original solitary waves are destroyed. We focus mainly on the formation process of secondary solitary waves and the role of boundaries on their properties.

Fig.1 shows the schematic setup of the numerical experiment in which two identical solitary waves that start off at the ends of a chain of N monodisperse grains and propagate through the system at equal speeds, collide, and continue on.

This paper is organized as follows: first we describe the numerical procedure used in our simulations to directly solve the equations of motion for the grains in the granular alignment. Next, we discuss the propagation and the interaction of solitary waves and discuss the formation of secondary solitary waves. We conclude by describing the basic properties of the eventual quasi-equilibrium state of the system.

II. THE MODEL AND SIMULATION DETAILS

We consider a linear arrangement of N identical spherical grains of radius R and mass m, interacting through a Hertzian contact force. The system is without any pre-compression. According to Hertz law, any two adjacent pair of beads labeled as i and $i+1$ interact as follows,

$$V(\delta_{i,i+1}) = \begin{cases} a\ \delta_{i,i+1}^{n}, & \delta > 0, \\ 0, & \delta \leqslant 0, \end{cases} \tag{1}$$

where n is 5/2 for spherical grains [8], $a = \frac{2}{5D}\sqrt{\frac{R}{2}}$, where $D = 3(1-\sigma^2)2Y$, is a constant which depends on the Young's modulus, Y, and the Poisson's ratio σ of the grains and $\delta_{i,i+1} \equiv 2R - (z_{i+1} - z_i)$, where z_i denotes the displacement of grain i from the equilibrium position. In granular systems, n depends upon the nature of the contact and $n > 2$. Eq. (1) is valid for grains made of an elastic material. However, the resulting interaction is non-linear due to the geometrical properties of the grains.

The equation of motion for the i-th grain in the chain can be written as,

$$m\ddot{z}_i = na\left(\delta_{i,\ i-1}^{n-1} - \delta_{i+1,\ i}^{n-1}\right). \tag{2}$$

A formal solution to Eq. (2) was first attempted by Nesterenko [15] and later by Sen and Manciu [16]. Here we describe the creation of secondary solitary waves by the collision of two identical solitary waves. The creation of secondary solitary waves by collision of a solitary wave against a wall is described in Ref. [5]. We start with two identical impulses directed into the chain at the initial time, $t = 0$, by assigning $v_1(0) = -v_0$ and $v_N(0) = v_0$, with $v_0 > 0$. The other grains are at rest at the initial time. These impulses lead eventually to the formation of identical solitary waves that are initiated near the ends of the chain. The initial impulse is all kinetic energy. It takes the system some space and time to convert this kinetic energy pulse into a solitary wave. Studies have shown that for spherical beads, where $n = 5/2$, the system takes about 10 grain diameters to form a solitary wave. The waves are about 7 grain diameters wide.

The system dynamics is obtained by direct time integration of the coupled Newtonian equations of motion via the 3^{rd} order Gear algorithm [17]. We choose 10^{-5} m, 2.36×10^{-5} kg and 1.0102×10^{-3} s as the units of distance, mass and time, respectively. The integration time step, dt, used was chosen small enough to resolve the finest details. For $n = 2.5$, i.e., spheres, we use $dt = 5 \times 10^{-7}$. The grain diameter is set to 100, i.e., 1 mm, $2R = 1$ and $a = 5657$ [18], a value ($= 4.14 \times 10^7$ N/m$^{\frac{3}{2}}$)which is the range of elasticity of silicate materials. In the cases here, we use an even chain made of $N = 500$ and $v_0 = 5 \times 10^{-4}$. In the discussions on quasi-equilibrium, we present our time domain results in microseconds to emphasize the exceptionally long times taken by these granular alignments to reach an equilibrium-like state.

III. FORMATION OF SECONDARY SOLITARY WAVES

By using the method described above, we perform extensive simulations to investigate the collision of solitary waves. Once each pulse is initiated at the ends of the chain, the pulses propagate as solitary waves. The pulses are 7 grain diameters wide. This size is independent of both, amplitude and grain size [19]. Fig. 2 shows the velocity profiles of the two solitary waves in incoming trajectories prior to the collision. Another important feature is that their propagation velocity scales with amplitude by an exponent $\frac{1}{5}$. This is consistent with results obtained by Nesterenko [15] and by Sen and Manciu [16]. The solitary waves approach each other and cross at the edge of the two central grains in the chain with even N or at the center of the central grain in a chain with odd N. After the crossing occurs, the solitary waves continue until they reach the opposite ends of the chain.

Now we turn our attention to the detailed dynamics of the crossing event which leads to the formation of the so-called secondary solitary waves. During the collision the original solitary waves do not cancel each other at the intersection region. In general, during the collision all the beads in the chain move out from their original position. Only the central grain in an odd chain remains static at the time of collision. In the even chain all the participating grains, including the one in the region where the crossing occurs, move out from their equilibrium positions during the complete interval of time. Therefore, immediately after the collision occurs, there is more kinetic energy available in the even case.

During the collision, solitary waves break down and reform; which means that during a short interval of time the profiles of the solitary waves lose their initial shape and are reformed again to their original shape with secondary solitary waves as a by-product [5]. In Fig. 3 we can see the precise moment when secondary solitary waves are formed.

After the crossing occurs, we carefully examine the region behind the crossed solitary waves. Using higher resolution to observe the kinetic energies of the individual grains, we find that multiple solitary waves of progressively decreasing amplitudes form in the collision region after the collision. The less energetic the solitary wave is, the slower it moves. These waves are called secondary solitary waves. In Fig. 4 we see the secondary solitary waves created as a by-product after the collision. It is worth observing that the system cannot transport energy via sound waves in this sonic vacuum system. Thus, all energy must eventually be bundled into solitary waves. Given that these waves are 7 grain diameters wide, it is easy to see that at least 7 grain collisions would be needed for these waves to be born. Thus, the time interval in which the waves are created seem not to be according to any simple pattern. These waves are several order of magnitude smaller than the original ones. Secondary solitary waves are formed in pairs of the same amplitude but move away from each other. Subsequently more secondary solitary waves are formed with decreasing amplitudes. Depending on the collision region, secondary solitary waves can be up to three to four orders of magnitude less energetic than the original solitary waves [12]. The amplitudes of secondary solitary waves depend on the details of the collision and also on the boundaries. The energies associated with the secondary solitary waves depend also on the softness of the inter-grain interaction. Steeper potentials produce more secondary solitary waves.

When the collision happens with a wall, again secondary solitary waves are created as a result of the collision. The amplitudes of the secondary solitary waves can be controlled by tuning the Young's modulus of the wall; a softer wall promotes stronger secondary solitary waves than harder ones [5].

IV. THE QUASI-EQUILIBRIUM STATE

The collision of solitary waves with one another and with the walls, whether the walls are infinitely massive or are characterized by softer potentials, leads to the partial decimation of the original waves and the formation of the secondary solitary waves. Our simulations strongly suggest that after very long times from the start of the formation of the secondary solitary waves, the memory of the existence of the original solitary waves is lost. This issue is addressed in detail in Refs. [10, 11, 14]. In this long-time regime, the dynamics of the system appears to be characterized by the continuous formation [19] and breakdown [9] of solitary waves all over the system.

We find that the range of velocities experienced by the average grain in this long time regime is a robust Gaussian as shown in Fig. 5. This result is consistent with the Maxwell distribution of velocities that is typically realized in many body systems. Of course, Gaussian distribution of velocities is a consequence of the central-limit theorem and is hence expected to be generally valid. Our confirmation of the Gaussian distribution of velocities for the grains (we have done these studies for all the grains although data is shown for a few grains) hence serves to check the correctness of the calculations.

One can now ask whether the equipartition theorem is satisfied in these systems. If so, and if the state of the system in the long time regime is independent of the initial conditions, one can claim that the system is in the equilibrium state.

The results shown in Figs. 6 and 7 depict kinetic energy (in gray scale) of the grains in a $N = 20$ system with end walls as a function of time. Note the differing time scales. In Fig. 6, we show results for a system with $n = 2$ (i.e., a one-sided harmonic system) and in Fig. 7 we show a $n = 2.5$ (i.e., the granular sphere system), which is an alignment of granular spheres. In Fig. 6 we find that the energy pulse quickly disperses in the chain. It is evident by looking at the time axis that the energy in the $n = 2$ system disperses rapidly. In the $n = 2.5$ system, the long time state reveals a significant amount of fluctuations, more so than what exists in the $n = 2$ system at much earlier times. Studies reported elsewhere demonstrate that the fluctuations against the expected equipartition energy can be larger in systems with $n > 2$ compared to the $n = 2$ system. These fluctuations can be as high as $10 - 30\%$ in systems as large as $N = 100$. Increasing system size reduces the fluctuations but does not lead to decay of the fluctuations in time. The departure from equipartition becomes increasingly pronounced as n increases [20].

V. CONCLUSION

In closing we summarize that granular alignments provide us with new and unforeseen challenges to explore in the boundary between strongly nonlinear dynamics of many body systems and of equilibrium and non-equilibrium statistical mechanics as we know it today. The existence of solitary waves, the interaction between these solitary waves and between these waves and system boundaries allow us to question whether the concept of equilibrium as we know it, meaning (a) that the state of a system is independent of initial conditions, (b) that velocity distribution is Maxwellian and (c) that equipartition is satisfied, is indeed the most general state. Our studies suggest that equipartition may not be realized in systems where there is no sound propagation. Nevertheless we find that such systems still exhibit a state that is very similar to the equilibrium state and yet with large kinetic energy fluctuations, so large in fact that a temperature cannot be easily defined for such systems and hence no thermodynamics is truly possible in the traditional sense in such systems. We suggest that this “quasi-equilibrium” state is a more general equilibrium state that exists in systems where there is no sound propagation.

VI. ACKNOWLEDGEMENT

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VII. FIGURE CAPTIONS

FIG. 1: Schematic setup of a granular chain at initial time. Two incoming pulses of equal velocity start simultaneously at the ends of the chain.

FIG. 2: Snapshot of the two solitary waves in an early stage traveling in incoming trajectories. (a.u.) on the y-axis stands for arbitrary units. The inset shows in detail one of the pulses with a constant width of 7 diameters.

FIG. 3: Formation of secondary solitary waves. The central region in the y-axis has been amplified 10 times to show the finest detail of the formation. (a.u.) on the y-axis stands for arbitrary units.

FIG. 4: Secondary solitary waves created after the collision of two solitary waves in a granular chain made of an even number of beads. (a.u.) on the y-axis stands for arbitrary units.

FIG. 5: Distribution of velocities for different grains.

FIG. 6: Kinetic energy (in gray scale) of the grains in a $N = 20$ system with $n = 2$.

FIG. 7: Kinetic energy (in gray scale) of the grains in a $N = 20$ system with $n = 2.5$.

VIII. FIGURES

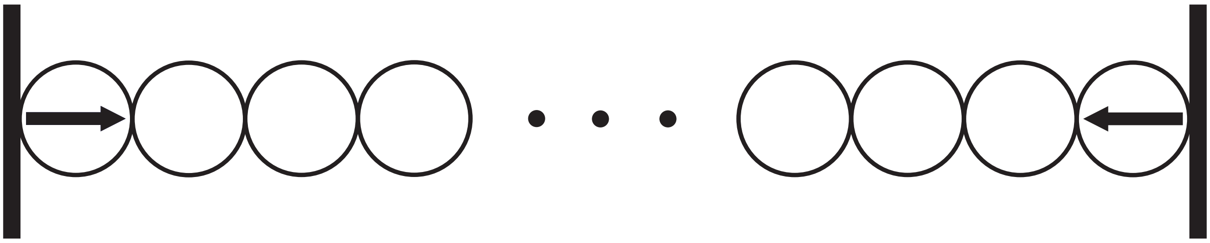


FIG. 1:

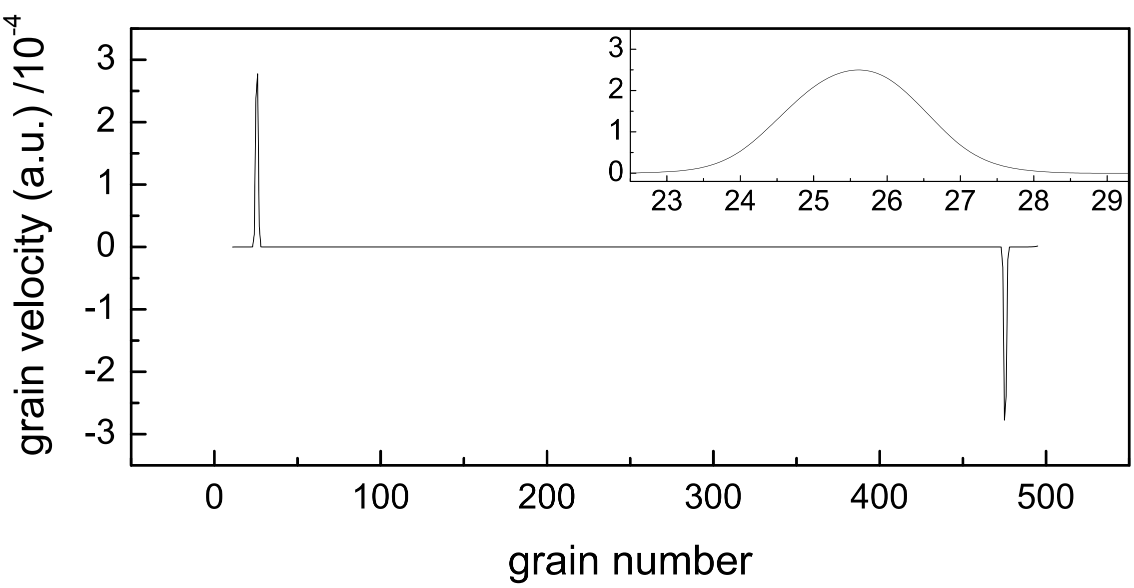

grain velocity (a.u.) /10^{-4}
3
2
1
0
-1
-2
-3
0
100
200
300
400
500
grain number
3
2
1
0
23
24
25
26
27
28
29

FIG. 2:

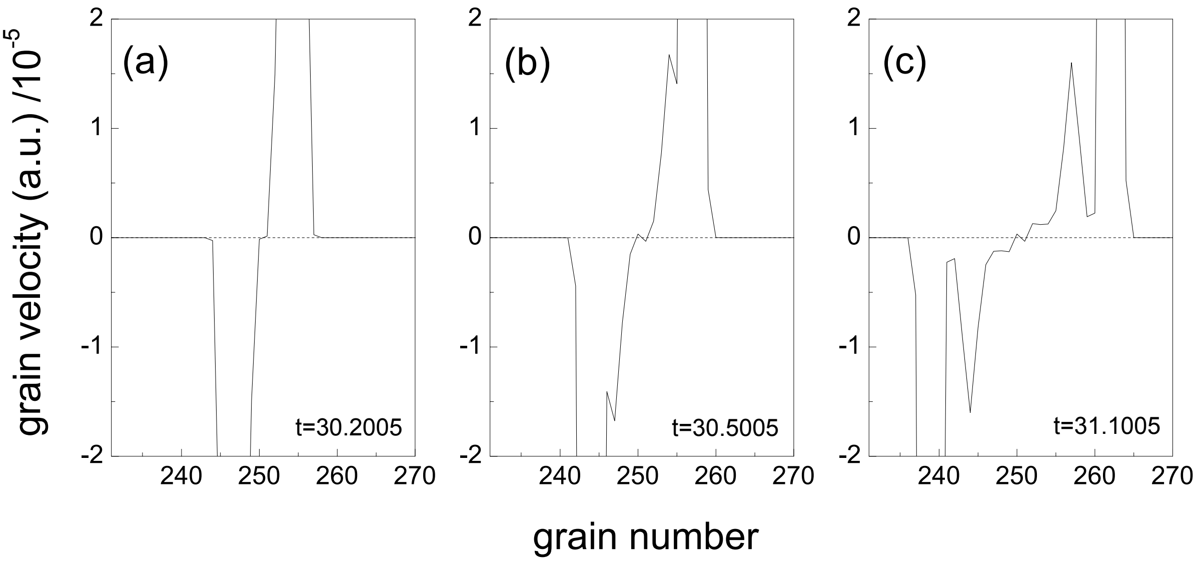

(a)
(b)
(c)
t=30.2005
t=30.5005
t=31.1005
grain velocity (a.u.) /10^{-5}
grain number
2
1
0
-1
-2
240
250
260
270

FIG. 3:

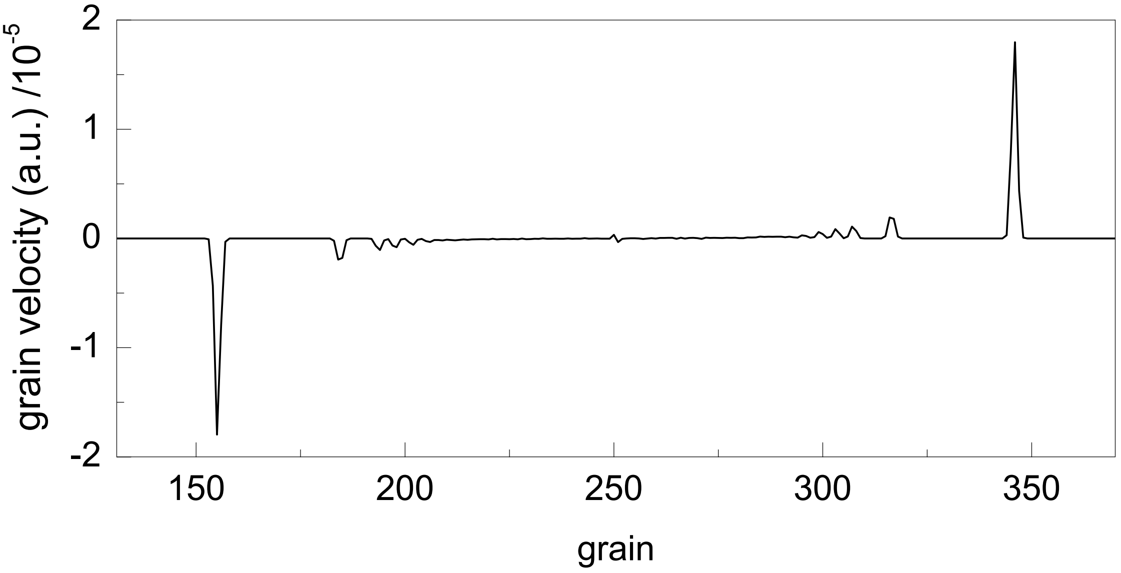
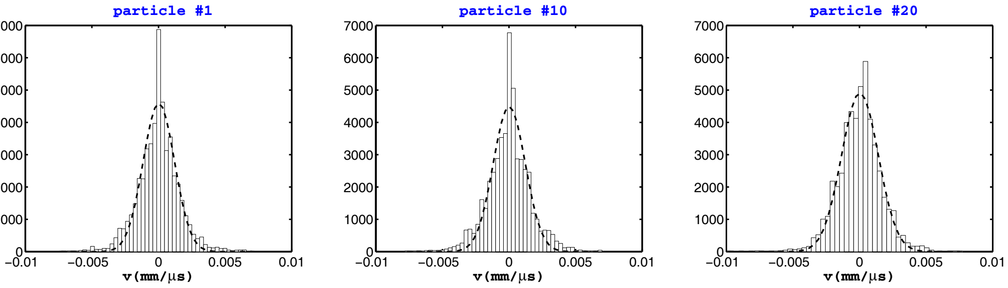


FIG. 4: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particle #10
particle #20
7000
6000
5000
4000
3000
2000
1000
0
−0.01
−0.005
0
0.005
0.01
v(mm/μs)

FIG. 5:

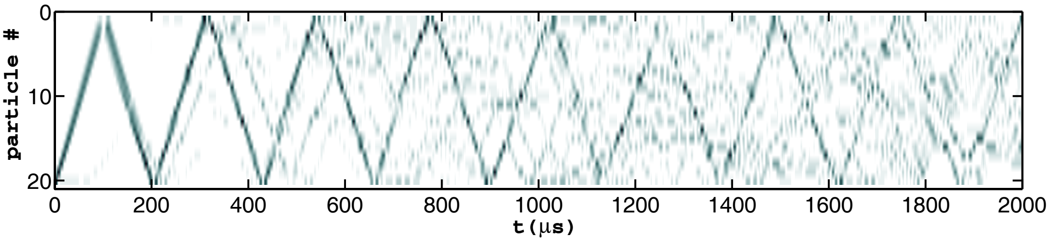
0
10
20
particle #
0
200
400
600
800
1000
1200
1400
1600
1800
2000
t(μs)

FIG. 6:

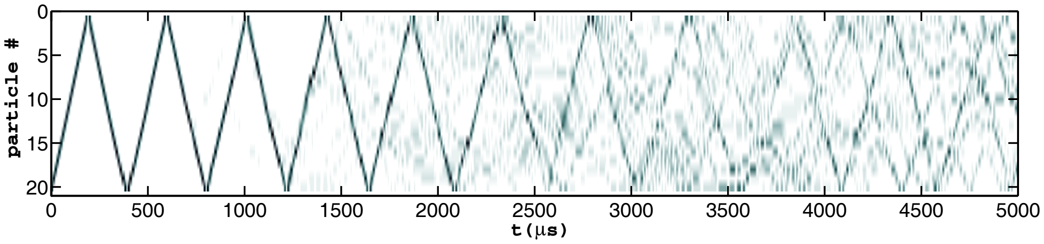
particle #
0
5
10
15
20
0
500
1000
1500
2000
2500
3000
3500
4000
4500
5000
t(μs)

FIG. 7: