Mechanical energy fluctuations in granular chains: The possibility of rogue fluctuations or waves

Ding Han, Matthew Westley, and Surajit Sen
Department of Physics, State University of New York, Buffalo, New York 14260-1500, USA

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The existence of rogue or freak waves in the ocean has been known for some time. They have been reported in the context of optical lattices and the financial market. We ask whether such waves are generic to late time behavior in nonlinear systems. In that vein, we examine the dynamics of an alignment of spherical elastic beads held within fixed, rigid walls at zero precompression when they are subjected to sufficiently rich initial conditions. Here we define such waves generically as unusually large energy fluctuations that sustain for short periods of time. Our simulations suggest that such unusually large fluctuations ("hot spots") and occasional series of such fluctuations through space and time ("rogue fluctuations") are likely to exist in the late time dynamics of the granular chain system at zero dissipation. We show that while hot spots are common in late time evolution, rogue fluctuations are seen in purely nonlinear systems (i.e., no precompression) at late enough times. We next show that the number of such fluctuations grows *exponentially* with increasing nonlinearity whereas rogue fluctuations decrease *superexponentially* with increasing precompression. Dissipation-free granular alignment systems may be possible to realize as integrated circuits and hence our observations may potentially be testable in the laboratory.

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I. INTRODUCTION

Rogue waves or freak waves in the open ocean have been the subject of significant interest for centuries [1] and perhaps more intensely so within the past five decades in the context of deep water waves, Bose-Einstein condensates, and financial markets [2–16]. These waves have been responsible for sinking numerous large vessels and killing hundreds of people even in recent times [17]. Clearly, the study of these waves is important.

There have been several studies on the properties of the nonlinear Schrödinger equation (NLSE) [18] which is believed to describe deep water waves [19–24]. The present understanding points to disorderly driving from strong winds and nonlinear effects such as modulational instabilities [25] as the underlying reasons for the appearance of fleeting large amplitude waves in deep water systems [8]. To be clear, by "rogue wave," one means that the wave height from crest to trough is more than about twice the significant wave height, which is the average wave height of the largest one third of nearby waves. Inspired by the many studies, one wonders if very large amplitude energy fluctuations—something similar to rogue waves but in a different context—can be seen in other nonlinear systems at sufficiently late times. We will call these fluctuations *rogue fluctuations*. This article attempts to address that question by considering the long-time dynamics in an alignment of spherical elastic beads [26] held between rigid end walls [27,28]. This system has turned out to be relatively simple, yet discrete and nonintegrable, and furthermore supports the existence of a rich array of strongly nonlinear phenomena [29–35].

Let us start with two elastic grains, which repel upon intimate contact [36–38]. This repulsion is intrinsically nonlinear in nature, i.e., there are no harmonic terms in the potential representing the interaction between two grains in contact [39]. The mechanical energy transport behavior through such granular alignment with N adjacent grains in gentle contact and held between rigid walls represents one of the simplest nonlinear many body systems we can consider. Any velocity perturbation initiated at one end of the chain travels as a nondispersive energy bundle (a solitary wave) in this system [26,28]. In order to satisfy causality, as explained elsewhere, the solitary waves must break and reform in every collision [40,41]. Such a process leads to the formation of tiny secondary solitary waves. All of these waves have the same spatial widths [30,42]. Their velocities depend on their energy contents [27,43]. In the absence of dissipation, at late times, the system ends up in an equilibriumlike state, called the quasiequilibrium state [31,44–48]. In the quasiequilibrium state, the grain velocities satisfy a Gaussian distribution (as dictated by the central limit theorem), the equipartitioning of energy is not satisfied, and the system may or may not show dependence on initial conditions. Large energy fluctuations are seen in the quasiequilibrium state. The objective of this work is to explore whether, for the right kind of initial conditions, large enough energy fluctuations are possible. If the energy fluctuations exceed six times the typical fluctuation (which is already quite large in the quasiequilibrium state), we choose to call such a wave a *rogue fluctuation* in this work.

In Sec. II we describe the model. The results of our study are presented in Sec. III. We conclude with a summary of the findings and a discussion of the implications of this work in Sec. IV.

II. THE MODEL

Let R be the radius and m be the mass of each of the spherical elastic grains in contact that make up the system. Let us assume these grains are placed in mutual contact along a line and let $z_1, z_2 \cdots$ represent the actual displacements from the original equilibrium positions. We assume that the Young's modulus Y and the Poisson's ratio σ describe the elastic grains. The grains barely touch one another at $t = 0$ and the system is assumed to be held between fixed end walls which are rigid. If the two spheres i and $i + 1$ are in contact, they repel according to Hertz's law [36] given by

$$V_{i,i+1} = a\delta_{i,i+1}^{5/2}, \tag{1}$$

where $\delta_{i,i+1} \equiv 2R - (z_{i+1} - z_i)$ and $a = \frac{2}{5D}\sqrt{\frac{R}{2}}$, where $D = \frac{3(1-\sigma^2)}{2Y}$. In general, instead of using the exponent 5/2 in Eq. (1), one can insert any nonlinear behavior with $n > 2$. As discussed extensively elsewhere, various values of n can be associated with various types of contact interfaces between the grains, and hence pertain to contact between identical grains of nonspherical but regular shapes. Indeed a depends on n. However, in each study involving identical grains, a translates to a fixed number which will relate to the characteristic energy transport time in the system, and for this reason we will keep matters simple and regard a as simply a constant in our studies.

The equation of motion for each grain except the boundary grains is

$$m\frac{d^2 z_i}{dt^2} = na[(\Delta + \delta_{i,i-1})^{n-1} - (\Delta + \delta_{i,i+1})^{n-1}], \tag{2}$$

where Δ denotes equal precompression applied to all the grains and n is the index of the power law that describes the nonlinear potential, for example, for the Hertz problem $n = 5/2$. Since we will consider various values of n in our study below, it makes sense to define the equations of motion in Eq. (2) rather broadly. We will carry out studies of our system with $\Delta = 0$ and $n > 2$ and for $n = 5/2$ and $\Delta > 0$.

The dynamical simulations are performed via the velocity Verlet algorithm [49,50]. In long dynamical runs it is easy to incur round-off errors. We have made a strong effort to make sure the errors are small enough such that the results are reliable by insuring that energy conservation holds as perfectly as possible. Over $\sim 10^8$ time steps, the computed total energy of our energy conservation varies about one part in 10^9 in typical simulation runs. Our integration time step was typically $\Delta t = 10^{-10}$ s, which would generally be in keeping with most of our dynamical simulation based work thus far [51]. We have also tried step sizes that are as small as 10^{-12} s but it turns out that such refinements did not influence the accuracy of our calculations. In nonlinear systems, the dynamics is strongly amplitude dependent and hence it can be hard to get a sense of how an actual system behaves without relating the physical parameters broadly to some system. With that in mind, in our studies, the grain radius is set to $R = 15$ mm, $\rho = 4.42\ \mathrm{mg/mm^3}$, $\sigma = 0.34$, and $Y = 400\ \mathrm{kN/mm^2}$ or 400 GPa, numbers that would be representative of an ultrahard ceramic [51]. The reason for choosing a hard system is to be able to initiate large velocity perturbations which would still yield modest grain compressions and, at the same time, allow many cycles of fast back and forth movement of the system energy within readily achievable simulation times.

The number of grains is $N = 500$ throughout this study. This turns out to be an adequate spatial extent for the system to "settle down." The velocity perturbations chosen at $t = 0$ vary uniformly randomly between $-0.1\ \mathrm{mm}/\mu\mathrm{s}$ and $0.1\ \mathrm{mm}/\mu\mathrm{s}$ (or, between -100 m/s and $+100$ m/s). This way we can be sure that large fluctuations, if present, would eventually emerge as the system evolves in time. Of course we assume that for ultrahard materials such high velocity perturbations still create small enough precompressions to justify the use of the Hertz law. The reason for this assumption is simple. Reducing the magnitudes of the initial perturbation velocities would not necessarily rule out the possibility of formation of very large fluctuations, but would push their formation deeper in time. Since accuracy is an important aspect of these simulations, probing deep into time becomes a problem with regard to both calculation accuracy and simulation times needed. To strike a compromise and have a sense of numbers we choose the system described above.

We ignore dissipation in this work as dissipation would quickly decimate all energy in the system. It should be noted that it is possible to mimic the behavior of dissipation-free granular systems by using equivalent circuits, though an $N = 500$ system's circuit may be hard to fabricate and work with [52].

III. RESULTS

In this section we will consider the dynamics of the grains in the system in the quasiequilibrium phase at late times. In these systems the word "late" does not have a simple meaning as the characteristic time scale is defined by the input energy and the system properties. By choosing a hard material and a large set of input velocities we have ensured that the system gets to late times fast enough such that we may be able to see such fluctuations within our simulation time, so within $t \sim 1$ ms or so. Most of our results are shown for times that are far beyond 1 ms. Henceforth by N_t we will denote the total number of time steps through which the system is being iterated. Typically, $N_t = 2 \times 10^8$ in most of our simulations.

We focus henceforth on the kinetic energy fluctuations in the system. The idea is to identify very large fluctuations by assuming that "large" means at least six times the typical kinetic energy fluctuation, which is usually defined as

$$\delta\langle E_K\rangle \equiv \sqrt{\frac{1}{N_t(N-1)}\sum_{i=1}^{N}\sum_{j=1}^{N_t}\left[E_{K_i}(j) - \langle E_K\rangle\right]^2}, \tag{3}$$

where $\langle E_K\rangle$ is the average kinetic energy as dictated by the virial theorem which in this case would be $\frac{5}{9}E$, E being the total energy in the system. The identification of the large fluctuations is done using an algorithm as follows. The space-time data containing the kinetic energy of each grain of the N grains at each instant of time are analyzed through 6×6 space-time grids. Only those points with energy $\langle E_K\rangle + 6\delta\langle E_K\rangle$ are assigned a value of 1 with the remaining points being assigned a value of zero. We next identify at least six consecutive hot spots spanning one or more grids and then identify the set of hot spots as a rogue fluctuation. Clearly, the definitions of hot spots and rogue fluctuations are arbitrary. However, it is not usual for most systems to have too many hot spots and hence one would expect the number of hot spots to far exceed the number of rogue fluctuations. As we shall see, systems that are linear and nonlinear show some hot spots. However, rogue fluctuations do not appear to be common in linear or nearly linear systems.

Let us first recall that the initial conditions used in this work are special, being a uniform random distribution of large velocity perturbations at time $t = 0$. Intuitively, such an initial condition may be assumed to mimic a system that has been

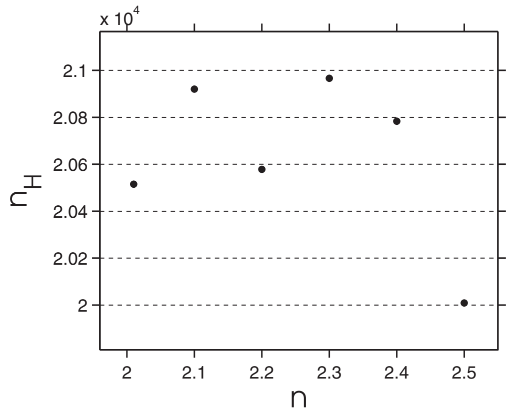

FIG. 1. The number of hot spots n_H for $n = 2.01$, 2.1, 2.2, 2,3, 2.4, 2.5 are shown. The number of hot spots has been calculated for periods across the total run time of 2 ms in our nondissipative ultrahard systems. The number of hot spots is strongly dependent upon the definition used to find them.

very roughly perturbed. Figure 1 shows the typical number of hot spots obtained in the manner described above for the entire length of the simulation, about 2 ms, for various values of $n > 2$. Though not shown here, we have carried out searches for hot spots for $n = 2$ and interestingly we found hot spots in those systems as well with the number of hot spots being not very different from the ones shown in Fig. 1. Further, a close look at the data shows that large kinetic energy fluctuations are not very uncommon and appear to come about with roughly comparable likelihood across all times in a great many systems. However, a large fleeting fluctuation may not result in what we call a rogue fluctuation in analogy with rogue waves that are encountered in open oceans and have been of much interest in the study of the nonlinear Schrödinger equation. We address our findings with regard to rogue fluctuations below.

Rogue fluctuations are also somewhat common in our system when the strongly perturbed system is observed across long enough times such as done here. Unlike in the case of hot spots, there is, however, a very clear trend in how these rogue fluctuations become more prevalent as n increases as shown in Fig. 2. The analyses reveal that the number of rogue waves n_R grows exponentially with increasing n. Our results are consistent with

$$n_R \sim e^{\gamma n}, \tag{4}$$

where $\gamma = 6.41 \pm 0.81$, in other words a *strongly exponential increase in the number of rogue fluctuations with increasing* n. In strongly nonlinear Hertz-like systems such as the ones characterized by Eq. (2), we now know that the magnitude of n is related to the width of the solitary wave W as $W \sim (n-2)^{-1/3}$. Larger n and hence smaller W means large amplitude solitary waves are possible within shorter length scales. Hence for a system of fixed N, the number of rogue waves will go up drastically as suggested by Eq. (4). It is intriguing that n_R increases exponentially in n, however. While it would be desirable to look for rogue fluctuations for $n \gg 5/2$, it turns out that such large nonlinearity studies incur significant enough round-off errors that it is difficult to extract reliable statistics for rogue fluctuations in such systems.

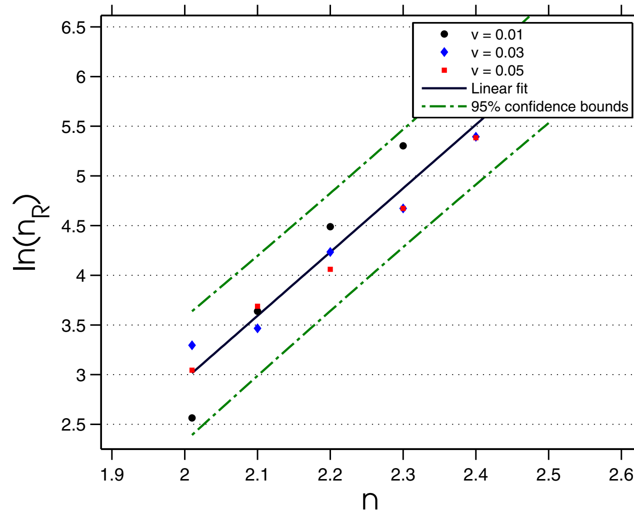

FIG. 2. (Color online) Plot shows how the number of rogue waves n_R grows with increasing n, for various perturbation velocity amplitudes v (0.01 mm/μs, 0.03 mm/μs, and 0.05 mm/μs). The exponential growth in n_R is robust (see text for details).

Regardless, rogue fluctuations in such systems are of great interest and are presently under investigation.

It is natural to ask when these rogue fluctuations form and how they possibly grow in time. We have analyzed the growth in n_R over time for $n = 2.5$. Our results suggest that n_R grows roughly linearly in t for large enough t (i.e., this relation does not hold at short enough times).

Until now we have kept precompression $\Delta = 0$ in Eq. (2). We now let $\Delta > 0$. Raising Δ/R has the effect of introducing harmonic and *other* nonlinear terms to the grain-grain interaction in our system. Thus, the finite Δ problem has parallels with the Fermi-Pasta-Ulam system. For large enough Δ, one can imagine the system acquires strongly harmoniclike features and hence n_R would decrease with increasing Δ. This is indeed

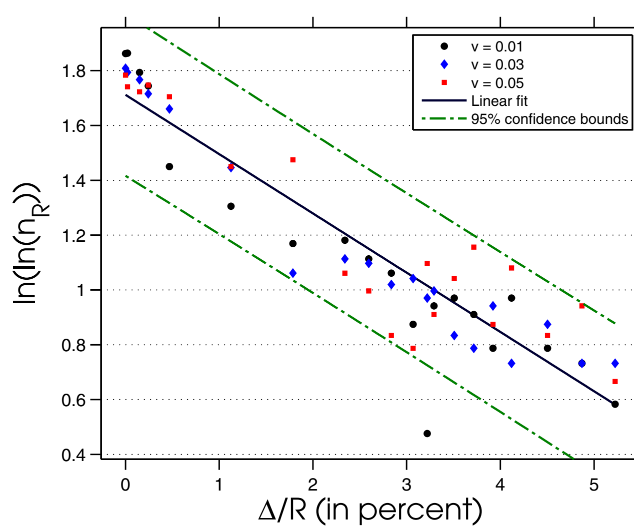

FIG. 3. (Color online) The number of rogue waves n_R decays superexponentially with increasing precompression $\frac{\Delta}{R}$ (see text for details).

what we see in Fig. 3. The simulations suggest that

$$n_R \sim \exp\left[\exp\left(-\kappa\frac{\Delta}{R}\right)\right], \quad (5)$$

where $\kappa = 0.216 \pm 0.022$, which is sometimes referred to as *superexponential decay.* To our knowledge, such decays are not common in physics. However, our simulations strongly suggest that rogue fluctuations go down rapidly with weakening nonlinearity even though the number of hot spots is not much affected.

IV. SUMMARY AND CONCLUSIONS

A great deal of work has been reported on the properties of rogue waves in the oceans. These waves have been extensively probed using the nonlinear Schrödinger equation. Our contention was to show that rogue-wave-like objects may not be unique to the nonlinear Schrödinger equation, and that similar large energy fluctuations, which we call rogue fluctuations, may show up in other systems.

It is well known that any perturbation matures into a solitary wave in unloaded granular alignments that are held between fixed rigid end walls. In a strongly perturbed system, one expects a large number of solitary waves of different amplitudes to be present. It is hence very likely that in the absence of dissipation there would be scenarios where the various solitary waves would come together to realize regions of very large energy fluctuations. This was the logical basis behind our contention.

We studied the long term dynamics of a granular alignment that is held between fixed rigid walls. The system's dynamics in all of our dynamical simulations were initiated by uniformly randomly perturbing each grain between an upper and a lower bound. The perturbation was kept sufficiently strong such that the mechanical energy could bounce back and forth through the system many times over relatively modest time intervals. We defined a hot spot as a point in space and time where the magnitude of kinetic energy was equal to or larger than the average kinetic energy plus six times the kinetic energy fluctuation. The results show that a large number of hot spots form in these systems at late enough times. The results also show that there are many regions of consecutive hot spots in time. We regard these regions as those with rogue fluctuations, in analogy with rogue waves. Rogue fluctuations hence represent long-lived hot spots. We have next shown that the number of rogue fluctuations grows exponentially for increasing nonlinearity of the system under conditions of zero precompression and that the number of rogue waves decays superexponentially with precompression at fixed nonlinearity.

Since all real granular alignments are dissipative in nature, it may not be possible to experimentally observe rogue waves in material systems unless they are appropriately driven in the presence of dissipation. However, it is possible to realize granular alignments in terms of large scale integrated circuits and those systems can be set up in such a way that they behave as effectively nondissipative systems. In due course it may be possible to explore the existence of these rogue fluctuations in such circuits.

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