Description of the surface contour and dispersion relation of subharmonical waves in Q-2D granular media.

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Abstract. When a granular media having a subharmonic pattern is simulated, the first challenge is to define the surface contour of the granular media. This work proposes a method to define this contour. After define this contour, we propose an automated method to detect the presence or absence of the subharmonic oscillation pattern. Finally, with this information, we used the results to study the dispersion relation of the subharmonic pattern and its dependence with the depth of the granular media, resulting in a coincidence with the dispersion relation for shallow water.

1. Introduction
In the last decades several works have been carried out to study the behavior of the granular media [1, 2, 3, 4]. A granular media is composed of particles interacting with each other by energy dissipating interactions, if no energy is injected into the granular media, then the granular media rapidly decants and is immobilized. One of the mechanisms for injecting energy into the granular media is to vibrate the vessel in which the granular media is located and fluidize it [5]. This method, under certain circumstances, causes the granular media to oscillate subharmonically with respect to base oscilation [6]. In this work, a granular media is computationally simulated, we propose a method to define the contour of a granular media, we propose a method to automatically discriminate the presence of the subharmonic pattern and finally the dispersion relation of the subharmonic wave pattern and its dependence with the depth of the granular media.

2. Characterization of the surface contour of a granular media
If we have a distribution of two-dimensional grains inside a rectangular box in which the grains have been compacted around one of the walls of the box, which we will call ”background”, it may be convenient for our investigation to define the surface contour of the granular media. This compaction could be due to the fact that the granular media has been compacted in the lower part of the box by the effect of an external gravitational force or other external force. If the information we have is the position of the geometric center of each grain, then we can define the surface contour as follows:

Once all the X and Y positions of all the particles inside the box are known, we separate the arrangement into \( N_x \) horizontal boxes of \( D_x \) width. For each of the boxes we consider only
the particles whose geometric center is inside the box and in each box we calculate the average vertical position and corresponding standard deviation of the set of particles inside of the box. Finally we define the upper surface of the granular media within the box as the sum of the average vertical position plus the corresponding standard deviation of the particles within the box by a factor of $\sqrt{3}$. This surface will be associated with the horizontal position of the center of the box $x_n$. By repeating this process in all the boxes we can obtain a discretized function $C_s(x)$ to we define the upper contour of the granular media as shown in the figure 1. Likewise, if for some reason the granular media has been separated from the bottom, we can also define the lower bound by subtracting from the average the standard deviation by the factor of $\sqrt{3}$. If the granular media is in evolution, repeating this method for different instants of time we can define a surface contour $C_s(x, t)$ dependent on both the horizontal position and time. With this tool we can study the spatial and temporal evolution of the surface of a granular media.

If the granular media is subject to some fluidization mechanism, it is very likely that some particles of the granular media will be distanced from the total grain set. In this case, the distant particles will increase the standard deviation distorting the surface contour, reason why we must use a criterion to ignore the particles that are far removed from the others.

Before calculating the upper contour as already described, the distance between each of the particles of the system is evaluated. If a particle is less than a certain distance of discrimination $d_0$ from another particle, we will say that the other particle is its neighbor. If a particle does not have at least two neighbors, then that particle is not taken into account for the calculation of the contour. In this way, the particles that are sufficiently close together are part of the granular media and the particles that move away from the whole are excluded except in the rare case where three isolated particles are very close. The distance $d_0$ that we recommend is of two particle diameters, in this way, two particles are considered to be neighboring if it is impossible for another particle to pass between them.

![Figure 1. Example of discretization of the granular media and creation of the upper contour. The red line represents the surface contour and the red spheres are the particles that are considered outside the granular media because they do not have enough neighbors.](image)

3. **Automatic identification of surface pattern**

A useful method for finding patterns in some feature of a system is by studying the autocorrelations of the fluctuations of that feature. If the system to be studied repeats a
sinusoidal characteristic, the autocorrelation of the fluctuations will also be a sinusoidal function. On the other hand, if the characteristic does not present a defined pattern and any fluctuations are a product of system noise, then the autocorrelation will tend to be a delta centered at 0. For the case that we are studying first we need to extract surface fluctuations. If the granular media has decanted because gravity or another homogeneous external field, the equilibrium surface without fluctuations should be a line $C_p(x) = mx + n$ perpendicular to the external field. This straight line is easily obtained from $C_s(x)$ using a basic linear fit. This straight line is not necessarily parallel to the base of the box, so if the box is inclined or subject to some asymmetry along it, it is expected that the slope $m$ is different from 0. Then, the function of spatial fluctuations with respect to equilibrium will be the function $C_f(x) = C_s(x) - C_p(x)$. Once we have our contour of fluctuations, we compute our autocorrelation function (ref eq: autocorrela), using the values $x_n$ corresponding to the position of the centers of the boxes used in calculating the surface contour.

$$A(d_n) = \sum_{i=1}^{N-n} \frac{C_f(x_i)C_f(x_{i+n})}{N-n} \quad n = 0, ..., N \quad d_{n+1} - d_n = x_{n+1} - x_n \quad d_0 = 0 \quad (1)$$

Once we have calculated the autocorrelation function $A(d)$, we proceed to extract significant values from it. One of them is that if we assume that the surface contour has the sinusoidal shape, then the average amplitude $a$ will be defined by $a = \sqrt{2A(0)}$. Another value to extract is the dominant wavelength $\lambda_1$, this wavelength is the distance for the autocorrelation function in which the first local maximum other than $A(0)$ is found. In addition, we define the discrimination factor $f_{di}$ as the ratio between the value of the autocorrelation function for the dominant wavelength and the value of the autocorrelation function at distance zero $f_{di} = A(\lambda_1)/A(0)$, so if the fluctuations have perfectly sinusoidal behavior, then $f_{di} = 1$ whereas if the fluctuations only respond to a noisy behavior, then $f_{di} = 0$, an example of this criterion can be observed in the figure 2.
Figure 2. Example diagram of upper contour and autocorrelation of fluctuations, where $C_s(X)$ is the upper contour, $A(X)$ the autocorrelation of the fluctuations of $C_s(X)$ and $\lambda_1$ is the dominant wavelength.

Using the factor $f_{di}$ we can begin to discriminate the existence or non existence of a periodic pattern in the contour. For this study we will use the criterion that if $f_{di} > e^{-1}$ will assume that there is a pattern, and otherwise there is no pattern. In the case of a subharmonic oscillation pattern, along the oscillation cycle this method detects that the pattern appears and disappears two times per period. In such a case, we can keep track of the amplitude $a$ over time, detect the time instant in which $a$ is a maximum for the first time in each cycle, and thus do a stroboscopic study of the granular media having as reference the phase of the cycle in which the pattern reaches its maximum amplitude.

4. Dispersion relation and its dependence on depth

In this study, multiple simulations were executed in a vertically vibrated granular media, using an event driven molecular dynamics algorithm [7, 8]. The simulations were carried out within a box of width $L_X = 200$ and height $L_Y = 100$ containing a set of particles of diameter $d$ and coefficient of restitution 0.6. To fluidize the granular media, the box is vertically vibrated with an angular frequency $\omega_B$ and an amplitude $A_B$. In each of the simulations the non-dimensional acceleration $\Gamma = A_B \omega_B^2 / g$, the dimensionless velocity $\zeta = A_B \omega_B / (\sqrt{dg})$ was varied, and the amount of particles, which becomes a change in the mean depth of the granular media $h/d = \frac{Nd}{L_x}$. For all these simulations the previous criterion was applied to discriminate the existence of the subharmonic pattern to preserve only the results in which the pattern exists, also considering that the pattern generated is subharmonic, then the oscillation frequency of the granular media will be $\omega = \omega_B/2$. In studying this dataset and testing different settings, we find a good fit for $\omega^2(k, h)$ (2):
\[ \omega_f^2 = 1.1 \pm 0.1 g k \tanh(0.8 \pm 0.2 h k) \] (2)

Figure 3. Quotient \( \omega_f^2/\omega^2 \) versus wave number \( k \) for different values of \( h \).

This dispersion relation and its dependence on depth is very similar to the dispersion relation for shallow water. In the manner in which \( h \) is defined, this value should be 1 for a crystallized compaction ordered as squares and 0.81 for a triangular compaction. Our value is closer to 0.81, which coincides with the fact that, upon striking the base, the granular media is compacted triangularly. This result is quite interesting, since considering that the dispersion relation is comparable to the dispersion relation for shallow water implies that a large part of the causes that generate this dispersion ratio occur when the base is impacted, since the dispersion ratio for shallow water requires that the liquid media always remain in contact with the bottom of the vessel, which in this medium only occurs when the granular media impacts the bottom of the box.

5. Conclusion and comments
We have proposed a method to define the surface contour of a granular media from the individual position of each grain. Using this method, we were able to study the dispersion relation for a vibrated granular media in which there is a subharmonic vibration which gives us the same dispersion relation for shallow water, which leads us to suppose that the guiding mechanism for the subharmonic waves occur when the granular media strikes the vibrating base. However, in the case of the surface waves of a liquid, its dispersion relation requires that the medium has a surface tension, which makes us assume that for the case of the granular media there could be some phenomenon that plays the role of the surface tension.
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