Acoustic resonances in a confined set of macroscopic disks

Juan F. González-Saavedra, Álvaro Rodríguez-Rivas, Miguel A. López-Castaño and Francisco Vega Reyes

Departamento de Física and Instituto de Computación Científica Avanzada (ICCAEx), Universidad de Extremadura, 06071 Badajoz, Spain
e-mail: juanfrangs@unex.es

Abstract. We study in this work a system of granular disks enclosed in a rectangular region. Granular disks are arranged, at high particle density, in a hexagonal lattice. Specifically, we are interested in the conditions for mechanical signal transmission. Two different potentials are considered. Our results are obtained by means of soft disks computer simulations. We analytically determine the eigenfrequencies spectra of the system from the corresponding Hessian matrix. Alternatively, the eigenfrequencies can also be obtained from the time evolution of molecular dynamics simulations. Previous works have shown that mechanical signal transmission in granular matter can be used to develop acoustic switches. Our results reveal that the working range of the granular switch changes dramatically for different interaction models. In particular, strong anisotropies in signal transmission may appear for certain interparticle forces.

1 Introduction

Signal transmission devices are ubiquitous in mechanical engineering applications [10,6]. They are used as vibration insulators [7], acoustic cloaks [20], sound propagation [5], signal rectification [4], etc. In this context, highly dense granular systems can be used to perform these tasks [19]. In particular, granular crystals have proven to be efficient for clean signal transmission [3]. In fact, some recent works show that they can work as switches [19], rectifiers [3] and a range of logic elements [12].

Hence, granular crystals can be used to modify and transmit mechanical energy signals [1]. These applications are analogous to the electrical switches that can control electromagnetic waves propagation [2]. Control of acoustic and thermal information using this type of switches can lead to applications in fields such as thermoelectric systems, communication or ultrasonic imaging [8].

As it is known, dense granular systems of identically shaped particles can develop crystalline structures [13]. Usually, the critical density for the appearance of ordering depends strongly on the values of the other relevant physical magnitudes: granular temperature [15], degree of inelasticity in collisions [18], the
specifics of the physical processes involved in particle collisions [14], the type of interaction with the boundaries [9], the kind of energy input necessary to thermalize the granular particles [11], etc. Experimental and computational work has put in evidence these effects.

We study in this work a system consisting of macroscopic disks by means of molecular dynamics simulations. In order to assess the influence of interparticle collisions, we consider two interaction potentials: a potential that is quadratic in the distance between particles [19], and a Lennard-Jones-type potential [16].

The paper is organized as follows. The second section is devoted to the system description, including the initial configuration used in this work, together with the computational and theoretical methods used to obtain the results. Finally, Section 3 presents the results and a discussion, together with a description of possible future extensions of our results.

2 Description of the system and computational methods

Let us imagine a rectangular region defined by two parallel rigid walls and two parallel periodic boundaries, as sketched in Fig. 1. There is no gravitational field acting on the system. Rigid walls-disks interactions are modelled with the same potential as for disk-disk interactions. More specifically, rigid walls are modelled by assuming the existence of a particle of the same size and mass behind the wall, when the wall is within the interaction range of a real particle. The \( x \) position of this wall particle coincides at all times with the \( x \) position of the corresponding real particle. On the contrary, the \( y \) position of the wall particle center is always located at a particle radius away from the wall surface.

Two different types of interaction are used. The first one is parabolic-like, with the form

\[
U(r_{ij}) = \begin{cases} 
\frac{\epsilon}{2} \left(1 - \frac{r_{ij}}{\sigma}\right)^2 & \text{if } r_{ij} \leq \sigma \\
0 & \text{if } r_{ij} > \sigma
\end{cases}
\]

whereas the second potential is a Lennard-Jones type potential [16]

\[
U(r_{ij}) = \begin{cases} 
4\epsilon \left[ \left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^6 \right] + \epsilon & \text{if } r_{ij} \leq r_c \\
0 & \text{if } r_{ij} > r_c
\end{cases}
\]

where \( \epsilon \) sets the energy scale, \( \sigma \) is the diameter of the disks, \( r_{ij} \) is the distance between centers of disks \( i \) and \( j \) and \( r_c \) is the energy cut distance, set in our simulations to \( 2^{1/6} \sigma \).

In order to obtain the eigenfrequencies of the system, we computed the eigenvalues \( \omega_k^2 \) of the dynamical matrix \( \mathcal{D} \), whose elements are [19] [17]

\[
\mathcal{D}_{ij} = \mathcal{M}_{ik}^{-1} \mathcal{H}_{kj}
\]

with

\[ \mathcal{H}_{ij} = \frac{\partial^2 U}{\partial x_i \partial x_j}, \quad M_{ij} = m_{L,H} \delta_{ij} \] (4)

where \( M_{ij}, \mathcal{H}_{ij} \) are the corresponding Hessian matrix [17] and the particle mass diagonal matrices, respectively, and \( m_L, m_H \) are the masses of the particles. The eigenvalues were obtained by: a) considering an initial equilibrium state of the system; b) from the average positions of the particles for a simulation run.

In the simulations, a 2D system of particles (disks with equal diameter \( \sigma \)) inside the rectangular box is considered. The dimension of the box is such that an integer number of horizontal layers can be perfectly accommodated into a hexagonal lattice, as it can be seen in Fig. 1. The total number of particles is 100, each of them with a diameter \( \sigma \), which we take as length unit. We consider particles with two different masses, the mass ratio being \( m_H/m_L = 10 \). The particle distribution is such that we have 25 light disks (with mass \( m_L \)) and 75 heavy disks (with mass \( m_H \)). The initial configuration is the mechanically stable packing of the disks.

![Fig. 1. Initial setup of the light (blue) and heavy (red) disks, with 10 × 10 particle layers. x stands for the horizontal axis and y for the vertical axis.](image)

Initial particle velocities are drawn from a Maxwell-Boltzmann distribution whose standard deviation is determined by the system initial temperature. In our case, this temperature is a control parameter in the simulations. The evolution of the system is obtained from molecular dynamics simulations using leap-frog method [16]. The pressure can also be modified by approaching the rigid walls to each other.

3 Results and discussion

In Fig. 2 we can see the corresponding eigenvalues for both parabolic [1] and Lennard-Jones [2] potentials. The equilibrium positions are considered as \( p = 0 \) configurations. This state can be modified by approaching the top and bottom walls. In this case, the disks will overlap, and, as a consequence, repulsion forces
between them appear. By means of this procedure, we can slightly increase the pressure to \( p = 0.1 \). As we can see, the eigenvalues display significant discontinuities. This produces frequency gaps which can be tuned by modifying the pressure of the system. It is this behavior which allows for the use as a switch. Put in other words, a mechanical signal with a given frequency \( \omega \) will be transmitted only if it does not lie within a forbidden frequency gap (for a given value of the system pressure \( p \)).

As we can see in Fig. 3 the normalized velocity autocorrelation function \( \left\langle (\mathbf{v}(t_0 + t) \cdot \mathbf{v}(t_0))/\mathbf{v}(t_0) \cdot \mathbf{v}(t_0) \right\rangle \) has finite decay length and is isotropic for the parabolic potential whereas for the Lennard-Jones potential does not decay and there are significant differences between the \( x \) and \( y \) directions. The peculiar behavior in the case of the Lennard-Jones may be due to its steep repulsive term, as compared to the parabolic potential.
Acoustic resonances in a confined set of macroscopic disks

Fig. 4. Power spectra distribution (Fourier transform of the velocity autocorrelations) in the \( x \) and \( y \) directions for the parabolic (left panel) and the Lennard-Jones potentials (right panel) at temperature \( T = 10^{-4} \).

A way to look at the behavior of an eventual granular switch is to calculate the power spectra density

\[
D(\omega) = \int_0^\infty dt \frac{\langle \mathbf{v}(t_0 + t) \cdot \mathbf{v}(t_0) \rangle}{\langle \mathbf{v}(t_0) \cdot \mathbf{v}(t_0) \rangle} e^{i\omega t} \tag{5}
\]

In Fig. 4, we can see the corresponding Fourier transform of the panels in Fig. 3. It is interesting to note that the isotropy properties of the autocorrelation function show up here as well. More specifically, for the Lennard-Jones potential (right panel), the high frequency peak disappears in the \( x \) direction for \( T < 10^{-4} \). This is illustrated in more detail in Fig. 5 where \( D(\omega) \) is displayed for a range of initial temperatures for both potentials.

Finally, in Fig. 5 we can see the different behavior of \(|D(\omega)|^2\) for the parabolic and Lennard-Jones potential in the \( x \) and \( y \) directions. We can remark the anisotropy that emerges for the Lennard-Jones potential. Notice also that for the Lennard-Jones potential more and stronger frequency peaks appear, compared with the parabolic one.

4 Conclusions

Summarizing, we have analysed in this paper the mechanical signal behavior for two granular systems. More concretely, our system is composed by two sets of granular particles whose masses are different. Otherwise, the particles have identical properties. Two different potentials have been analysed. They are arranged in an hexagonal lattice and from the corresponding Hessian matrix we have calculated the inherent eigenfrequencies. In addition, we inspected the behavior of the velocity autocorrelations functions finding important anisotropic behavior in the case of the Lennard-Jones potential for which clearly the transmission is more intense in the \( y \) direction (perpendicular to the thermal walls). In addition, the high frequency peak of the velocity autocorrelation Fourier transform disappear in the \( x \) direction for the Lennard-Jones potential.
Fig. 5. Power spectra distribution (Fourier transform of the velocity autocorrelations): for the parabolic potential in the $x$ direction (a) and $y$ direction (b), and the Lennard-Jones potentials in the $x$ direction (c) and $y$ direction (d).

Our results show that the properties of the interaction forces and the initial temperature conditions can significantly change the properties of the mechanical signal transmission in a forced granular system.

References

1. Alagoz, S., Baykant Alagoz, B.: Sonic crystal acoustic switch device. J. Acoust. Soc. Am. 133, EL485–EL490 (2013)
2. Bardeen, J., Brattain, W.H.: Phys. Rev. 74, 230 (1948)
3. Boechler, N., Theocharis, G., Daraio, C.: Nat. Mater. 10, 665 (2011)
4. Boechler, N., Theocharis, G., Kevrekidis, P.G., Daraio, C.: J. Appl. Phys. 109, 074,906 (2011)
5. Cummer, S.A.: Science 343, 495 (2014)
6. Devaux, T., Cebrecos, A., Richoux, O., Pagneux, V., Tournat, V.: Acoustic radiation pressure for nonreciprocal transmission and switch effects. Nature Commun. 10, 3292 (2019)
7. Gantzounis, G., Serra-Garcia, M., Homma, K., Mendoza, J.M., Daraio, C.: Granular metamaterials for vibration mitigation. J. Appl. Phys. 114, 093,514 (2013)
8. Li, F., Anzel, P., Yang, J., Kevrekidis, P.G., Daraio, C.: Granular acoustic switches and logic elements. Comput. Sci. Eng. 5, 5311 (2014)
9. Lobkovsky, A., Vega Reyes, F., Urbach, J.: Eur. Phys. J. Special Topics 179, 113–122 (2009)
Acoustic resonances in a confined set of macroscopic disks

10. Lu, Y.J., Ge, Y., Yuan, S.Q., Sun, H.X., Liu, X.J.: Acoustic logic gates by a curved waveguide with ultrathin metasurfaces. Journal of Physics D: Applied Physics 53, 015,301 (2020)
11. M. A. López-Castaño, González-Saavedra, J.F., Rodríguez-Rivas, A., Vega Reyes, F.: Statistical properties of a granular gas fluidized by turbulent air wakes (2019). E-print arXiv:1911.01384
12. Mahboob, I., Flurin, E., Nishiguchi, K., Fujiwara, A., Yamaguchi, H.: Nat. Commun. 2, 198 (2011)
13. Melby, P., Vega Reyes, F., Prevost, A., Robertson, R., Kumar, P., Egolf, D.A., Urbach, J.S.: The dynamics of thin vibrated granular layers. J. Phys.: Condens. Matter 17, S2689–S2704 (2005)
14. Olafsen, J.A., Urbach, J.S.: Clustering, order and collapse in a driven granular monolayer. Phys. Rev. Lett 81, 4369–4372 (1998)
15. Prevost, A., Melby, P., Egolf, D., Urbach, J.S.: Phys. Rev. E 17, 050,301(R) (2005)
16. Rapaport, D.C.: The art of molecular dynamics simulation. Cambridge University Press, Cambridge, UK (2004)
17. Tanguy, A., Wittmer, J.P., Leonforte, F., Barrat, J.L.: Continuum limit of amorphous elastic bodies: A finite-size study of low-frequency harmonic vibrations. Phys. Rev. B 66, 174,205 (2002)
18. Vega Reyes, F., Urbach, J.S.: Clustering, order and collapse in a driven granular monolayer. Phys. Rev. E 78, 051,301 (2008)
19. Wu, Q., Cui, C., Bertrand, T., Shattuck, M.D., O’Hern, C.S.: Active acoustic switches using two-dimensional granular crystals. Phys. Rev. E 99, 062,901 (2019)
20. Zigoneanu, L., Popa, B.I., Cummer, S.A.: Nat. Mater. 13, 352 (2014)