Role of defects in the onset of wall-induced granular convection

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We investigate the onset of the wall-induced convection in vertically vibrated granular matter by means of experiments and two-dimensional computer simulations. In both simulations and experiments we find that the wall-induced convection occurs inside the bouncing bed region of the parameter space in which the granular bed behaves like a bouncing ball. A good agreement between experiments and simulations is found for the peak vibration acceleration at which convection starts. By comparing the results of simulations initialised with and without defects, we find that the onset of convection occurs at lower vibration strengths in the presence of defects. Furthermore, we find that the convection of granular particles initialised in a perfect hexagonal lattice is related to the nucleation of defects and the process is described by an Arrhenius law.

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between the disks and via static friction \[28\]. This model and its parameter values (See Tab. 1) have been chosen because they reproduce the contact properties \[29\] of granular beads, and give results for the dynamics of an intruder in a vertically oscillated granular bed, which are in good agreement with experiments \[20\].

The simulation box is driven sinusoidally, i.e., the bottom of the container is moved in time according to

\[ z_b = -\frac{1}{2}L_z + A \sin(\omega t), \]

where \( z_b \) is the height coordinate of the bottom of the container, \( A \) is the amplitude of the oscillation, \( \omega \) is the frequency and \( t \) is the time.

We traced the dynamical phase diagram for a fixed oscillation frequency \( \omega = 1.00 \text{s}^{-1} \) and lateral wall separation \( L_x/\sigma = 20 \). Reduced units are used throughout the article: the particle mass \( m \), the particle diameter \( \sigma \) and the gravitational acceleration \( g \) are our fundamental units. Consequently, the derived units are the time \( t_0 = \sqrt{\sigma/g} \), velocity \( v_0 = \sqrt{g\sigma} \), force \( f_0 = mg \), elastic constant \( k_0 = mg/\sigma \) and damping coefficient \( \gamma_0 = g/\sigma \). Further details of the model are given in appendix A.

The external driving force is characterised by a dimensionless acceleration \( \Gamma = A\omega^2/g \), corresponding to the maximum acceleration due to Eq. (1) divided by the gravitational acceleration \( g \). Alternatively, we use the dimensionless energy parameter \[30\] \( K_m = A^2\omega^2/\sigma g \), i.e., the maximum kinetic energy per particle 'injected' in the system every period of oscillation \[31\].

The experiment is conducted with a monolayer of spherical polished opaque glass beads (SiLiBeads P) with a diameter of \( 2 \pm 0.02 \) mm. A rectangular cell made up of two glass plates \( 40 \text{ mm} \) width by \( 200 \text{ mm} \) height separated by a distance of \( 2.3 \text{ mm} \) is used to create a quasi-two-dimensional configuration. The cell is mounted on an electromagnetic shaker (Tira TV50350) with the sinusoidal frequency and amplitude controlled by a function generator (Agilent FG33220). The acceleration is obtained by an accelerometer (Dyson 3035B2). In order to avoid the influence from electrostatic forces, the side walls of the container are made of aluminium. With a backlight illumination, the mobility of the particles are captured with a high speed camera (IDT MotionScope 50350) which is externally triggered so as to take images at fixed phases of each vibration cycle. The snapshots captured are subjected to an image processing procedure to locate all spheres based on a Hough transformation \[32\]. Tracer particles are used to determine the convection threshold (see appendix B for details).

In order to compare the results of the simulations with the experiments, we produced results for fixed numbers of particles, namely \( N = 200, 400, 800, 1200, 1600 \). The different sets are identified via the linear density \( N_l = N/L_x \). This number gives an approximate value for the number of particle layers and hence, the height of the granular bed. In reality the height depends on the local structure of the granular bed, namely, the orientation of the hexagonally-ordered particles, and the type and amount of defects.

### III. Initialisation

In the experiment the system is initialised with a strong agitation to create a completely fluidized state, followed by a slow ramping down of the vertical acceleration. In the simulation the initial configuration is prepared with two distinct procedures. In the crystalline initialisation, the particles are placed in a perfect hexagonal lattice resting at the bottom of the container. In the random initialisation, the particles are placed randomly in the box. Via molecular dynamics we evolve the system until all particles have fallen under gravity and have reached a rest position.

![Figure 1. (colour online) Simulation snapshots of the typical initial configurations for \( N_l = 60 \). The colour indicates the local order of the particles according to an analysis with the \( q_6 \) order parameter \[33\]. Green (light grey) indicates hexagonal order, red (dark grey) indicates a square local order while other colours indicate a disordered configuration.](image)

The resulting configurations are shown in Fig. 1. We note that in both simulations initialised randomly and the experiments a large amount of particles have local hexagonal order with many topological defects, such as dislocations and grain boundaries. For a two dimensional system there are two favoured orientations of the hexagonal lattice, when in contact with a flat wall. In Fig. 2b) the Orientation A with the [111] direction parallel to the wall is shown. In Fig. 2b) the orientation B has the [010] direction parallel to the wall. In the crystalline initialisation we chose to place the particles according to orientation A. After the random initialisation processes, we find...
that in the experiment almost all particles have orientation B, while in simulation the orientation A seems to be favoured, but grain boundaries between the different orientations are visible. Figure 1 shows the configurations obtained in the three cases.

IV. DYNAMICAL PHASES

We have systematically investigated the onset of convection at different dimensionless accelerations/energies and heights of the granular bed. Figure 3 shows the location of the dynamical phases as a function of the dimensionless acceleration $\Gamma$ and the energy parameter $K_m$ for different values of the linear density $N_l$. The parameter $N_l\sigma$ is also a measure of the number of layers in the granular bed, and therefore of its height.

The transition from the comoving to bouncing bed phase occurs, as expected, at $\Gamma \approx 1$ with the critical value of the acceleration increasing slightly with increasing number of layers. We find good agreement between simulations started with defects (green triangles) and experiments (connected squares). On the other hand, for simulations without initial defects we find a stronger dependence on the number of layers (blue circles). Inside the bouncing bed regime, we observe a transition from a bouncing bed phase without convection to a bouncing bed phase with convection. For the number of layers $N_l\sigma \geq 40$, we find reasonable agreement between experiments and the simulations initialised randomly. On the other hand, for $N_l\sigma=10$ and 20 the model overestimates the amount of energy necessary for the convection to start. At small heights of the granular bed, the effective force that drives the onset of convection, i.e., the frictional force between particles and walls, reduces because the normal stress to the side walls reduces. This is reminiscent of the Janssen’s law for the static case [34, 35]. As a consequence, one expects a higher agitation strength for the onset of convection for small number of layers.

On the other hand, the experimental box is not exactly two-dimensional and the presence of a front and a back wall effectively increases the amount of wall surface available with respect to the simulations. We believe this is the reason behind the lack of the increase in the critical acceleration for $N_l\sigma=10$, and 20. For simulations that start without topological defects we consistently detect the onset of convection (blue circles) at higher values of the acceleration with respect to the experiments and to the simulations started with defects. The enhancement of the convection due to the presence of defects explains the observation of Pöschel and Herrmann [11] that an intruder can initiate convection. The presence of an intruder induces topological defects [36] that initiate the convection and segregation.

V. ONSET OF CONVECTION

In crystalline materials collective particle movements occur via crystalline plane slips [10]. The same occurs in our granular systems, but we noted some differences in slip behaviour between simulation and experiments. In simulation the slip occur primarily along the oblique directions, while in the experiment it occurs mainly along the vertical direction. The difference can be explained by the different orientation of the hexagonal crystal in the two cases. The granular particles experience a shear stress due to the wall of the container along the vertical direction. In the experiments the particles are oriented
like in Fig. 2b), and slips occur preferentially in the vertical direction. On the other hand, in simulations we find more particles with an orientation like in Fig. 2a) and the pyramidal slip planes will be activated first. As long as plane slips are concerned, the worst case scenario is represented by a perfect crystal with orientation A. Since no defects are initially present, slips along the pyramidal planes can only occur if defects are nucleated first. Another difference is that in experiments we often observe single convective rolls similar to the observation in a two-dimensional rotating cell [37]. This type of convective motion is not detected in simulation and the reason for the discrepancy is likely due to a small tilt of the side walls [9].

In order to clarify the role of defects in the onset of convection, we analyse in computer simulations the granular temperature \( T_g \) in relation to the average input energy \( K_m \). The granular temperature is defined as

\[
T_g = \frac{m}{N} \left( \sum_{i=1}^{N} \frac{1}{2} (v_i(t) - v_{cm}(t))^2 \right) \tag{2}
\]

where \( v_{cm} \) is the centre of mass velocity and \( v_i(t) \) is the velocity of particle \( i \) at time \( t \) and \( \langle \rangle \) indicates a time average. Figures 4a-b show the behaviour of the reduced granular temperature \( T_g^* = T_g/(mg\sigma) \) as a function of the dimensionless energy parameter \( K_m \) for systems initialised with and without defects, respectively. In both cases the temperature increases monotonically over many periods of temperature behaviour, we investigate the slip probability \( \sigma \) and its dependence on \( K_m \).

We divide the energy \( K_m \) parameter space in regions with different slopes of the temperature curves. For the random initialisation (Fig. 4a) we find two regions: A and B. The transition occurs at \( K_m \approx 3.3 \) as signalled by a change in slope of the temperature curve. Comparing the energy value for this transition with the diagram of Fig. 3, we note that it corresponds to the energy value at the onset of convection.

On the other hand, for the case initialised without defects (Fig. 4b) we can distinguish three regions. Following the naming convention used in Fig. 4a, we indicate with \( A_1 \) the region where convection is detected. The region \( A_2 \), without convection, is now divided in two subregions \( A_1 \) and \( A_2 \).

In order to clarify the origin of the different regions of temperature behaviour, we investigate the slip probability of a particle in the bulk of the granular bed, i.e. away from the top free interface [35]. The slip of a particle is detected if a displacement larger than 0.2 \( \sigma \) is measured for at least two nearest neighbours after one oscillation. We define the slip probability \( p_s \) as the fraction of particles which undergo a slip in one oscillation period. The value of \( p_s \) is averaged over 200 periods of oscillation. The slip probability as a function of \( 1/K_m \) is shown in Figs. 4a-b for the random and crystal initialisation, respectively. For the random case we do not observe a change in the slip behaviour between regions \( A \) and \( B \). On the other hand a quite dramatic change of behaviour is observed for the crystal case. In particular, in region \( A_1 \) the number of detected slip is exactly zero, while region \( A_2 \) is characterised by a quite steep increase of slip events, which slows down considerably upon onset of convection (region B).

In all cases the curves can be fitted to an Arrhenius law, \( p_s \propto \exp(-E_b/K_m) \), indicating the presence of activating mechanisms. The energy parameter \( E_b \) is a measure of the barrier height and the dimensionless energy \( K_m \) assumes the role of a reservoir temperature. For the random case just a single curve can be fitted to the entire range of inverse energies. From the fit we find an average dimensionless barrier height \( E_b = 7 \pm 1 \). For the case initialised with the crystal, we find a barrier \( E_b = 130 \pm 20 \) in region \( A_2 \), and a barrier \( E_b = 7 \pm 1 \) in region \( B \).

Since the barrier height is the same for the system with initial defects, independent of the presence of convection, we can speculate that the activation mechanism indicated by the Arrhenius equation is the activation of slip events in a crystal with topological defects. Interestingly, the same barrier is measured for the system without initial defects in region B, suggesting the same activation mechanism. But in order for this to occur defects must first nucleate inside a perfect crystal, and we speculate that the very high barrier in region \( A_2 \) is due to the nucleation of defects in a perfect hexagonal crystal.

![Figure 4](image.jpg)

**Figure 4.** (colour online) Granular temperature \( T_g^* \) versus dimensionless energy parameter \( K_m \). The dashed lines separate regions with different slopes of the temperature curves. a) For the system initialised randomly, i.e. with defects. b) For the system initialised in a perfect hexagonal lattice, i.e. without initial defects.
VI. CONCLUSIONS

In conclusion, using two-dimensional computer simulations and experiments we locate the wall-induced convection in the bouncing bed region in the dynamical phase diagram of vertically vibrated granular matter.

For the onset of convection, we find an overall good agreement between the experimental results and those from simulations initialised with defects, for a linear density/number of layers of $N_l\sigma \geq 40$. On the other hand, for $N_l\sigma = 10$, and 20 the model overestimates the amount of energy necessary for the convection to start. We believe the reason behind the discrepancy is the presence of a front and a back wall in the experimental box, which effectively increase the amount of wall friction “available” for convection to start. Other phenomenological differences between simulations and experiments are observed for the favoured crystal orientation and slip events. We think that these differences are due to a small tilt of the experimental box and small variations of the experimental box width $L_x$.

For a system initialised in a perfect crystal, i.e., without initial defects, we consistently observe the wall-induced convective motion to occur at higher values of the dimensionless energy parameter (shaking strength) than the experimental box width and small variations of the experimental box width.

In conclusion, using Molecular Dynamics simulations at fixed time step $dt$, for two translational degrees of freedom and one rotational degree of freedom for a system of soft disks. An illustration of the model is shown in Fig. 6. Two particles at positions $r_i$ and $r_j$ with velocities $v_i$ and $v_j$ and angular velocities $\omega_i$ and $\omega_j$ define a system with an effective mass $m_{eff} = m_i + m_j$ and a normal unit vector $n_{ij} = \frac{r_i - r_j}{|r_i - r_j|}$. The tangential direction is defined as $t_{ij} = \frac{v_{ij}}{|v_{ij}|}$, where

$$v_{ij} = v_i - v_j - \frac{1}{2}(\sigma_i \omega_i + \sigma_j \omega_j) \times n_{ij},$$

with $v_{n_{ij}} = (v_{ij} \cdot n_{ij}) n_{ij}$.

We define the displacement in the two directions $\delta_{n_{ij}} = d - |r_i - r_j|$, with $d = 1/2(\sigma_i + \sigma_j)$, and $\delta_{t_{ij}} = v_{t_{ij}} dt$. For the disk-disk interactions we use a linear model with forces

$$F_{n_{ij}} = (\kappa_n \delta_{n_{ij}} n_{ij} - \gamma_n m_{eff} v_{n_{ij}}),$$

$$F_{t_{ij}} = (-\kappa_t \delta_{t_{ij}} n_{ij} - \gamma_t m_{eff} v_{t_{ij}}),$$

in the normal and shear tangential directions, respectively. The parameters $\kappa_n$ and $\kappa_t$ are the stiffness co-

Appendix A: Details of the Model

We carry out Molecular Dynamics simulations at fixed time step $dt$, for two translational degrees of freedom and one rotational degree of freedom for a system of soft disks. An illustration of the model is shown in Fig. 6. Two particles at positions $r_i$ and $r_j$ with velocities $v_i$ and $v_j$ and angular velocities $\omega_i$ and $\omega_j$ define a system with an effective mass $m_{eff} = m_i + m_j$ and a normal unit vector $n_{ij} = \frac{r_i - r_j}{|r_i - r_j|}$. The tangential direction is defined as $t_{ij} = \frac{v_{ij}}{|v_{ij}|}$, where

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in the normal and shear tangential directions, respectively. The parameters $\kappa_n$ and $\kappa_t$ are the stiffness co-
coefficients in the normal and tangential direction, respectively. The energy dissipated during the contact is regulated by the damping coefficients $\gamma_n$ and $\gamma_t$. In addition we model the static friction by keeping track of the elastic shear displacement $\delta_{nij}$ over the contact lifetime and truncate it such that the Coulomb condition $|F_{tij}| < |\mu F_{nij}|$ is satisfied, where $\mu$ is the static friction coefficient. The same kind of interaction is used between the particles and the container wall. We also consider the gravitational force $g = -ge_z$, where $e_z$ is the unit vector pointing in $z$ direction.

Once the forces on all particles are known the total force and torque $\tau_i$ on a particle $i$ is determined by

$$F_i = mg + \sum_j (F_{nij} + F_{tij}) \quad (A4)$$

$$\tau_i = -\frac{1}{2} \sum_j \sigma_j n_{ij} \times F_{tij}.$$

### Table I. Numerical values of the simulation parameters.

| Coefficient                  | Particle-Particle | Wall-Particle |
|------------------------------|-------------------|---------------|
| Normal stiffness $k_n$       | $10^6 (k_0)$      | $10^6 (k_0)$  |
| Tangential stiffness $k_t$   | $10^4 (k_0)$      | $10^4 (k_0)$  |
| Static friction $\mu$       | 0.6               | 0.6           |
| Normal damping $\gamma_n$   | 100 ($\gamma_0$) | 100 ($\gamma_0$) |
| Tangential damping $\gamma_t$| 100 ($\gamma_0$) | 100 ($\gamma_0$) |

The typical numerical values of simulation parameters are shown in Table I. In this linear model it is possible to calculate the contact duration [10]

$$t_c = \pi \left( \frac{k_n}{m_{eff}} - \frac{\gamma_n^2}{4} \right)^{-0.5} \quad (A5).$$

In order to obtain an accurate integration of the equation of motion during contact, the time step of the simulation is chosen to be $\delta t \approx t_c/50$ [11].

### Appendix B: Detection of the dynamical phases

The detection of the bouncing bed dynamical phase is performed visually, in both computer simulations and experiments. In the experiments the distance between the granular bed and the bottom of the container depends on the phase lag between the camera and the shaker, which can be adjusted to inspect the collective motion of the granular bed over the whole vibration cycle.

The detection of the convective motion is done in simulation by colouring the particles according to their initial height as shown in Fig. 7. After few oscillation cycles we determine visually the presence, or not, of the typical structures of the convective rolls.

In the experiments, convection is detected with the help of tracer particles. From the occurrences of slip events for tracer particles at the side walls within a period of 1000 vibration cycles, we determine the convection threshold. An example is shown in Fig. 8.

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Figure 8. (colour online) A sequence of experimental snapshots showing convection of the granular particles (black spheres) under sinusoidal vibrations with an agitation frequency $f = 10$ Hz and $\Gamma = 4.53$. Red (dark grey) and yellow (light grey) spheres mark the tracer particles that are moving up and down, respectively. a) At $t=0$. b) $t=1$ s. c) $t=2$ s.

[1] H. M. Jaeger, S. R. Nagel, and R. P. Behringer, Rev. Mod. Phys. 68, 1259 (1996).
[2] S. Luding, Nonlinearity 22, R101 (2009).
[3] H. Miyamoto, H. Yano, D. J. Scheeres, S. Abe, O. Barnouin-Jha, A. F. Cheng, H. Demura, R. W. Gaskell, N. Hirata, M. Ishiguro, T. Michikami, A. M. Nakamura, R. Nakamura, J. Saito, and S. Sasaki, Science 316, 1011 (2007).
[4] J. Duran., Sands, powders, and grains: An introduction to the physics of granular materials. (Springer Verlag, 2000).
[5] N. Mohabuth and N. Miles, Resources, Conservation and Recycling 45, 60 (2005).
[6] A. Rosato, K. Strandburg, F. Prinz, and R. Swendsen, Phys. Rev. Lett. 58, 1038 (1987).
[7] M. Schröter, S. Ulrich, J. Kreft, J. Swift, and H. Swinney, Phys. Rev. E 74, 011307 (2006).
[8] D. Hong, P. Quinn, and S. Luding, Phys. Rev. Lett. 86, 3423 (2001).
[9] J. Knight, H. Jaeger, and S. Nagel, Phys. Rev. Lett. 70, 3728 (1993).
[10] W. Cooke, S. Warr, J. Huntley, and R. Ball, Phys. Rev. E 53, 2812 (1996).
[11] T. Pöschel and H. J. Herrmann, Europhysics Letters 29, 123 (1995).
[12] A. Kudrolli, Rep. Prog. Phys. 67, 209 (2004).
[13] M. Majid and P. Walzel, Powder Technology 192, 311 (2009).
[14] A. Mehta and J. Luck, Phys. Rev. Lett. 65, 393 (1990).
[15] S. Douady, S. Fauve, and C. Laroche, Europhysics Letters 8, 621 (1989).
[16] A. Uegawa and O. Sano, Journal of the Physical Society of Japan 72, 1390 (2003).
[17] O. Sano, Phys. Rev. E 72, 051302 (2005).
[18] P. Eshuis, R. Bos, D. Lohse, D. Van der Meer, and K. Van der Weele, Phys. of Fluid 19, 123301 (2007).
[19] P. Eshuis, D. van der Meer, M. Alam, H. J. van Gerner, K. van der Weele, and D. Lohse, Phys. Rev. Lett. 104, 038001 (2010).
[20] J. Sun, F. Battaglia, and S. Subramaniam, Phys. Rev. E 74, 061307 (2006).
[21] E. Clément, J. Duran, and J. Rajchenbach, Phys. Rev. Lett. 69, 1189 (1992).
[22] J. B. Knight, E. E. Ehrichs, V. Y. Kuperman, J. K. Flint, H. M. Jaeger, and S. R. Nagel, Phys. Rev. E 54, 5726 (1996).
[23] Y.-h. Taguchi, Phys. Rev. Lett. 69, 1367 (1992).
[24] S. Luding, E. Clément, A. Blumen, J. Rajchenbach, and J. Duran, Phys. Rev. E 50, R1762 (1994).
[25] M. Bourzutschky and J. Miller, Phys. Rev. Lett. 74, 2216 (1995).
[26] D. Risso, R. Soto, S. Godoy, and P. Cordero, Phys. Rev. E 72, 011305 (2005).
[27] D. Frenkel and B. Smit, Understanding Molecular Simulation (Academic Press, London, 2002).
[28] P. A. Cundall and O. D. L. Strack, Géotechnique 29, 311 (1979).
[29] J. Schafer, S. Dippel, and D. Wolf, Journal De Physique I 6, 5 (1996).
[30] H. Pak and R. Behringer, Physical Review Letters 71, 1832 (1993).
[31] This parameter is also called dimensionless shaking strength [18].
[32] C. Kimme, D. H. Ballard, and J. Sklansky, Comm. As-
soc. Comp. Mach. 18, 120 (1975).
[33] P. Steinhardt, D. Nelson, and M. Ronchetti, Phys. Rev. B 28, 784 (1983).
[34] H. A. Janssen, Z. Ver. Dt. Ing. 39, 1045 (1895).
[35] U. M. B. Marconi, A. Petri, and A. Vulpiani, Physica A 280, 279 (2000).
[36] V. W. de Villeneuve, R. P. Dullens, D. G. Aarts, E. Groeneveld, J. H. Scherff, W. K. Kegel, and H. N. Lekkerkerker, Science 309, 1231 (2005).
[37] F. Rietz and R. Stannarius, Phys. Rev. Lett. 108, 118001 (2012).
[38] We have chosen to exclude particles closer than 10 σ to the free interface.
[39] K. Huang, G. Miao, P. Zhang, Y. Yun, and R. Wei, Phys. Rev. E 73 (2006).
[40] J. Schaefer, S. Dippel, and D. Wolf, J. Phys. I France 6, 5 (1996).
[41] J. Lee, J. Phys. A 27, L257 (1994).