Shear-induced solid-fluid transition in a wet granular medium

Michael Schulz and Beatrix M. Schulz
Abteilung Theoretische Physik, Universität Ulm, D-89069 Ulm, Germany

Stephan Herminghaus
Abteilung Angewandte Physik, Universität Ulm, D-89069 Ulm, Germany

(Received 4 April 2002; revised manuscript received 13 February 2003; published 7 May 2003)

We present a numerical study of a shear-induced solid-fluid transition in wet granular matter. The simulation is based on a simple model that considers both the cohesive forces induced by the adsorbed liquid amount and the repulsive forces due to the excluded volume interaction of the granules. Dissipation is assumed to be entirely due to the hysteretic character of the cohesive forces. In particular, we analyze the dynamics of the system close to the phase transition from solidlike behavior to a mobile ergodic state under the influence of an external force field F, when the latter exceeds a critical force F_c. Diffusion coefficients, dissipation, and kinetic order parameters can be expressed as characteristic scaling laws.

DOI: 10.1103/PhysRevE.67.052301 PACS number(s): 45.70.Mg, 05.65.+b

Granular matter, such as sand, soil, or gravel, has been studied closely by scientists and engineers for over a hundred years [1–5]. However, since these materials are inherently far from thermal equilibrium, attempts to treat granular matter with the methods of statistical physics are comparatively new [6–8]. Significant progress in the field has been possible only with the help of modern computers [9–19].

By far most of the work has been concerned with dry granular matter. These systems consist only of elastic beads, with some internal and surface friction in the general case. However, the much more complicated case of wet granular material is also the much more important one. Any finite humidity leads to a thin layer of water on virtually all surfaces. Dramatic effects such as soil liquefaction, with devastating landslides as a possible consequence, are believed to be due to the interplay of the liquid with the grain piling [20].

As a handy illustration, let us consider a sand castle [21]. It is clear that its stability is due to its moisture content, since from dry sand no stable shape can be created. Similarly, stability is lost as well if the sand is immersed in water. It is thus obviously the presence of liquid-vapor interfaces which provides the mechanical stability. In fact, gravitational shear induces no flow at all, since the sand castle will not yield at any perceivable rate to gravity. This state of the material may be called solid. If, however, it is subject to a critical shear force, it starts ''flowing,'' i.e., yielding to the applied force by changing its shape. This state will be called fluid (not to be confused with the liquid moistening the grains). If the moisture content is small but finite, there is a liquid bridge between any two grains touching each other, which exerts an attractive central force upon the grains.

Two possible mechanisms come to mind which may be responsible for the increased stability of the pile. On the one hand, a shear will entail the extension, and eventual rupture, of some of the bridges. This energy cost acts against the shear and thus stabilizes the pile. On the other hand, the central force exerted by a liquid bridge presses the adjacent grains together, thus increasing the critical tangential force necessary for overcoming the friction between them. It is of fundamental interest to know what characteristic properties of wet granular matter can be attributed to which mechanism. In the present study, we assume the grains to be completely frictionless, such that all of the dissipation is due to the rupture of liquid bridges.

A first analysis of the statics and dynamics of sandpiles shows [22–24] that the addition of small adhesive forces between the grains causes the site of failure in the bulk or, more precisely, at the bottom of the sandpile rather than at the surface. On the other hand, several experimental results show that the flow in cohesive powders or cohesive piles mainly appears on the top [25]. Furthermore, segregation of multidisperse particles is sharply reduced [26] and preferential clumping of small particles is observed when a small volume fraction of fluid is added.

We introduce a simple model of wet granular matter, which allows a quantitative analysis of the underlying particle dynamics. To this end we consider a dense system of $N \sim 10^4$ spherical beads with no mutual friction, in a cubic box with cyclic boundary conditions. The radii of the beads are chosen at random within a moderate range $\delta R/R \sim 0.1$, in order to avoid crystallization. The particles are assumed to be frictionless with the exception of dissipation effects related to liquid bridges. The characteristic feature of our system is a hysteretic force modeling the liquid bridges between the beads [27]. This force is set to zero as long as the center of mass distance, δx_{ab}, of two approaching particles of radii R_a and R_b is larger than $R_a + R_b$. As soon as $\delta x_{ab} = R_a + R_b$, a liquid bridge is formed, and the interaction force

$$F_{ab} = F_0[\Phi(\xi) - 1] \tag{1}$$

is switched on, with $\xi = \delta x_{ab}/(R_a + R_b)$. $\Phi(\xi)$ models the mutual hard core repulsion of the beads. Continuity at the contact point requires $\Phi(1) = 1$. Because the repulsion remains effective only on a small interval much smaller than the liquid layer thickness, the detailed functional structure of $\Phi(\xi)$ is widely irrelevant. The only condition is that close to the reduced contact distance $\xi = 1$, the repulsion force should

increase sufficiently strongly with decreasing particle distance ξ. For our simulations, we chose $\Phi(\xi)=\xi^{-13}-(\xi-1)\xi_0^{-13}/(\xi_0-1)$ for $\xi<\xi_0$ and $\Phi(\xi)=0$ for $\xi>\xi_0$ with $\xi_0=1.05$, which ensures a differentiable form avoiding numerical instabilitites. The constant attractive force is an idealized representation which neglects the curvature of the liquid layers, the roughness of the granules, and all effects related to the conservation of the liquid volume [22,27]. However, the main effect is well represented by this simple assumption. If the distance δx_{ab} exceeds for the first time after the collision the critical value $R_a+R_b+R_{\mathrm{crit}}$, the liquid bridge snaps, and the interaction is reset to $F_{ab}=0$. The hysteresis spanning the range between R_a+R_b and $R_a+R_b+R_{\mathrm{crit}}$ is the only source of dissipation in our model. In our simulations, we have set $R_{\mathrm{crit}}/R\sim 0.2$.

Shear is applied to the system by means of a space dependent external force field $\mathbf{F}(\mathbf{x})$, which acts upon each particle individually. A cosine profile, $\mathbf{F}(\mathbf{x})=\mathbf{e}_x F\cos(2\pi z/L)$, is chosen. The system is characterized by three relative length scales (width of the radius distribution $\delta R/R\sim 0.1$, the maximum length of a liquid bridge $R_{\mathrm{crit}}/R\sim 0.2$, and the characteristic length of the cosine profile $L/R\sim 40$, where R is the average radius of the granules) and one relative force scale F/F_0. In what follows, we set $F_0=1$.

On the basis of this model, we have performed standard molecular dynamics simulations with variable values of the applied shear F and found three regimes. At small values on F, we observe a solidlike behavior, where no substantial displacement of beads is observed. After a short relaxation time, an arbitrary initial configuration reaches a frozen microstate. Dissipation, i.e., the rupture of liquid bridges, takes place only at the initial stage, and the total number of bridges finally acquires a constant value. The final state is then characterized by small fluctuations of the particles around their stationary position, whereby energy is conserved. At large amplitudes F, the system exhibits fluidlike behavior. A constant rate of bridge formation and rupture is observed. The trajectory of each individual particle is reminiscent of Brownian motion at large time scales, and can be well described by a self-diffusion coefficient. Clearly, due to the symmetry breaking with respect to the external field, we have to distinguish between diffusion coefficients D_x, D_y, and D_z. The most interesting regime is the crossover from the solidlike regime to the fluid regime, which occurs in the vicinity of a critical force, $F_c\approx 0.42$. As F_c is approached from below, the system develops a propensity to form avalanches. This can be seen in the mean square displacement obtained from an average over all beads of one system, where diffusive behavior alternates with long intervals where the particles are largely at rest. It is illustrative to plot the total kinetic energy in the system as a function of time, as shown in Fig. 1. Long periods of ''background'' fluctuations characterizing a quasisolid state alternate with cascades of spontaneous bursts.

For a quantitative analysis of this cascading effect, we define an order parameter characterizing the strength of the observed cascades. Cascades correspond to significant jumps of the total kinetic energy over a relatively short time interval $\Delta t=t_{m+1}-t_m$. It should be noted that these jumps are not

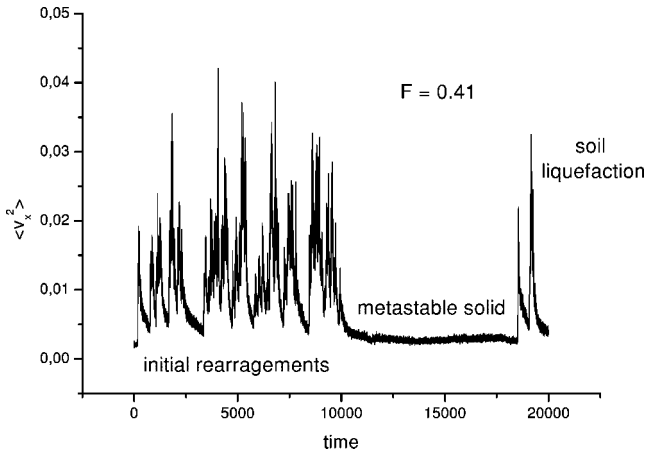

FIG. 1. Typical behavior of the total kinetic energy as a function of time at the critical threshold F_c. Regimes of temporary solidification alternate abruptly with regimes of global mobility.

real discontinuities. They become strong but regular changes of the kinetic energy for $\Delta t\to 0$ are observed because of the underlying Newtonian equations of motion. We stress the weight of the cascades by defining the kinetic order parameter

$$\chi^{(n)}=\left\langle \sum_{t_m=0}^{t_{\max}} |E(t_{m+1})-E(t_m)|^n \right\rangle, \tag{2}$$

where n is sufficiently large. As demonstrated in Fig. 2, the data are in agreement with a power law, $\chi^{(n)}\sim|F-F_c|^{-\gamma_n}$, over more that three decades in $F-F_c$. The critical exponent γ_n of the divergence depends, in principle, upon n. However, as shown in Figs. 3 and 4, it acquires a rather stable value of $\gamma_n/n=0.24$ in a wide range $n=4,\ldots,12$. Larger values of n favor some few cascades and degrade the statistics, while the influence of small energy fluctuations

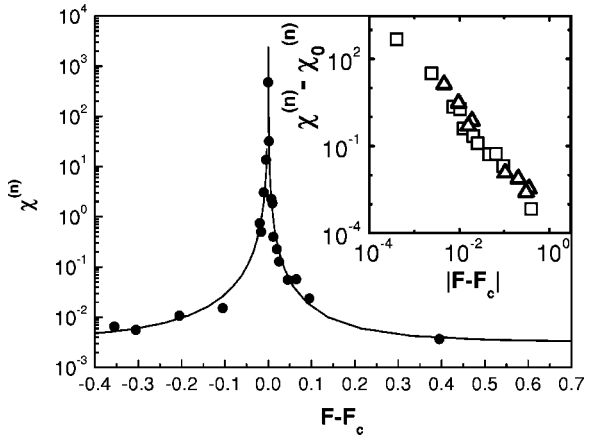

FIG. 2. Kinetic order parameter χ as a function of $F-F_c$ for $n=8$. The cascadelike motion dominates close to the critical threshold and pushes the order parameter. The full lines are fits corresponding to $\chi^{(8)}=\chi_0^{(8)}+C|F-F_c|^{\gamma_8}$ with $\gamma_n^+=1.94\pm 0.08$ for $F>F_c$ and $\gamma_n^-=1.93\pm 0.11$ for $F<F_c$. The inset shows the wide range of the algebraic behavior (triangles, $F<F_c$; squares, $F>F_c$).

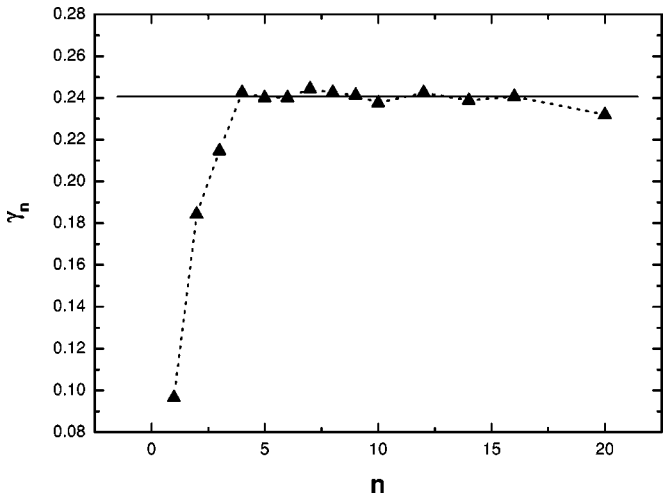

FIG. 3. The critical exponent of χ as a function of n. There is a clear plateau at 0.24.

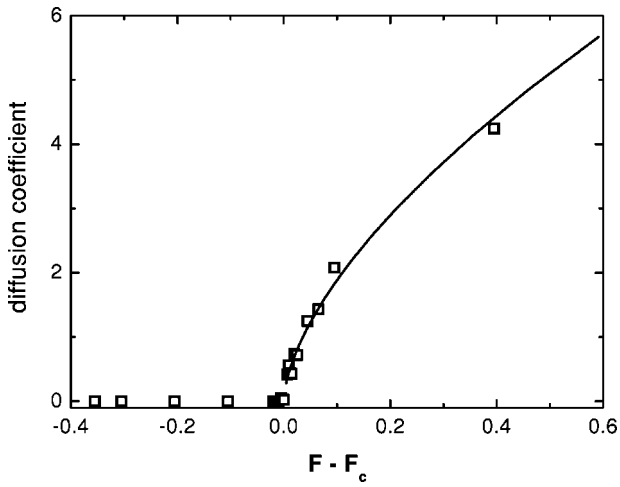

FIG. 4. Ensemble averaged diffusion coefficients in the direction of the force field orientation. The diffusion coefficients are determined from the long time behavior of the mean square displacement. A scaling law is obtained for the vicinity of the critical force, F_c.

increases rapidly for $n<4$. Cascades can be also observed above the threshold, but here they are confined to the initial stage of the simulation. The frequency of their occurrence then decreases rapidly, such that a more or less continuous flow of the granular medium is rapidly established. Conversely, below the critical threshold the frequency of cascades decreases due to the gradual solidification of the system.

Let us now turn to the ensemble averaged diffusion coefficients as a function of F. These are plotted in Figs. 3 and 4, and it is apparent that they can be expressed by a power law $D\sim|F-F_c|^{\beta}$, with $\beta=0.62\pm0.05$. Within our (limited) accuracy, there is no difference in the scaling behavior for the three directions of motion (x, y, and z), suggesting an isotropic state. This is another justification to call this state a fluid. Another critical behavior can be obtained for the time averaged number Γ of ruptured liquid bonds per unit time. We obtain the scaling behavior $\Gamma\sim|F-F_c|^{\bar{\beta}}$ with $\bar{\beta}=0.73\pm0.06$. These results indicate that the solid-fluid transition of our model system, and potentially of wet granular matter in general, can be interpreted as a dynamical critical phenomenon.

Finally, we should try to understand the value of the critical force. Assuming, for the sake of simplicity, that the piling of the beads has a hexagonal close packing structure, the maximum absolute shear force between neighboring granular layers is given by $2\pi Fh/L$, where $h=2R\sqrt{2/3}$ is the distance between the layers. The critical point is reached if the external forces and the attractive forces due to the liquid bridges are in balance. The geometrical constraints require $2\pi F_c h/L=2F_0\sqrt{3}$. Hence, if there are liquid bridges between all of the neighboring beads, the maximum critical force is $F_c=F_0L/(2\pi R\sqrt{2})$. Considering $L/R\sim40$ as in our system, we get $F_c/F_0\sim5$. However, only a small fraction of liquid bridges is on, which may be estimated as $R_{\mathrm{crit}}/\sqrt{3}R\sim0.1$. Consequently, we obtain $F_c/F_0\sim0.5$, which is quite close to what we found in the simulation. It is clear that the actual pile is weaker, since the piling is random instead of hexagonal, which entails a smaller coordination number.

Finally, it should be noted that the size distribution of the particles does not remain unaffected by the fluid motion. Figure 5 shows the lateral distribution of grain sizes, averaged in the (y,z) plane. While for large forces we observe an ideal mixture, a redistribution is observed as F_c is approached from above, which tends to accumulate small particles predominantly in regions of large force gradients. A similar phenomenon can be detected qualitatively also below F_c, but segregation is not complete there because of the increasing solidification of the system. Segregation in granular materials is rather common [26], but it should be noted that it spans only a small fraction (about 10%) of the width of the size distribution of the beads.

In conclusion, we state that a dynamic solid-fluid transition, which is very reminiscent of the typical mechanical behavior of wet sand or soil, can be observed in a very simple model that neglects internal friction, and has a hys-

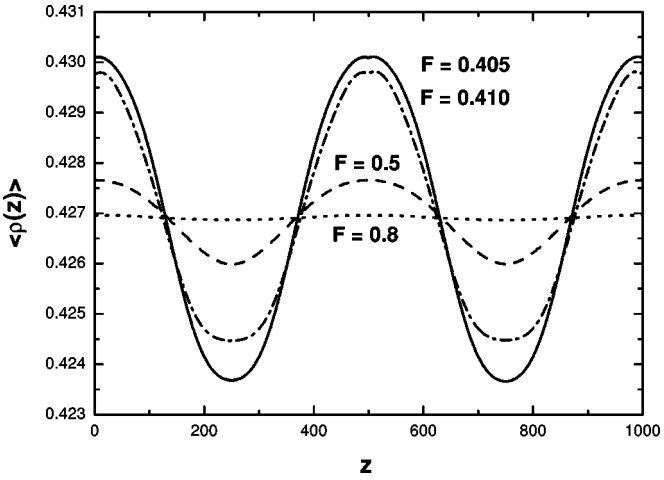

FIG. 5. Distribution of the mean particle radius in the stationary fluid state as function of a rescaled coordinate z for various force amplitudes F. The distribution is slightly smoothed by use of standard wavelet techniques.

teretic interaction force as the only source of dissipation. The transition can be characterized by rather well defined critical exponents in all relevant quantities investigated. It is clear that further investigation is required to characterize the universality class of this fascinating phenomenon. In particular, it is necessary to study whether the critical exponents are universal or depend upon the form of the force law, or other characteristic parameters, such as the rupture distance R_{crit}. This will be left to further work.

This work was supported by the Deutsche Forschungsgemeinschaft (Grant No. SFB 569 and Priority program 1052).

[1] R.A. Bagnold, Proc. R. Soc. London, Ser. A **225**, 49 (1954).
[2] H.M. Jaeger, S.R. Nagel, and R.P. Behringer, Rev. Mod. Phys. **68**, 1269 (1996).
[3] *Granular Matter: An Interdisciplinary Approach*, edited by A. Mehta (Springer, New York, 1993).
[4] *Physics of Dry Granular Media*, edited by H. J. Herrmann, J.-P. Hovi, and S. Luding (Kluwer, Dordrecht, 1998).
[5] J. Duran, *Sands, Powders, and Grains* (Springer, New York, 1999).
[6] S.F. Edwards and R.B.S. Oakescott, Physica A **157**, 1080 (1989).
[7] A. Mehta and S.F. Edwards, Physica A **157**, 1091 (1989).
[8] S.F. Edwards and D.V. Grinev, Physica A **302**, 162 (2001).
[9] H.J. Herrmann, K. Kroy, and G. Sauermann, Physica A **302**, 244 (2001).
[10] A. Coniglio and M. Nicodemi, Physica A **296**, 451 (2001).
[11] D.S. Dean and A. Lefevre, Phys. Rev. Lett. **86**, 5639 (2001).
[12] B. Painter and R.P. Behringer, Phys. Rev. E **62**, 2380 (2000).
[13] F. Melo, P. Umbanhowar, and H.L. Swinney, Phys. Rev. Lett. **72**, 172 (1994).
[14] G. Straßburger and I. Rehberg, Phys. Rev. E **62**, 2517 (2000).
[15] A. Barrat, J. Kurchan, V. Loreto, and M. Sellitto, Phys. Rev. Lett. **85**, 5034 (2000).
[16] H.M. Jaeger and S.R. Nagel, Science **255**, 1523 (1992).
[17] K. Velten and W. Best, Phys. Rev. E **62**, 3891 (2000).
[18] P.B. Umbanhowar, F. Melo, and H.L. Swinney, Nature (London) **382**, 793 (1996).
[19] C. Josserand, A. Tkachenko, D.M. Mueth, and H.M. Jaeger, Phys. Rev. Lett. **85**, 3632 (2000).
[20] *Proceedings of the 11th Asian Regional Conference, Seoul, Korea, 1999*, edited by S. W. Hong, M. M. Kim, G. S. Yang, S. R. Lee, S. S. Chung, C. C. Ihm, H. T. Kim, and J. B. Park (Balkema, Rotterdam, 1999).
[21] D.J. Hornbaker, R. Albert, I. Albert, A.-L. Barabasi, and P. Schiffer, Nature (London) **387**, 765 (1997).
[22] T.C. Halsey and A.J. Levine, Phys. Rev. Lett. **80**, 3141 (1998).
[23] L. Bocquet, E. Charlaix, S. Ciliberto, and J. Crassous, Nature (London) **396**, 735 (1998).
[24] N. Fraysse, H. Thome, and L. Petit, Eur. Phys. J. B **11**, 615 (1999).
[25] M.A.S. Quintanilla, A. Castellanos, and J.M. Valverde, Phys. Rev. E **64**, 031301 (2001).
[26] A. Samadani and A. Kudrolli, Phys. Rev. Lett. **85**, 5102 (2000).
[27] Willett, C.D. Willet, M.J. Adams, S.A. Johnson, and J.P.K. Seville, Langmuir **16**, 9396 (2000).