Journal of Statistical Physics, Vol. 68, Nos. 5/6, 1992

The Langevin Dynamics of Vibrated Powders

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Received February 21, 1992

We present a microscopic theory of the relaxational behaviour of a granular pile submitted to vibration, elucidating the different roles of collective and independent-particle relaxation. We write down and solve Langevin equations for these processes, which have an explicit coupling. The analysis of the solution in terms of independent-particle and collective relaxations provides a consistent framework for the interpretation of experimental results.

KEY WORDS: Langevin equations, powders, sandpiles, cooperative dynamics, relaxational phenomena.

Powders have been of interest to engineers[1] for a long time, but it is only recently that they have become an important and exciting area of theoretical[2–7] and experimental[8,9] physics. In addition to phenomena exhibited by other amorphous systems, their randomness of shape and texture strongly influences their static and dynamic properties. Powders are highly nonlinear and hysteretic, as a consequence of which they show complexity, so that the occurrence and relative stability of a large number of metastable configurations govern their behavior. They exhibit behavior that is neither completely solidlike nor completely liquidlike, but which is intermediate between the two. Like liquids, powders can take the shape of their containing vessel, but unlike them, they can also adopt a variety of shapes when they are free-standing. This leads to the everyday (but nonintuitive!) phenomenon of the angle of repose, which is the angle that a sandpile makes with the horizontal. In reality, the angle of response is not unique,

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0022-4715/92/0900-1131$06.50/0

but depends on the history of the sandpile[3]: this is related to, among other things, the phenomenon of dilatancy,[1] which is the ability of granular materials to sustain different degrees of packing. The compactivity X, which was defined in recent statistical mechanical treatments of powders,[2] measures the efficiency of packing, so that powders with a high X are strongly dilatant.

One of the most interesting aspects of powders is their relaxational behavior, because it manifests many of the features referred to above. In this paper, we unify earlier computer simulation approaches[5,10] within the framework of a microscopic theory of relaxation in a vibrated granular pile. This is based on a qualitative picture of competition and cooperation between independent-particle and collective relaxation put forward in earlier work[3]: in this short communication we quantify these ideas, and show that they give rise to quite distinctive behavior in the time dependence of the slope of the pile. Our results are in qualitative accord with recent experimental work.[9]

Consider a pile of grains on a vibrating table. The state of the pile may be described by the macroscopic angle of tilt θ and ϕ, the local deviation from θ, caused by surface roughness, which is based on the definition of the Bagnold dilatancy angle.[1] The Bagnold angle, as originally defined, was the average extent to which clusters of particles protruded from the surface, which was in turn a measure[1] of the dilatancy; we choose to work, instead, with $\Phi^2 \equiv \langle \phi^2 \rangle_{\text{pile}}$ and below will quantify Bagnold's idea by making an explicit connection between Φ^2 and the compactivity X [see Eq. (3b)]. As will be seen from Fig. 1, small Φ corresponds to a well-packed pile (with low X) with a smooth surface, whereas large Φ corresponds to a loosely packed pile (with high X) with a rough surface.

It is well established[1] that any experimental measurement of the macroscopic angle of tilt θ lies between two limits, the so-called maximum angle of stability θ_m and the minimum angle of repose θ_r; the difference between these two angles is Δ, the Bagnold angle, which, as has been pointed out by other authors,[9] is a measure of the hysteresis. We make this idea more quantitative by interpreting Δ as the maximum value of Φ. In other words, Φ is a variable whose value is bounded by Δ, so that small values of Φ will lead to measured angles θ nearer θ_r, while large values of Φ will lead to measured angles θ nearer θ_m. It is worth mentioning that the origin of Φ is dynamical, in that dynamics on the surface leads to disorder, which is the origin of hysteresis in the configurational properties of the pile.[3,6]

In the presence of an applied vibration of intensity H (scaled by the gravitational acceleration),[3] θ and Φ will be time-dependent. If H is greater than the binding energy of the particles to their clusters, they are

ejected (*independent-particle relaxation*) from their clusters and travel in avalanches down the pile. The rate of change of θ is predominantly governed by these avalanches: therefore we view θ as representing the motion of independent particles. Conversely, if H is small relative to the binding energies of the particles, they are not ejected: in this case the grains reorganize within a cluster (*collective relaxation*) to minimize voids. Since a finite value of Φ is a reflection of the presence of dilatant clusters on the

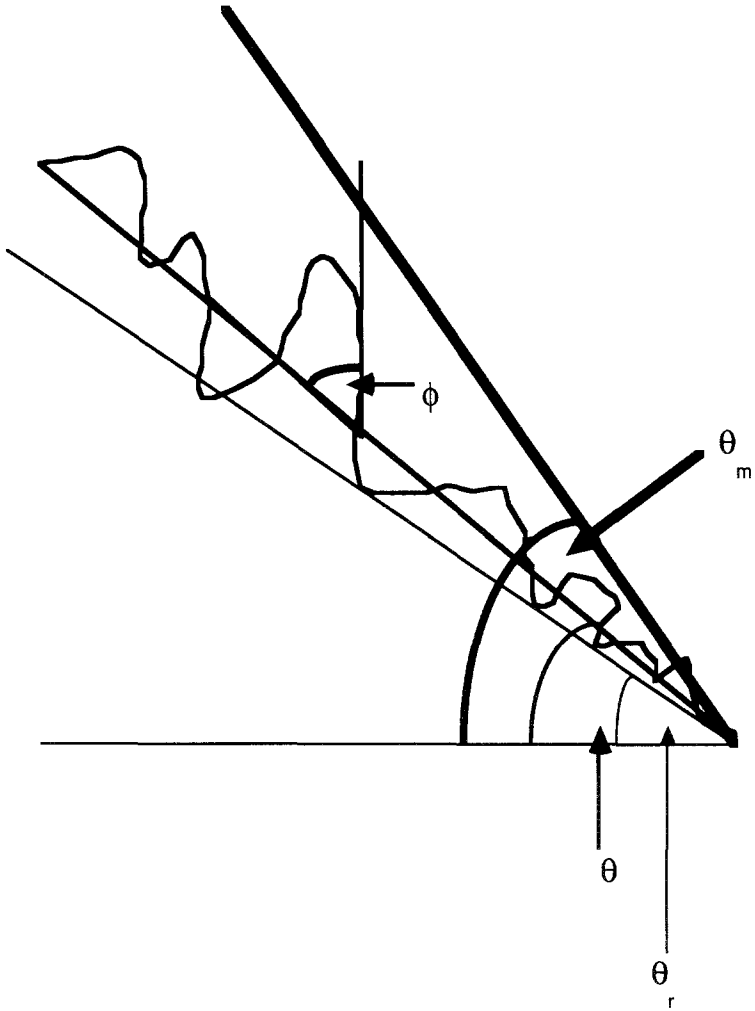


Fig. 1. The surface of a granular pile. The angles θ_r and θ_m are shown, corresponding respectively to the angles of repose and maximum stability; the measured angle θ varies between these two limits. The angle ϕ is the local deviation from θ.

surface, it is natural to associate the collective motion of these clusters with $d\Phi/dt$. We expect that for high intensities of vibration, the dominant process is independent-particle relaxation at the surface leading to avalanches down the slope, whereas collective relaxation dominates at low intensities. Because independent-particle relaxation occurs via cascades of particles, it will not lead[10] to the most efficient packing or to the smoothest surface. In contrast, we expect that when collective relaxation dominates, the macroscopic slope will relax slowly or not at all, and the slow collective reorganization of particles will lead to efficient void-filling, i.e., to a low compactivity and a smooth surface.

Although we have interpreted $d\theta/dt$ and $d\Phi/dt$ as though the corresponding relaxation processes were independent, we expect them to be coupled. Physically this coupling arises because a large roughness (large Φ^2) will increase the value of θ as explained above, and a steeper slope (large θ) will sustain less roughness (small Φ^2). In keeping with the above discussion, we write down coupled Langevin equations for θ and Φ:

$$d\theta/dt = -\gamma\theta - c\Phi^2 + \zeta(t) \tag{1}$$

$$d\Phi/dt = -\Gamma\Phi - c'\theta\Phi + \xi(t) \tag{2}$$

where γ and Γ are the rates controlling the θ and Φ relaxation processes, and c and c' are, respectively, the coupling constants relating the independent-particle and collective processes. The second term on the rhs of Eq. (1) represents the contribution to $d\theta/dt$ (to lowest order) of the roughness: this can be viewed as representative of the average mismatch between the dilatancies of neighboring clusters. The sign of this coupling is argued to be negative, as large mismatches (associated with large roughness) will enhance the value of θ, as discussed above, leading to an increase in the rate of decay of the slope. Correspondingly, the second term on the rhs of Eq. (2) is bilinear in θ and Φ, and has a negative sign because large values of θ contribute to a decay of Φ, because steeper slopes can sustain less roughness. It is evident from Eqs. (1) and (2) that the coupling term in the equivalent Landau–Ginzburg formulation of this problem is proportional to $\theta\Phi^2$. The respective noise terms ζ and ξ have the usual spectral properties:

$$\langle \zeta(t)\,\zeta(t') \rangle = 2\langle \theta^2 \rangle_{\text{eq}}\,\gamma\,\delta(t-t'), \qquad \langle \theta^2 \rangle_{\text{eq}} \propto H \tag{3a}$$

$$\langle \xi(t)\,\xi(t') \rangle = 2\langle \Phi^2 \rangle_{\text{eq}}\,\Gamma\,\delta(t-t'), \qquad \langle \Phi^2 \rangle_{\text{eq}} \propto X \tag{3b}$$

where the subscript eq refers to the long-time limit in the presence of vibration. Equations (3a) and (3b) are the fluctuation-dissipation relations for a driven granular system, with effective temperatures proportional to H and

X, respectively (throughout we take the constants of proportionality to be unity). Equation (3a) ties in with earlier work[3,5,10] as well as with the concept of granular temperature[4]; in Eq. (3b) we have made the reasonable assumption that the effective temperature associated with the relaxation of clusters is related to the density of packing, so that, for instance, clusters are able to rearrange more freely in loosely packed piles.

Let us now discuss the physical significance of the rate of independent-particle relaxation γ: we expect this to be governed by an activated process over a random distribution of barrier heights U related[3] to the configurational properties of a cluster. A suitable approximation is

$$\gamma(U) = \gamma_0 \exp(-U/H) \tag{4}$$

Note that the effective temperature controlling these kinetics comes out naturally from Eq. (3a). The rate of collective relaxation Γ is expected to be a similar function of the compactivity X; however, the energy barriers are much larger for cluster rearrangement, which leads to far larger magnitudes of the exponent in the analogue of Eq. (4) for Γ. Therefore only the smallest energy barriers contribute, so that we consider Γ to be a parameter, not a distribution over energies.

In the absence of the coupling and the noise ζ, the solution of Eq. (1) is

$$\langle \theta(t) \rangle_U = \theta(0) \int_0^\infty \exp[-\gamma(U)t]\, \rho(U)\, dU \tag{5}$$

where the subscript U denotes an average over the distribution $\rho(U)$. If we make the assumption, for simplicity, that $\rho(U)$ is a constant $1/U_0$ up to a cutoff U_0, we obtain upon integration

$$d\langle \theta(t) \rangle_U / dt = H\theta(0)\{\exp(-\gamma_0 t) - \exp[(-\gamma_0 t(\exp(-U_0/H)]\}/U_0 t \tag{6}$$

In the experiments described in ref. 9, a logarithmic decay of the slope θ was reported when the intensity of vibration was large; if we consider time scales such that $\gamma_0^{-1} \ll t \sim \gamma_0^{-1} \exp(U_0/H)$, the second term in the brackets of Eq. (6) vanishes, while the first term is of order one.[11] Then, $d\langle \theta(t) \rangle_U / dt \propto 1/t$, leading to a logarithmic decay of $\langle \theta(t) \rangle_U$ with time. This situation is illustrated in Fig. 2a, and will be discussed later.

We now move on to the full solution of Eqs. (1) and (2) in the presence of coupling. The relaxation time of a cluster is much larger than that of a particle (i.e., $1/\Gamma \sim N/\gamma$, where N is the number of grains in a cluster), so that the collective motion of the cluster, represented by Φ, forms a slowly evolving dynamical "cage" for the motions of the individual grains. Consequently we use a mode-decoupling scheme for the "slow" variable Φ, analogous to that used in another context.[12]

We first solve Eq. (2) for $\Phi^2(t)$, and substitute into Eq. (1), to obtain

$$d\theta/dt = -\gamma(U)\theta + \zeta(t) - c\Phi^2(0)\exp(-2\Gamma t) + 2c\int_0^t dt' \exp[-2\Gamma(t-t')]\,[c'\theta(t')\,\Phi^2(t') - \Phi(t')\,\xi(t')] \quad (7)$$

Next we average over the noise term $\xi(t)$, and use a simple scheme to decouple the θ and Φ processes; this involves, first, evaluating the noise-averaged and decoupled $\Phi^2(t)$ from Eqs. (2) and (3b) as

$$\langle \Phi^2(t) \rangle_{\mathrm{dec},\xi} = \Phi^2(0)\exp(-2\Gamma t) + X[1-\exp(-2\Gamma t)] \quad (8)$$

and then replacing $\Phi^2(t)$ in the integrand of Eq. (7) by its decoupled average $\langle \Phi^2(t) \rangle_{\mathrm{dec},\xi}$. Finally, we average over the noise $\zeta(t)$, and get

$$d\theta_{\mathrm{av}}/dt = -\gamma(U)\theta_{\mathrm{av}} - c\Phi^2(0)\exp(-2\Gamma t) + 2cc'X\int_0^t dt' \exp[-2\Gamma(t-t')]\,\theta_{\mathrm{av}}(t') + 2cc'\exp(-2\Gamma t)\,[\Phi^2(0)-X]\int_0^t dt'\,\theta_{\mathrm{av}}(t') \quad (9)$$

where the subscript av denotes the average over both $\xi(t)$ and $\zeta(t)$. Despite its complexity, Eq. (9) may in fact be solved exactly. This is done by differentiating with respect to time, and eliminating the integrals in Eq. (9) by substitution; after some algebra, this reduces to the modified Bessel equation.[13] The final solution is

$$\theta_{\mathrm{av}}(t) = \exp[-\alpha(U)t]\,\{A(U)\,I_\nu[\beta\exp(-\Gamma t)] + B(U)\,K_\nu[\beta\exp(-\Gamma t)]\} \quad (10)$$

where $I_\nu(x)$ and $K_\nu(x)$ are the modified Bessel functions, and

$$\alpha(U) = \Gamma + \gamma(U)/2$$

$$\beta^2\Gamma^2 = 2cc'[\Phi^2(0) - X]$$

$$\Gamma\nu(U) = +\{[\Gamma - \gamma(U)/2]^2 + 2cc'X\}^{1/2}$$

The coefficients $A(U)$ and $B(U)$ can be obtained by using the initial values of θ_{av} and $d\theta_{\mathrm{av}}/dt$, so that

$$B(U) = \frac{-c\Phi^2(0) + \theta_{\mathrm{av}}(0)\{\alpha(U) - \gamma(U) + \beta\Gamma[I_{\nu+1}(\beta)/I_\nu(\beta)] + \nu\Gamma\}}{\beta\Gamma\{[K_\nu(\beta)\,I_{\nu+1}(\beta)/I_\nu(\beta)] + K_{\nu+1}(\beta)\}}$$

$$A(U) = \frac{\theta_{\mathrm{av}}(0) - B(U)\,K_\nu(\beta)}{I_\nu(\beta)}$$

These equations represent the full analytical solution to the decoupled problem. However, since Eqs. (10) are all functions of U, we now need to integrate over U, as was done in Eq. (5). This was done numerically, and some representative plots are shown in Fig. 2, which show the form of $\theta_{av}(t)$ for large and small values of H, the intensity of vibration. However, for ease of discussion, and in view of the complexity of the form of the above solution, we look at its form for large times:

$$\langle \theta_{av}(t) \rangle_U \cong \int_0^{U_0} dU\, \rho(U) \{ [(\beta/2)^\nu A(U) \exp[-z_+(U)t]]/\Upsilon(\nu+1) + \tfrac{1}{2}(\beta/2)^{-\nu}\, \Upsilon(\nu)\, B(U) \exp[-z_-(U)t] \} \tag{11}$$

$$z_\pm(U) = \alpha(U) \pm \Gamma\nu(U)$$

where $\Upsilon(\nu)$ is the incomplete gamma function.[13] We now analyze the above results; note that $\gamma(U)$ is bounded by $\gamma_{max} = \gamma_0$ and $\gamma_{min} = \gamma_0 \exp(-U_0/H)$. When the intensity of vibration is large, i.e., γ_{min} is much larger than the other rate parameters such as Γ or $(2cc'X)^{1/2}$, then $z_+(U) \to \gamma(U)$ and $z_-(U) \to 0$. Also, it is readily seen that the coefficient of $\exp[-z_-(U)t]$ goes to zero in this regime. The form of Eq. (5) is then recovered and its solution, described in Eq. (6), is illustrated in Fig. 2b. Although the decay in this figure is not logarithmic over the whole range, its form for times t such that $\gamma_0^{-1} \ll t \sim \gamma_0^{-1} \exp(U_0/H)$ *is* logarithmic. When, on the other hand, H is lowered, γ_{min} decreases: the term involving $A(U)$ in Eq. (11) continues to dominate over the one involving $B(U)$ until a time t sufficiently large that the former becomes vanishingly small, leading to a slower rate of decay. Thus, although the decay of $\langle \theta_{av} \rangle_U$ starts off being logarithmic even for small intensities of vibration, there is a crossover in its behavior leading to a decrease in the slope of the graph (Fig. 2c); this persists for a considerable time before the eventual decay to zero.

Let us now interpret these findings in the context of the experimental results. In the experiments,[9] the regime of large-intensity vibrations was characterized by an apparently logarithmic decay. In our theory, the solution for large H in a given region of time is logarithmic (Fig. 2a), but the functional form for arbitrary times is more complex. In the large-H regime (Fig. 2b), the decay is predominantly independent-particle-like, and the "log" decay over a relatively large range of times is a signal of this. The regime of small intensities of vibration is more interesting: we interpret the initial decay as being due to independent particles ("log" decay), albeit with a slower rate. Soon, the collective motion of the clusters takes over, so that there are essentially no avalanches due to independent-particle

motion; this occurs in the flat portion of the curve of Fig. 2c, where there is almost no decrease of slope. These slow motions of the clusters, when continued over a long time, generate overburdens at the surface that are metastable (because H is small, there is insufficient energy for particles to be ejected): however, when the cumulative effect of these overburdens becomes mechanically unstable, the pile collapses. In this limit, we see a complicated mix of collective and independent-particle motion. In the experiments,[9] flattening of the θ vs. $\log t$ curve at long times for small-intensity vibrations was also seen, but it proved impossible to go far enough out in time to observe the final behavior in the slow regime. It seems that our theory provides an excellent framework within which to interpret those experimental results, and suggests what one might see at longer times than those so far observed experimentally.

We now return to the subject of hysteresis: as mentioned in the introduction, this is a particular characteristic of granular materials. Our theory shows the effect of hysteresis in the pile, via the "memory kernel" of

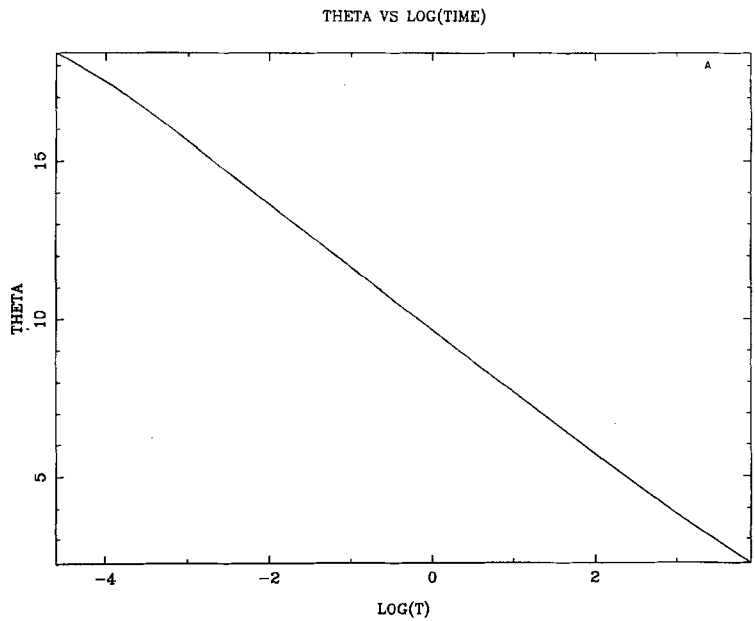
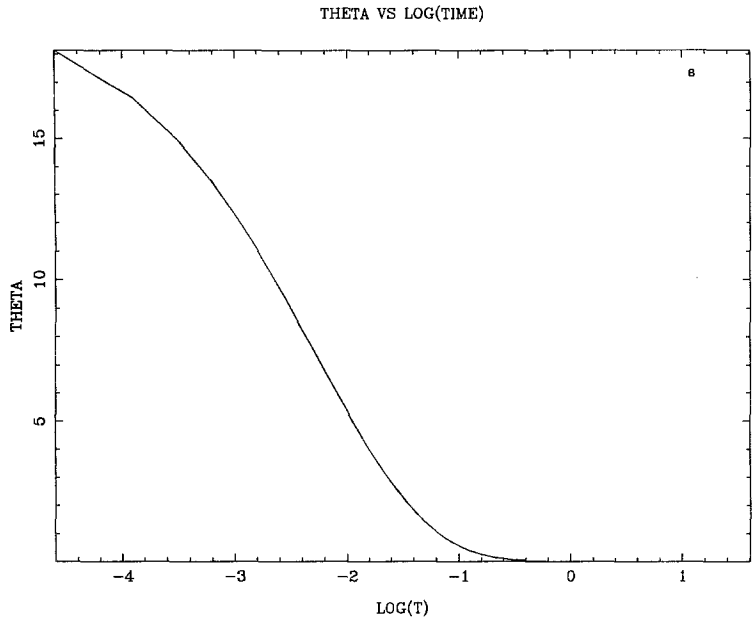


Fig. 2. θ_{av} versus $\log t$, with $\theta_{av}(0) = 20$ in each case: (a) in the absence of coupling, with $H = 10$. (b) for large H ($H = 10$) in the presence of coupling. The decay is rapid, and is logarithmic for the time scales specified in the text. (c) in the presence of coupling, for small H ($H = 0.1$). The initial decay is logarithmic until a crossover occurs, indicated by the flattening. Eventually, as predicted by Eq. (9), θ_{av} drops to zero.



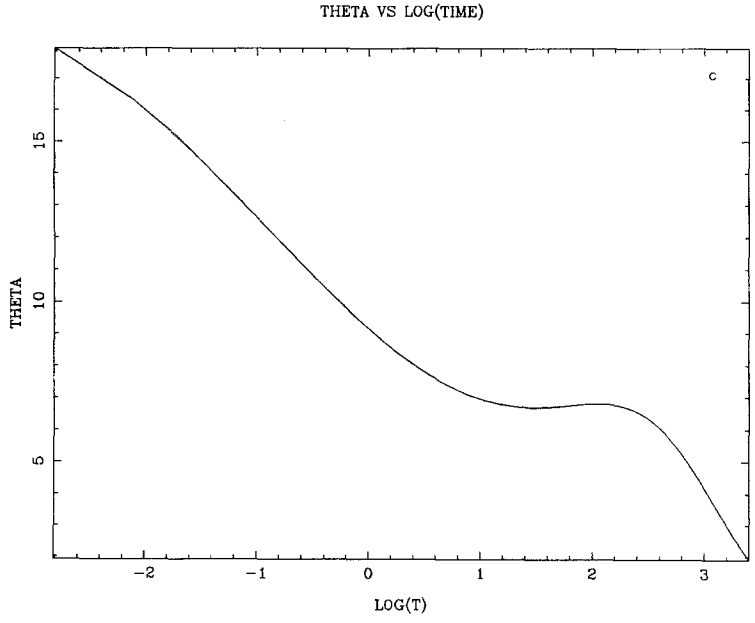


Fig. 2. (*Continued*)

Eq. (9); since Γ is small, the effects of the initial roughness $\Phi^2(0)$ and slope $\theta_{av}(0)$ persist for a long time. In addition to the coefficients $A(U)$ and $B(U)$, the *arguments* of the modified Bessel functions in Eq. (10) contain these quantities, thus showing their importance for the relaxation processes; it may readily be shown from Eqs. (10) and (11) that these effects are particularly significant for small intensities of vibration, when the coupling of the two processes is comparable to the intensity H of the driving force. This is in accord with physical intuition; for small intensities of vibration, the predominantly collective relaxation process leads to slow configurational changes, so that the memory of initial conditions persists for far longer times than is the case when H is large.

In conclusion, we have devised a novel theory of the relaxation of a pile of granular material subjected to vibration. We have defined coordinates for independent-particle and collective processes within the pile, and written down coupled Langevin equations for them. The preexisting concepts of granular temperature[4] H and compactivity[2] X have been unified within the framework of a consistent theory, which links each one to a dynamical variable via fluctuation-dissipation relationships. Our theory provides a quantitative illustration of two of the special features of powders, viz. dilatancy and hysteresis. The solution of the Langevin equations, obtained using a simple decoupling scheme, shows rich and complex behavior, which arises from the competition and cooperation between independent-particle and collective relaxations. This solution, and our analysis of it, unifies earlier work[3,5,10] and provides a reasonable basis for the interpretation of experiments.[9]

ACKNOWLEDGMENTS

We thank Mike Cates for useful comments on the manuscript; A.M. thanks Dietrich Stauffer very warmly for his encouragement and many useful remarks. A.M. and R.J.N. thank the Science and Engineering Research Council, U.K., for support.

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Communicated by D. Stauffer