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Theory of Stress Distribution in Granular Materials: the Memory Formalism

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A theoretical approach to the description of stress distribution in granular compacts is presented on the basis of a memory function formalism. Experiments which have motivated the approach are mentioned. The formalism is shown to provide an explanation of observed features of stress distribution in compacts, and to lead to existing theories in extreme limits, thereby providing a unification of the theories. The memory functions are shown to be intimately related to characteristic spatial correlations in the granular system and are discussed on the basis of stochastic considerations.

I. INTRODUCTION: EXPERIMENTAL MOTIVATION AND THE MEMORY APPROACH

Major areas of current research in granular materials include avalanches, patterns in flow, segregation, sound propagation, and spatial distribution of stress [1-6]. This article deals with the last of these. The study of stress distribution in static piles of granular material is characterized by undisputable importance from the applications point of view, enormous difficulty in the clear construction of theories as well as in experimental measurement of relevant observables, and, currently, by an unfortunate absence of communication between various groups working in the field. The importance of the field stems, e.g., from the requirement of understanding and control of stress distribution in pre-sintering compacts in almost any manufacturing situation. The difficulty in theory arises from the complexity of the system, involving as it does, friction, as well differing shapes and sizes of the granular particles: for instance, almost nothing is known definitively about the so-called constitutive relations among the stresses. The difficulty in experiment lies in the design of direct probes of stress in the *bulk* of the granular material: it is relatively easy to measure stress at the surfaces of a compact but values of stress in the interior must be often deduced from density distributions or other indirect observations¹.

The focus of the present article is a method we have developed recently [8-10] for the theoretical description of stress distribution on the basis of what is called a memory formalism. The original motivation for the investigation was provided by reported observations of curious features such as spatial oscillations in stress down the center line in compacts. These features are apparent in recent experimental results [11] as well as in data that have been available in the literature for many years [12-15]. Experimental information about the distribution of stress in a powder compact has been difficult to obtain unambiguously. Observations have employed, in some cases, direct measurement of the stress with the use of sensors or strain gauges [14,20] within, or at the edge of, a compact to measure the forces that evolve during pressing. Other cases have involved indirect deduction of the stress distribution from the density distribution within the compact. The first approach suffers from a lack of accuracy and the second from the need for specific assumptions of a local stress-density relation at every point in the compact [16-19]. Nevertheless, it is quite clear that characteristic unexplained features such as the non-monotonic variation of the stress with depth along the centerline of the compact emerge regularly (but not universally), and that a theoretical description of these features is not trivial. Indeed, Aydin et al. [11] have referred to the *failure* of existing theories to account for the oscillatory behavior. The reader is referred to ref. [9] for a detailed description of the experimental background.

The method of approach we have developed [8-10] is based on two ingredients: (i) the $t-z$ transformation which singles out one spatial direction in the granular material and treats it for the purpose of description as if it were time, and (ii) a spatially non-local formalism which employs integrodifferential equations of the Volterra type incorporating memory functions which characterize spatial correlations in the granular material. The $t-z$ transformation has appeared in investigations earlier than ours, notably in the work of Bouchaud, Cates and collaborators [7]. The transformation simplifies the mathematical treatment considerably, provides physical intuition based on knowledge of initial value problems in other fields, but, as a result of accompanying approximation procedures, forces certain limitations on the applicability of the entire formalism. The memory formalism [8-10] has a great deal of analytic power, particularly for the unification of disparate approaches and for the description of intermediate cases, and was suggested by work in the rather distant area of exciton transport in molecular aggregates [21]. It can be viewed as

¹The third current characteristic, the absence of communication between different sets of workers, is difficult to account for, but could be arising from the fact that the background of the investigators is rather varied, ranging from engineering through physics to applied mathematics.

arising from a mathematical generalization of constitutive relations such as those employed in ref. ([7]) but, as will be remarked below, is best looked upon as arising from the stochastic properties (spatial correlations) of the granular system.

The first step in our description is, thus, the choice of the z direction as the direction of gravity and/or of the applied stress, along with an attempt to write a closed evolution equation for the scalar field σ_{zz} which represents the zz -component of the stress tensor. The second step, and indeed the characteristic ingredient of our approach, is the use of an 'evolution equation' which is non-local in z :

$$\frac{\partial \sigma(x, y, z)}{\partial z} = D \int_0^z dz' \phi(z - z') \left[\frac{\partial^2 \sigma(x, y, z')}{\partial x^2} + \frac{\partial^2 \sigma(x, y, z')}{\partial y^2} \right] \quad (1)$$

The bridge function ϕ which connects the derivatives of the stress at various depths z is the *memory function*, and is a measure of important spatial correlations of the granular material which arise from the granularity (variations in shape and size of the grains) and other properties such as friction. Those properties also determine the value of D . For the sake of simplicity we will refrain from discussing in this paper starting points more general than (1) in which the depth coordinate and the other spatial coordinates are intermingled in the memory description.

The three succeeding sections of this article deal, respectively, with how an equation such as (1) helps in the unification of diverse existing approaches to stress distribution, how they lead to the understanding of observed features such as spatial oscillations of the stress in compacts, and how the memory functions are related to properties of the compact.

II. HOW MEMORIES HELP I: UNIFICATION OF EXISTING APPROACHES

Three particular cases of (1) deserve mention. In the first, we take the memory function to be independent of z : $\phi(z) = c^2/D$. Equation (1) reduces, then, to the wave equation

$$\frac{\partial^2 \sigma_{zz}(x, y, z)}{\partial z^2} = c^2 \nabla^2 \sigma_{zz}(x, y, z) = c^2 \left[\frac{\partial^2 \sigma_{zz}(x, y, z)}{\partial x^2} + \frac{\partial^2 \sigma_{zz}(x, y, z)}{\partial y^2} \right], \quad (2)$$

and thus to the starting point of the analysis of Bouchaud et al. [7]. The parameter c denotes what may be termed the wave speed, which is directly related to the slope of the so-called light cones. This perfect memory situation represents the fact that the stress applied on one particle is transmitted along the lines of contact between particles and there is no loss of information about the original strength and direction of the applied force.

In the second case, we take the memory function to be decaying so rapidly with depth that it may be replaced by a δ -function: $\phi(z) = \delta(z)$. Equation (1) yields the diffusion equation

$$\frac{\partial \sigma_{zz}(x, y, z)}{\partial z} = D \nabla^2 \sigma_{zz}(x, y, z) = D \left[\frac{\partial^2 \sigma_{zz}(x, y, z)}{\partial x^2} + \frac{\partial^2 \sigma_{zz}(x, y, z)}{\partial y^2} \right]. \quad (3)$$

It is possible to show in detail, as we have done elsewhere [8] that the above equation is identical to a simplified version² of the starting point of the analysis of Liu et al. [23].

The diffusive limit of the evolution has been used in the past for developing mean field treatments [23] and addressing the magnitude distribution of the stresses rather than their spatial variation. The wave limit has been discussed primarily via ray tracing arguments [7] in what may be termed the geometrical limit of the wave equation. Our own approach has been quite different. We have obtained actual solutions of these equations for the propagators (Greens functions) through explicit initial value and boundary value treatments and, with their help, attempted to address the *spatial* distribution of stress in granular systems. Our especial emphasis has been to present an intermediate starting point which combines the physics inherent in the extreme limits of wave-like and diffusive behavior and is capable of describing the *entire* range in between. Therefore, we focus attention on memory functions which are neither constant nor have infinitely fast decay. A simple intermediate situation is the exponential $\phi(z) = \alpha \exp(-\alpha z)$. In the respective limits of small and large α (the latter limit being actually $\alpha \rightarrow \infty$, $c \rightarrow \infty$, $c^2/\alpha = \text{const.}$), the wave and the diffusive case emerge trivially. The intermediate case gives the telegraphers equation

²The simplification consists in assuming a lack of dependence of D on z as well as on x, y .

$$\frac{\partial^2 \sigma_{zz}(x, y, z)}{\partial z^2} + \alpha \frac{\partial \sigma_{zz}(x, y, z)}{\partial z} = c^2 \nabla^2 \sigma_{zz}(x, y, z) \quad (4)$$

with $D = c^2/\alpha$.

Whereas the wave limit of Bouchaud et al. [7] corresponds to identical, frictionless spherical particles arrayed in a perfectly ordered lattice, the intermediate situation above describes a more realistic granular system in which random-shaped particles of random sizes are packed in a random arrangement. For the sake of simplicity, we will consider here only a two-dimensional system and thus use, instead of (4), the equation

$$\frac{\partial^2 \sigma_{zz}(x, z)}{\partial z^2} + \alpha \frac{\partial \sigma_{zz}(x, z)}{\partial z} = c^2 \frac{\partial^2 \sigma_{zz}(x, z)}{\partial x^2}. \quad (5)$$

The easy unification of the extreme limits provided by our memory approach may be appreciated either directly as explained above or through explicit solutions such as those of (5). Take the applied stress $\sigma_{zz}(x, 0)$ at the 'surface' $z = 0$ to be a delta function $\delta(x)$. The solution of (5) is then given by

$$\sigma_{zz}(x, z) = e^{-\alpha z/2} \left[\frac{\delta(x + cz) + \delta(x - cz)}{2} + T \right], \quad (6)$$

where the term T vanishes identically for $cz \leq x$, and equals, for $cz \geq x$,

$$T = \left(\frac{\alpha}{4c} \right) \left\{ I_0 \left(\frac{\alpha}{2c} \sqrt{c^2 z^2 - x^2} \right) + \frac{cz}{\sqrt{c^2 z^2 - x^2}} I_1 \left(\frac{\alpha}{2c} \sqrt{c^2 z^2 - x^2} \right) \right\} \quad (7)$$

the I 's being modified Bessel functions. In the limit $\alpha = 0$,

$$\sigma_{zz}(x, z) = (1/2) [\delta(x + cz) + \delta(x - cz)] \quad (8)$$

as in ref. [7] and we immediately recover the phenomenon of 'light cones'. Our solution shows that, in addition, there is a nonvanishing stress distribution *within* the light cones. This stress is given by our term T . In the limit which reduces our theory to the opposite extreme of Liu et al. [23], the light cones spread out to coincide with the surface $z = 0$, and the entire region experiences stress:

$$\sigma_{zz}(x, z) = \frac{e^{-x^2/4Dz}}{(4\pi Dz)^{1/2}}. \quad (9)$$

It is also possible to analyze with the help of these solutions the well-known 'burial problem', i.e., the question of where one should bury oneself under a sandpile to minimize the stress. One way of addressing the problem is to consider, via the $t - z$ transformation, stresses arising from gravity forces to be applied to circular regions of radii increasing continuously from zero to a maximum at different times (depths), and to sum all the contributions, taking boundary contributions to be relatively negligible. The key quantity to analyze is, thus,

$$Q(x, z) = \int_0^z dz_1 \int_{-vz_1}^{vz_1} dx_1 \psi(x, x_1, z, z_1) \quad (10)$$

where ψ is the propagator (Greens function) and v describes the slope of the sandpile. The propagator is easily obtained from the memory functions, an explicit example being (6). The vanishing of $\frac{\partial Q(x, z)}{\partial x}$ at a given value of the depth z locates the extremum and the sign of the second derivative identifies the extremum as minimum or maximum. Unlike simple ray tracing arguments, which cannot address the fact that stress extrema appear under the apex in some sandpiles but not in others, the present memory analysis has the potential to show how factors such as the extent of coherence (the value of c/α in our telegraphers equation above) influence the extremum.

III. HOW MEMORIES HELP II: EIGENVALUE PROBLEM FOR COMPACTION IN DIES

We now return to the primary problem which motivated the memory approach: spatial oscillations of stress in compacts. The memory approach addresses this issue by developing an eigenvalue analysis of (1) in the compact. Details of the theory may be found in [8] and applications to experiment in [9]. Under the assumption that the extent in the z -direction is large, (5) can be solved through the application of the method of separation of variables:

$$\sigma_{zz}(x, z) = \sum_k (A_k \cos kx + B_k \sin kx) g_k(z) \quad (11)$$

$$g_k(z) = e^{-\frac{\alpha}{2}z} \left[\cosh \Omega_k z + \frac{\alpha}{2\Omega_k} \sinh \Omega_k z \right], \quad \Omega_k = \sqrt{\alpha^2/4 - c^2 k^2}. \quad (12)$$

First, let us take the stress to be vanishing on the boundaries of the die which we assume to extend from $x = -L/2$ to $x = L/2$. This is an artificial boundary condition which we consider only for illustrative purposes [8]. If a constant punch pressure p_0 is applied across the top surface of the compact, the center line stress can be evaluated exactly in the Laplace domain as

$$\tilde{\sigma}_{zz}(0, \varepsilon)/p_0 = \frac{1}{\varepsilon} \left[1 - \operatorname{sech} \left(\frac{L}{2c} \sqrt{\varepsilon^2 + \varepsilon\alpha} \right) \right] \quad (13)$$

where tildes denote the Laplace transform, and ε is the Laplace variable. In the wave limit $\alpha = 0$, the inversion is easy and gives the center line stress as a square wave $W(z)$ along the z coordinate. It is constant at the applied value p_0 for $0 < z < L/2c$, flips to $-p_0$ for $L/2c < z < 3L/2c$, flips back to p_0 for $3L/2c < z < 5L/2c$, and continues alternating in this fashion. In the diffusive limit, the center line stress distribution is given by

$$\sigma_{zz}(0, z)/p_0 = 2 \int_0^{1/2} d\nu \theta_1 \left(\nu \left| \frac{4Dz}{L^2} \right. \right), \quad (14)$$

where θ_1 is the elliptic theta-function of the first kind. The general expression for the intermediate region is

$$\sigma_{zz}(0, z)/p_0 = 1 + \int_0^z du e^{-(\alpha/2)u} \left[M(u) + (\alpha/2) \int_0^u ds I_1(s) M(\sqrt{u^2 - s^2}) \right] \quad (15)$$

where I_1 is the modified Bessel function and $M(z)$, the derivative $\frac{dW(z)}{dz}$ of the square wave $W(z)$ described above, can be expressed as an infinite sum of δ functions centered at multiples of $L/2c$.

This illustrative analysis shows oscillations in the center line stress but contains unphysical elements which arise from the vanishing boundary conditions at the die walls because of the wave element in the evolution. Realistic considerations involve a decrease of the stress at the pipe walls with increasing depth, and have been treated in [9]. In that treatment, $\sigma_{zz}(\pm L/2, z)$ is not taken to vanish, but rather to be a given function $h(z)$ of the depth:

$$\sigma_{zz}(x, z) \Big|_{x=\pm L/2} = p_0 h(z), \quad (16)$$

where p_0 is the average value of the applied stress at the top surface. The function $h(z)$ is taken directly from experiment. The solution of (5) with such initial and boundary conditions presents an unusual boundary value problem which is analogous to propagation problems in which the boundary condition is dependent on time [24]. We have provided a complete solution in ref. [9] which may be summarized as follows.

In a manner analogous to that used in the treatment of Thompson [17], the applied stress at $z = 0$ is taken to have a parabolic dependence,

$$\sigma(x, 0) = p_0 \left(c_0 + (1 - c_0) \frac{12x^2}{L^2} \right), \quad (17)$$

with $c_0 = \sigma(0, 0)/p_0$ to ensure that the integrated applied pressure is equal to p_0 . A typical set of observations taken from Duwez and Zwell [20] is found to be compatible with

$$h(z) = \beta + [(3 - 2c_0) - \beta] e^{-\gamma z}. \quad (18)$$

With the definition

$$a_m = \frac{4(-1)^m}{\pi(2m+1)}, \quad m = 0, 1, 2, \dots \quad (19)$$

the restriction $k = (2m+1)\frac{\pi}{L}$, and

$$A_k = p_0 a_m \left[c_0 + 3(1 - c_0) \left(\frac{k^2 L^2 - 8}{k^2 L^2} \right) \right], \quad (20)$$

the expression for the stress extended to realistic initial and boundary conditions is found to be

$$\begin{aligned} \sigma_{zz}(x, z) = & p_0 \beta + \sum_k (A_k - p_0 a_m \beta) g_k(z) \cos kx \\ & + p_0 ((3 - 2c_0) - \beta) \sum_k \frac{c^2 k^2 a_m}{(\gamma - \alpha/2)^2 - \Omega_k^2} \\ & \times \left\{ e^{-\gamma z} - g_k(z) + \frac{\gamma}{\Omega_k} e^{-\frac{\alpha}{2} z} \sinh \Omega_k z \right\} \cos kx \end{aligned} \quad (21)$$

Thus, with given distributions of stress along the top surface and the side walls, explicit solutions are found for the stress in the interior and compared successfully to experiment. Oscillations down the center line emerge naturally but not always, the factor governing their appearance being the ratio c/α . Closed contours signifying true wavelike behavior appear in some cases but not in others, also depending on the value of c/α . Practical matters such as the effect of lubrication of the walls and of changing the profile of the applied stress at the top of the compact can be addressed [9].

Careful analysis of the question of whether the diffusive limit alone would suffice to describe the observed stress distribution results in an unequivocal answer in the context of the experiments reported in refs. [11,14,15]. The wave ingredient of the telegrapher's equation is found to be essential to explain some of the data (as in uranium dioxide) where oscillations are clearly visible. Furthermore, even for cases which exhibit no such oscillations (as in magnesium carbonate and alumina), a careful analysis based on our predictions lead to the conclusion that the diffusive limit is inadequate for the experiments of refs. [11,14,15].

IV. WHERE DO THE MEMORIES ORIGINATE? - STOCHASTIC CONSIDERATIONS

Having understood how memories help in understanding experiment and in unifying diverse approaches to the calculation of stress distributions, it is necessary to understand how the memories arise. One way is to obtain them phenomenologically through more or less suggestive arguments involving generalizations of previous constitutive relations. Such arguments have been provided in ref. [8] but give only a mathematical justification with little physical content. To understand the physical origin of the memories, consider (for simplicity) a two-dimensional granular compact (z along the vertical and x along the horizontal) consisting of weightless circular discs of a given radius arranged in perfect order. Let a vertical force be applied to the top of one of the discs lying on the top layer of the compact. It is trivial to show, on the basis of Newtonian laws of statics, that the consequent force distribution, equivalently stress distribution, is down two lines in the compact, representative of what has been called [7,8] light cones. Viewed through the $t - z$ transformation, the representative point in the one-dimensional space of x travels ballistically with constant speed which we will call c . Consider next a more realistic situation. The array is now not perfectly periodic, there being irregularities stemming from changes in shape and size of the discs and/or presence of friction. The speed c will change from location to location, and the path of the representative point will be jagged: the speed c will become a *stochastic* variable. Restricting attention to its z -variation only, we write

$$\frac{dx}{dz} = c(z), \quad (22)$$

with $c(z)$ a given stochastic process. Defining a Liouville density for the process and averaging over all realizations of the stochastic process, it is possible to obtain [25] a variety of evolution equations for the averaged probability density $P(x, z)$ according to the particular stochastic characteristics of the process $c(z)$. In other words, the particular irregularities arising from the shape and size changes in the discs, or from their roughness, are reflected in $c(z)$ and thereby in the evolution of $P(x, z)$. The latter quantity, involving as it does an average over various realizations (the jagged paths) of the stochastic process, can be shown to correspond to the probable value of the stress, equivalently to the probability density of the stochastic process.

One simple example of the stochastic process is one in which $c(z)$ is stationary and Gaussian, with zero mean and a correlation function Δ :

$$\langle c(z)c(z_1) \rangle = \Delta(z - z_1). \quad (23)$$

It leads straightforwardly [25] to

$$\frac{\partial}{\partial t} P(x, z) = D(z) \frac{\partial^2}{\partial x^2} P(x, z), \quad (24)$$

where the depth-dependent diffusion constant $D(z)$ is given as

$$D(z) = \int_0^z dz_1 \Delta(z - z_1). \quad (25)$$

We observe that the depth-dependence of $D(z)$ arises from a direct integration of the correlation function $\Delta(z)$. If the correlation function decays extremely rapidly signifying that the stochastic process corresponds to a perfect random walk, the stress evolution equation is a simple diffusion equation as in (3). Our analysis thus provides an explicit derivation from stochastic considerations of the full (not simplified to a constant D) equation of Liu et al. [23], and clarifies the validity of that equation.

On the other hand, if the stochastic process is a random telegraph, with an exponential correlation, it is also possible [25] to show that, to a good approximation, the stress evolution equation is the telegrapher's equation (4). Generally, the complexities and irregularities of the grain-grain interactions in the compact will influence the details of the stochastic process and thereby the memory function. Computer simulations have been begun to obtain the spatial correlations inherent in $c(z)$ and thence the memory functions. Such simulations, along with attempts to measure the correlations experimentally through scattering experiments, give an *a priori* predictive character to the theory of stress distribution that we have developed. The memory functions are seen, in this manner, to be not merely a phenomenological construct but calculable in principle from microscopic considerations regarding the physical characteristics of the granular system.

There is yet another source of memory functions which has been described in ref. [10] in greater detail than possible here (because of space restrictions). It arises from an effective medium theory of the granularity of the material. The granularity demands that one replace x by a discrete index m and the randomness of shapes and sizes of the particles demands that the rates in the evolution equation be random functions. Even if we start from a diffusive (but discrete) extreme represented, e.g., by

$$\frac{dP_m(z)}{dz} = F_{m+1,m} [P_{m+1}(z) - P_m(z)] + F_{m,m-1} [P_{m-1}(z) - P_m(z)] \quad (26)$$

where P denotes the z -component of the stress, and m is the discrete index representing the horizontal x (or y) coordinate, the randomness of the rates leads to a memory function that arises from *disorder*:

$$\frac{dP_m(z)}{dz} = \int_0^z dz' \mathbf{F}(z - z') [P_{m+1}(z') + P_{m-1}(z') - 2P_m(z')] \quad (27)$$

Here $\mathbf{F}(z)$ is obtained through a mean field argument from the random distribution $\rho(F)$ of the rates. Equation (27) is evidently equivalent to (3) in the continuum limit, $\mathbf{F}(z)$ being proportional to $D\phi(z)$. The memory functions which arise from such effective medium considerations are characterized by a sum of two parts with differing decay constants, and to stress distributions different from those predicted by a diffusion or telegrapher's equation [10].

V. CONCLUSIONS

The formalism of memory functions for the description of stress distribution described in the present paper has achieved unification of diverse approaches such as those applicable in the extreme diffusive and wave limits, treatment of the entire range in between, and explanation of observed features such as oscillations in stress distribution. The memory function may be computed from given stochastic properties of the granular system arising from the varying shapes and sizes of the grains and from the grain-grain interaction. Information about these stochastic properties themselves may be obtained in principle from a combination of scattering experiments and computer simulations. The memory formalism has also been extended [26] to include nonlinearities of the kind relevant to reaction diffusion systems.

Among shortcomings of this approach in its present stage are the assumption that the present does not influence the past (in the sense of the $t - z$ transformation) which means that stresses at smaller depths are considered as not influenced by stresses at larger ones. This assumption is not always valid as the stochastic paths representing the variable $c(z)$ can in some cases turn upwards in a granular system. Indeed, stress distribution cannot be looked

upon universally as an initial value problem. This is a difficulty shared by the extreme approaches of Liu et al. [23] and of Bouchaud and Cates [7] as well as by our intermediate formalism. Related to this problem is the evident restriction that the stress analysis presented above for dies be used only in long pipes or media without a bottom. Termination in the z direction as in a compact introduces 'boundary conditions in time' which appear difficult to treat from evolution equations. In the true time evolution situation, we predict behavior at a later time, given spatial boundary conditions for all time and an initial condition. The incorporation of a 'final' condition, i.e., a boundary condition at large values of time seems difficult to implement. Another notable absence from the formalism is the inclusion of features peculiar to the granular system such as isostaticity [27]. This last is a very important matter which, it is hoped, will be incorporated in the analysis at a future time. Indeed, at the present stage, our formalism is too simplistic to address severe complexities peculiar to granular matter such as the dependence of stresses on the history of how the granular system is constructed [3,28,29].

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