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Elementary Preamble to a Theory of Granular Gases (*).

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1. Introduction.

Granular materials partake, almost dramatically at times, of the properties of solids and, under different circumstances, of some properties of gases. Some scientists have suggested that they represent a new state of matter, to be treated *per se*; because of their ambiguity the search of an overall continuum model for these media is quite intriguing. Even if one confines inquiry to fast flows of sparse granules (as in granular gases, see e.g. [2]), the range of phenomena that may occur and that should be described by an adequate theory is vast. Within this area one is lured into adopting such appealing terms as gross *granular heat* and gross *granular temperature*, though the appropriateness of the borrowing can be challenged as the definitions of those gross quantities involve kinetic entities, whose detailed evolution can be in part ascertained rather than being totally unpredictable on principle and, at most, appraised through statistics. In any case, when exploiting vague analogies with the thermodynamics of perfect gases, one must make allowance for the fact that, in generic granular flows, speeds of agitation need not be, as they are in gases, many orders of magnitude greater than the average velocity or the velocity of any reasonably behaved observer. Thus one must be wary of a naive transfer to each moving element in a continuum of properties inferred from experiments within containers fixed to the

(*) The paper completes, extends, hopefully makes more perspicuous topics covered by an earlier report of limited circulation [1]; the report itself was an excerpt of a talk given in Bologna in 1999.

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walls of a laboratory; questions of objectivity become important if not paramount. One way to avoid difficulties would be to evaluate the relevant variables from some intrinsic local frame. The traditional way in continuum mechanics is to appeal to gross position and velocity gradients, a way that cannot be satisfactorily pursued in our context. Notice that akin problems arise in the analysis of vibrations of large and very flexible space structures (or, more down to earth, of the motion of a misshaped soap bubble in wind): the centre of gravity need not be superposed to a place occupied by some element of the structure; even if perchance such superposition occurs, the movement in the vicinity of the centre might have little to do with the gross motion of the structure; hence the need of an alternative notion of gross rotation. A solution is easy to find: the set of balance equations of momentum, moment of inertia, moment of momentum can be interpreted as the tools that allow us to figure out the background against which an objective measure of residual energy of agitation can be achieved, with consequent satisfactory portrayal of «thermal» concepts.

Again, the many different scales of events possible in a generic granular flow entail a reconsideration of the ties of the concept of temperature with the kinetic circumstances of ensembles of granules having diverse (and not necessarily canonical) distributions of energy, thus including easily, for instance, negative and tensorial absolute temperatures.

Finally, when one pursues a continuum model of granular flows, one must abandon the fundamental tenet that it be possible to define, that is to identify for ever, each material element. Then test domains of minute diameter and the corresponding local averages take a central rôle; the question how to average near the frontier of the body and thus how to model boundary effects must be addressed. Moreover, in the formulation of constitutive relations, valid either in the interior or at the boundary of the body, local space and time-correlations might take precedence over material space-gradients and material time-derivatives.

However, whichever changes be necessary, ultimately some alternative paradigm should emerge and it is attractive to note, from a cursory review of some proposals for extended versions of continuum mechanics (e.g., the theory of hypoelasticity) or continuum thermodynamics, some stunning similarities in the evolution equations which are arrived at. True, those theories all presume the absence of local mesospin (which may be instead relevant in granular flows). However, next to the equation of continuity and Cauchy's equation an additional equation concerns the shuffling motions; it involves a stirring tensor and rules the evolution of a Reynolds' tensor, a symmetric tensor which both in hypoelasticity and in extended thermodynamics coincides with momentum flux.

Precisely, the theory of hypoelasticity [3], Grad's theory of 13 moments [4], extended thermodynamics [5], Jenkin's theory of fast flow of granular materials [6], all suggest the addition to the classical equation of balance of another equation which rules the evolution of the symmetric Reynolds' tensor H:

$$\varrho \overset{\Delta}{H} = S_I - div\ \boldsymbol{s} + S_E;$$

at the same time, for Cauchy's stress tensor T, a very simple constitutive law is suggested: $T = \varrho H$. ϱ is density, $\overset{\Delta}{H}$ the convected time derivative of H, $\mathbf{s}$ is the third order stirring tensor; the tensor S_I represents internal equilibrated actions, and S_E the external stir.

Here, within the mechanics of mass points, an elementary analysis which involves predominantly velocities rather than places, is shown to lead to a global equation of motion which suggests, by analogy, within continuum mechanics, just the last balance equation mentioned above. Precisely that equation may be relevant, in general, when modelling kinetic bodies (i.e., bodies which are in a permanent state of flux and possess no natural paragon placement) and, in particular, granular gases.

2. Adscititious topics in elementary mechanics.

Consider a system $\mathcal{S}$ of N mass points; let $x(\tau)$ the current centre of gravity of $\mathcal{S}$ and μ the total mass; $\mu^{(i)}$, the mass of the $i-$th point; $x^{(i)}(\tau)$, its current place; $\tilde{y}^{(i)}$, its position vector with respect to the centre of gravity in a paragon setting (e.g., the initial placement). Take for $R(\tau)$ a proper orthogonal tensor; split $x^{(i)}$ into the following sum:

$$x^{(i)}(\tau) = x(\tau) + R(\tau)\, s^{(i)}; \qquad s^{(i)} = \tilde{y}^{(i)} + \tilde{s}^{(i)}(\tau) \tag{1}$$

involving a global rigid displacement $(x(\tau), R(\tau))$ and an individual shuffle vector $\tilde{s}^{(i)}$.

In a motion the velocity of each point is given by the sum

$$\dot{x}^{(i)}(\tau) = \dot{x}(\tau) + \mathbf{e}\big(q(\tau) \otimes y^{(i)}(\tau)\big) + R(\tau)\ \dot{\tilde{s}}^{(i)}(\tau) \tag{2}$$

of speeds of entrainment (the first two addenda) and of agitation (the last addendum): here $y^{(i)} = x^{(i)} - x$, $\boldsymbol{e}$ is Ricci's permutation tensor, q is the speed of rotation so that $\dot{R}R^{-1} = \boldsymbol{e}q$.

Differentiating again (2) with respect to time one can exhibit explicitly entrainment, relative, Coriolis' components of acceleration:

$$\ddot{x}^{(i)} = \ddot{x} + \boldsymbol{e}(\dot{q} \otimes y^{(i)}) + q^2(I - c \otimes c)y^{(i)} + R\ddot{s}^{(i)} + 2\boldsymbol{e}(q \otimes R\dot{s}^{(i)})\,; \tag{3}$$

here c is the unit vector associated with q, i.e., $q = |q|c$, and I is the identity tensor.

The total kinetic energy $\mu\kappa$ is given by

$$\mu\kappa = \frac{1}{2}\mu\dot{x}^2 + \frac{1}{2}\mu q^2(I - c \otimes c)\cdot Y + \frac{1}{2}\sum_i \mu^{(i)}\big(\dot{s}^{(i)}\big)^2 + \sum_i \mu^{(i)}\big(R\dot{s}^{(i)}\big)\cdot\boldsymbol{e}\big(q \otimes y^{(i)}\big)\,, \tag{4}$$

where μY is Euler's inertia tensor

$$\mu Y = \sum_i \mu^{(i)} y^{(i)} \otimes y^{(i)}. \tag{5}$$

Notice that μJ, $J = (trY)\,I - Y$, is the usual tensor of inertia, and that $\mu(I - c \otimes c)\cdot Y = c\cdot Jc$ coincides with the moment of inertia around a baricentric axis parallel to c.

Actually, one could have started this elementary investigation taking for x any moving point and enquiring subsequently how $\dot{x}(\tau)$ should be chosen so that $\frac{\mu}{2}\dot{x}^2$ differ the least from the total kinetic energy; the answer would have been to choose $\dot{x}$ so that it coincide always with the speed of the centre of gravity. Similarly, one can choose q in such a way that the speeds $\boldsymbol{e}\big(q \otimes y^{(i)}\big)$ best fit the motion relative to $x(\tau)$, in the sense that the discrepancy in kinetic energy is minimal

$$\mu\kappa - \frac{1}{2}\sum_i \mu^{(i)}\boldsymbol{e}\big(q \otimes y^{(i)}\big)^2 = \min\,; \tag{6}$$

one needs only take for q the solution of the equation

$$Jq = k\,, \tag{7}$$

where μk is the moment of momentum with respect to the centre of gravity

$$\mu k = \sum_i \mu^{(i)} y^{(i)} \times \dot{y}^{(i)}. \tag{8}$$

With that choice of q the last term in (4) cancels out. The kinetic energy is split into the sum of the two, observer-dependent, usual terms as in a rigid motion and an observer-independent term due to agitation.
To prove the statements above notice that the last term in (2) could be written successively as follows:

$$q \cdot \sum_i \mu^{(i)} y^{(i)} \otimes \left(R\dot{s}^{(i)}\right) = q \cdot \left[\sum_i \mu^{(i)} (y^{(i)} \times \dot{y}^{(i)} - y^{(i)} \times (q \times y^{(i)})\right] =$$

$$= q \cdot \left[\sum_i \mu^{(i)} y^{(i)} \times \dot{y}^{(i)} - \mu J q\right],$$

whereas the second addendum in the right-hand side of (4) is exactly the contribution to $\mu\kappa$ of a rigid rotation around x.

Knowledge of $\dot{x}$ and q (and hence of x and R) offers the chance to fix a background against which the motion of agitation can be measured objectively. To determine $\dot{x}$ and q, appeal can be made to the global equations

$$\mu \ddot{x} = f, \qquad \mu \dot{k} = m, \tag{9}$$

where f and m are resultant and resultant moment of external forces on $\mathcal{S}$. Success is obvious if there is no agitation and the motion is trivially rigid. However, in general one is not so fortunate because there may be an influence of shuffle and agitation certainly on J and, perchance, on f and m; notice, in particular, that J depends critically on expansion/contraction of $\mathcal{S}$ because

$$\dot{J} = \left(tr\dot{Y}\right) I - \dot{Y} \tag{10}$$

and

$$\dot{Y} = 2 \text{ sym } K, \tag{11}$$

where

$$\mu K = \sum_i \mu^{(i)} y^{(i)} \otimes \dot{y}^{(i)} \tag{12}$$

is the tensor moment of momentum, the evolution of which must be known to evaluate the evolution of Y. In a rigid motion K depends on Y and q only, $K = -(\boldsymbol{e}q)\,Y$, and no further developments are required. Instead, in general, as remarked above, a deeper analysis of the motions of S needs be effected in advance. We need to modify the developments at the beginning of this section as a premise; rather than (1) take now

$$x^{(i)}(\tau) = x(\tau) + G(\tau)\, s^{(i)}(\tau)\,, \tag{13}$$

where G is a tensor with positive determinant; correspondingly,

$$\dot{x}^{(i)} = \dot{x} + By^{(i)} + G\dot{s}^{(i)}, \qquad B = \dot{G}G^{-1}, \tag{14}$$

and

$$\ddot{x}^{(i)} = \ddot{x} + \big(\dot{B} + B^2\big)\, y^{(i)} + 2BG\dot{s}^{(i)} + G\ddot{s}^{(i)}, \tag{15}$$

if $y^{(i)}$ is equal to $Gs^{(i)}$.

Thus, shuffle and agitation are now supposed to be remainders beyond an affine, rather than rigid, motion. The kinetic energy is given by the sum

$$\frac{1}{2}\mu\dot{x}^2 + \frac{1}{2}\mu tr(BYB^T) + \frac{1}{2}\sum_i \mu^{(i)}\big(G\dot{s}^{(i)}\big)^2 + \sum_i \mu^{(i)}\big(G\dot{s}^{(i)}\big)\cdot\big(By^{(i)}\big)\,. \tag{16}$$

However, if B is chosen so as to make $\mu\kappa - \sum_i \mu^{(i)}\big(By^{(i)}\big)^2$ a minimum, i.e., as to satisfy the condition

$$BY = K^T, \tag{17}$$

the last term in (16) vanishes; in fact, even the mixed kinetic tensor

$$\sum_i \mu^{(i)}\dot{s}^{(i)} \otimes By^{(i)} \tag{18}$$

vanishes, not only its trace, so that a relatively compact expression is available also for the kinetic energy tensor $\mu W = \frac{1}{2}\sum_i \mu^{(i)}\dot{x}^{(i)} \otimes \dot{x}^{(i)}$, as follows:

$$\mu W = \frac{1}{2}\mu\dot{x} \otimes \dot{x} + \frac{1}{2}\mu BYB^T + \frac{1}{2}\mu H\,. \tag{19}$$

where, if H_* is Reynolds's kinetic tensor of agitation, H is its transformed expression by G:

$$\mu H_* = \sum_i \mu^{(i)} \dot{s}^{(i)} \otimes \dot{s}^{(i)}, \qquad H = G H_* G^T. \tag{20}$$

It is important to notice, in particular for later developments, that all vectors $\dot{s}^{(i)}$ and the tensor H_* are absolute, i.e., not affected by changes or movements of the observer.

To determine $\dot{x}$ and B, appeal is now made to the first one of (9) and to the equation of balance of the tensor moment of momentum

$$\mu(\dot{K} - BK - H) = M - A\,, \tag{21}$$

where M and A are respectively the tensor moment of external and internal forces acting on S

$$M = \sum_i y^{(i)} \otimes f^{ext(i)}, \qquad A = -\sum_i y^{(i)} \otimes f^{int(i)}. \tag{22}$$

Because the vector moment of internal forces vanishes, A is a symmetric tensor. Remark that (11) can be read as the assertion that the «reference» tensor of inertia $Y_* = G^{-1} Y G^{-T}$ is constant irrespective of shuffle.

We still need the evolution equation for H; it is easily obtained from Newton's law, multiplying both members tensorially by $\dot{s}^{(i)}$, summing and transforming through G:

$$\mu(\dot{H} + BH + HB^T) = S - Z\,; \tag{23}$$

here S is the stirring tensor of external forces

$$S = 2 \text{ sym} \sum_i (G\dot{s}^{(i)}) \otimes f^{ext(i)}, \tag{24}$$

and a similar definition but with opposite sign applies to Z, involving internal forces. The queer choice of sign for A and Z has to do with a convention appropriate in a distinct, later context. Finally, if one remarks that

$$K = \text{sym } K + \frac{1}{2} \boldsymbol{e} k\,, \qquad M = \text{sym } M + \frac{1}{2} \boldsymbol{e} m\,, \tag{25}$$

the system of equations to explore becomes

$$
(26)\qquad \begin{cases} \mu \ddot{x} = f\,, \\ \dot{k} = m\,, \\ \mu\ \mathrm{sym}\left(\dot{K} - BK\right) = \mathrm{sym}\, M + \mu H - A\,, \\ \mu\left(\dot{H} + BH + HB^{T}\right) = S - Z\,. \end{cases}
$$

Strictly, the first two equations bear upon the preferred reference, if only its rotational speed q is defined through the relation

$$
q = J^{-1} k\,,
$$

whereas the last two lead to global hints on agitation; but, generally, the two sets are strongly linked. Actually, for some later purposes, it is more convenient to keep together the two equations for the symmetric and skew components of K and to add to the list the evolution equation for Y:

$$
(27)\qquad \begin{cases} \mu \ddot{x} = f\,, \\ \mu\left(\dot{K} - BK\right) = M - A + \mu H\,, \\ \dot{Y} = YB^{T} + BY\,, \\ \mu\left(\dot{H} + BH + HB^{T}\right) = S - Z\,. \end{cases}
$$

Notice, in the second and fourth equation, that the quantities between brackets express the convected time derivative $\overset{\Delta}{K}$ of K and $\overset{\Delta}{H}$ of H, based on the spin tensor B.

If all $\dot{s}^{(i)}$ vanish, then all $s^{(i)}$ maintain their initial values, H vanishes and the local motion is affine, or pseudo-rigid in the therminology of Cohen and Muncaster [7]. Their results could be borrowed here; one needs to study only the reduced system of the first three equations of (27) in x and B.

More generally, if f, M, A, Z and S depend at most on x, $\dot{x}$, G, B and H, then (26) can be interpreted as a differential system in x, G, and H.

Circumstances could be called *kinetic* when the system has no physically relevant paragon setting, its behaviour is ruled by abrupt responses to current circumstances and, as a consequence, in our model, f, M, and S need depend at most on $v = \dot{x}$, B and H; then (27) becomes a first order system in v, B, Y and H. This system would merit scrutiny on its own, perhaps under appropriate, special choices of f, M, A, Z and S.

A case of special interest is met when $A = \mu H$ or, at least the quantity $(A - \mu H)$ together with f and M depend at most on v, B and Y; then the first three equations can be dealt separately from the last.

More subtle is the case in when f, M and S depend also on $\kappa + \varphi_I$ where φ_I is the potential energy of internal forces, supposing that they all be conservative; or, rather, when they depend also on the manner the mass points of $\mathcal{S}$ can be classed in families of increasing total energy, or, more deeply, in families of approximately equal Reynolds tensor.

3. The kinetic energy theorem and some corollaries.

A tensor kinetic energy theorem can be derived easily from (2.28) by adding term by term first, second and fourth equation after tensorial multiplication of the first by $\dot{x}$, of the second by B, and after multiplication by $\frac{1}{2}$ of the fourth; finally, by taking the symmetric parts of all terms:

$$\mu \dot{W} = \operatorname{sym}[\mu \ddot{x} \otimes \dot{x} + \mu(\dot{B} Y B^T + B^2 Y B^T)] + \frac{1}{2}\mu \dot{H} = \tag{28}$$

$$= \operatorname{sym}\left[\mu \ddot{x} \otimes f + B(M - A)\right] + \frac{1}{2}(S - Z).$$

More particularly, but also with deeper meaning, if one takes the trace, one arrives at the more usual kinetic energy theorem

$$\dot{\kappa} = \dot{x} \cdot f + (M - A) \cdot B^T + \frac{1}{2} \operatorname{tr}(S - Z). \tag{29}$$

Remark that

$$M \cdot B^T + \frac{1}{2} \operatorname{tr} S = \sum_i \dot{y}^i \cdot f_E^i, \qquad -\left(A \cdot B^T + \frac{1}{2} \operatorname{tr} Z\right) = \sum_i \dot{y}^i \cdot f_I^i. \tag{30}$$

The standard requirement that the power of internal actions be invariant for any rigid change of speed, when B is an arbitrary skew tensor, also leads to the condition

$$A \in Sym\,,$$

which was already noticed on equivalent grounds.

If potentials φ_E, φ_I exist for external and internal forces, respectively, then

$$f_E^i = \frac{\partial \varphi_E}{\partial x^{(i)}}\,, \quad f_I^i = \frac{\partial \varphi_I}{\partial x^{(i)}}\,; \tag{31}$$

a theorem of energy conservation follows:

$$\kappa + \varphi = \text{const}\,, \qquad \varphi = \varphi_E + \varphi_I\,. \tag{32}$$

Notice that, on the one hand, for (14),

$$\dot{\varphi} = \sum_i \frac{\partial \varphi}{\partial x^{(i)}} \cdot \left(\dot{x} + By^{(i)} + G\dot{s}^{(i)}\right),$$

and, on the other hand,

$$\frac{\partial \varphi}{\partial x} = \sum_i \frac{\partial \varphi}{\partial x^{(i)}}\,, \qquad \frac{\partial \varphi}{\partial G} = \sum_i \frac{\partial \varphi}{\partial x^{(i)}} \otimes s^{(i)},$$

so that

$$\dot{\varphi} = \dot{x} \cdot \left(\sum_i \frac{\partial \varphi}{\partial x^{(i)}}\right) + \dot{G} \cdot \left(\sum_i \frac{\partial \varphi}{\partial x^{(i)}} \otimes s^{(i)}\right) + G \cdot \left(\sum_i \frac{\partial \varphi}{\partial x^{(i)}} \otimes \dot{s}^{(i)}\right).$$

Juxtaposition with the right-hand side of (29) suggests the «constitutive laws»

$$f = \frac{\partial \varphi}{\partial x}\,, \qquad M - A = \frac{\partial \varphi}{\partial G} G^T, \qquad S - Z = 2\ \text{sym}\left(\sum_i \dot{s}^{(i)} \otimes \frac{\partial \varphi}{\partial s^{(i)}}\right),$$

or, more precisely,

$$f = \frac{\partial \varphi_E}{\partial x}\,, \qquad M = \frac{\partial \varphi_E}{\partial G} G^T, \qquad A = -\frac{\partial \varphi_I}{\partial G} G^T,$$

$$S = 2\ \text{sym}\left(\sum_i \dot{s}^{(i)} \otimes \frac{\partial \varphi_E}{\partial s^{(i)}}\right), \qquad Z = -2\ \text{sym}\left(\sum_i \dot{s}^{(i)} \otimes \frac{\partial \varphi_I}{\partial s^{(i)}}\right). \tag{33}$$

φ_E may be influenced also by x and $\text{skw}\, G$, besides $\text{sym}\, G$ and $\dot{s}^{(i)}$; on the contrary, φ_I must be observer independent, hence it must not involve x

and may depend on G only through the product $C = G^T G$, so that

(34) $$A = -2G \frac{\partial \varphi_I}{\partial C} G^T.$$

Of course, in general, A and Z have also dissipative components beside the conservative components expressed, as above, through φ_I.

Sometimes there is an interest for a «reduced» theorem involving the «gross» kinetic energy tensor $\widetilde{W}$ per unit mass

$$\widetilde{W} = \frac{1}{2}\dot{x} \otimes \dot{x} + \frac{1}{2} BYB^T.$$

The theorem is signified by the reduced equation

$$\mu \dot{\widetilde{W}} = \operatorname{sym}[\mu \dot{x} \otimes f + B(M - A)],$$

and leads, by difference from (28) (and when the trace is taken), to a «principle» of energy balance. The latter is, in the present context, nothing else but a corollary of the last equation (27) but with a different promotion of terms, the leading rôle being played by the «internal energy»

(35) $$\varepsilon = \frac{1}{2} trH - \varphi_I.$$

As we can avail ourselves of the more powerful relation (28), we do not pursue here the consequences of that corollary. Actually, for later purposes, one can write the last equation (27) in an equivalent form which approaches the principle of conservation more closely, using a tensor of energy

$$E = \frac{1}{2}H + \frac{1}{3}\varphi_I I;$$

precisely

$$\mu(\dot{E} + BE + EB^T) = \frac{1}{2}(S - \widehat{Z}),$$

where

$$\widehat{Z} = Z - \frac{1}{3}\,\dot{\varphi}_I I - \frac{2}{3}\,\varphi_I \mathrm{sym}\, B =$$

$$= -2\ \mathrm{sym}\left[\sum_i \dot{s}^{(i)} \otimes \frac{\partial \varphi_I}{\partial s^{(i)}} - \frac{1}{6}\,\dot{\varphi}_I I - \frac{1}{3}\,\varphi_I \mathrm{sym}\, B\right].$$

4. Energy distributions.

The topics of this section are textbook affairs; because of the interest here in non-canonical instances, they are recalled nonetheless in essence and with the appropriate slant.

4.1. *The scalar case.*

When the mass points are very numerous, though with bounded total mass μ, the «averages» x, k, Y, etc. acquire prominent import. At the same time, as mentioned at the end of the previous section, the resultant actions on $\mathcal{S}$, expressed by f, M, S, may come to depend (not only on kinematic variables such as v, B, Y, H, but, as hinted, also) on the way mass-points can be parcelled out in families, each family comprising points with an energy of agitation falling within a limited range, say $[(j-1)\,\mu\varepsilon\delta, j\mu\varepsilon\delta]$, $j = 1, 2 \ldots$ (here δ is a positive number). The fraction $\frac{N_i}{N}$ of mass points belonging to the j-th family is measured by a non-negative constant γ_j.

Then an histogram can be drawn as a graph of a piecewise constant function $\overline{\gamma}(\xi)$ having the value γ_j for ξ within the interval $[(j-1)\,\delta, j\delta]$. Notice that there will always be a value, say J of the index, such that $N_J > 0$, whereas all N_j with index larger than J vanish; that it is so because the total energy $m\varepsilon$ is (approximately equal to and) not less than $\mu\varepsilon\delta \sum_j (j-1)\,N_j$; that each term in the sum cannot exceed δ^{-1}; that any non-null value of N_j is a positive integer, hence no less than 1; and, in conclusion, that $J - 1 \leqslant \delta^{-1}$.

The function $\overline{\gamma}(\xi)$ satisfies a normalization condition

$$\int_0^\infty \overline{\gamma}(\xi)\, d\xi = \delta \sum_j \gamma_{j-1} = \frac{1}{N} \sum_j N_j = 1\,.$$

A second important relation is derived easily; remark that

$$\int_0^\infty \xi\overline{\gamma}(\xi)\, d\xi = \sum_j \gamma_j \int_{(j-1)\delta}^{j\delta} \xi d\xi = \sum_j j\gamma_j \delta^2 - \frac{1}{2}\delta ,$$

and that, on the other hand,

$$\sum_j \mu\varepsilon\delta^2 (j-1)\gamma_j \leqslant \mu\varepsilon \leqslant \sum_j \mu\varepsilon\delta^2 j\gamma_j$$

or

$$1 \leqslant \delta^2 \sum_j j\gamma_j \leqslant 1 + \delta .$$

In conclusion,

$$1 - \frac{\delta}{2} \leqslant \int_0^\infty \xi\overline{\gamma}(\xi)\, d\xi \leqslant 1 + \frac{\delta}{2} .$$

Our analysis becomes more fluent if we proceed to smooth out the histogram (perhaps imagining that the range of δ is taken ever smaller) to become the graph of a (continuous, even smooth) function $\gamma(\xi)$ with the properties that $\gamma(\xi)\, d\xi$ gives the fraction of mass points with energy of agitation within the interval $(\mu\varepsilon\xi,\ \mu\varepsilon(\xi + d\xi))$ and that the following normalization conditions apply

$$\int_0^\infty \gamma(\xi)\, d\xi = 1 , \qquad \int_0^\infty \xi\gamma(\xi)\, d\xi = 1 .$$

It is easy to contrive distribution functions satisfying all conditions noticed so far for γ. Take any function $\lambda(\overline{\xi})$ defined over $[0, +\infty)$ with non-negative, not everywhere null values (even a measure) and integrable, together with $\overline{\xi}\lambda(\overline{\xi})$, over $[0, +\infty)$

$$\int_0^\infty \lambda(\overline{\xi})\, d\overline{\xi} = \varrho , \qquad \int_0^\infty \overline{\xi}\lambda(\overline{\xi})\, d\overline{\xi} = \sigma ; \qquad 0 < \varrho, \sigma < \infty .$$

By choosing

$$\gamma(\xi) = \frac{\sigma}{\varrho^2}\lambda\left(\frac{\varrho\xi}{\sigma}\right),$$

one obtains just one of the desired functions.

It is an easy matter to check that the following choices for γ satisfy all requirements mentioned above. It is appropriate to emphasize that the abscissa ξ for the histogram is chosen here as to be non-dimensional and such that mass points for which $\xi = 1$ have energy per unit mass exactly equal to the total energy per unit mass. The use of non-dimensional variables may give an impression of excessive specialization; in the formulae, in fact, the choice of constants is mandatory:

(i) Canonical:

$$\gamma = e^{-\xi}, \qquad \text{for all } \xi . \tag{36}$$

For some systems, such as monoatomic gases, this distribution is requisite under «quasi-static» conditions.

(ii) Power law:

$$\gamma = 24(2+\xi)^{-4}, \qquad \text{for all } \xi . \tag{37}$$

Remark that other negative powers different from -4, strictly less than -2 could be contemplated; the numerical factors would then be obviously different.

(iii) Piece-wise constant: For any constant $\beta \in [0, 1)$, take

$$\gamma(\xi) = 0, \quad \text{when} \quad 0 \leqslant \xi < \beta \quad \text{or} \quad \xi > 2-\beta ,$$

$$\gamma(\xi) = \frac{1}{2(1-\beta)}, \quad \text{when} \quad \beta < \xi < 2-\beta . \tag{38}$$

The limit for $\beta \to 1$ is a measure with an atom at $\xi = 1$.

(iv) Piece-wise linear: For any $\beta \in \left[\frac{3}{2}, 3\right]$, take

$$\gamma(\xi) = 0, \quad \text{when} \quad \xi > \beta ,$$

$$\gamma(\xi) = 2\beta^{-3}[3(2-\beta)\,\xi + (2\beta-3)\,\beta], \quad \text{when} \quad 0 \leqslant \xi \leqslant \beta . \tag{39}$$

(v) Piece-wise exponential: Given the constants β, positive; $\xi_1 \geqslant 0$, $\xi_2 > \xi_1$; and α real; take

$$\gamma(\xi) = 0, \quad \text{when} \quad 0 \leqslant \xi \leqslant \xi_1 \quad \text{or} \quad \xi > \xi_2,$$
$$\gamma(\xi) = \beta e^{-\alpha\xi}, \quad \text{when} \quad \xi \in [\xi_1, \xi_2],$$

where

$$\beta = \frac{\alpha}{e^{-\alpha\xi_1} - e^{-\alpha\xi_2}}$$

and α is a solution of the equation

(40) $$\alpha = \frac{(1+\alpha\xi_2)\, e^{-\alpha\xi_2} - (1+\alpha\xi_1)\, e^{-\alpha\xi_1}}{e^{-\alpha\xi_2} - e^{-\alpha\xi_1}}.$$

To lighten developments, we refer below only to the choice $\xi_1 = 0$, when

(41) $$\gamma(\xi) = \frac{\alpha}{1 - e^{-\alpha\xi_2}} e^{-\alpha\xi},$$

where α satisfies the equation

(42) $$\alpha - 1 = \frac{\alpha\xi_2}{1 - e^{\alpha\xi_2}}.$$

An inspection of (42) requiring only accurate evaluations of orders of magnitude shows that: There is one and only one value of α satisfying (42) for each choice of ξ_2 larger than 1. There are no values of α satisfying (42) for $\xi_2 < 1$. The function $\alpha(\xi_2)$, thus defined, is strictly increasing from $-\infty$ to 1; it vanishes for $\xi_2 = 2$; its approximate expression in the neighborhood of 2 is

$$\alpha \simeq \frac{3}{2}(\xi_2 - 2).$$

When ξ_2 tends to 1 and α to $-\infty$, the distribution (41) approaches a $\delta-$ function with an atom at $\xi = 1$. When ξ_2 tends to the value 2 and α to zero, the distribution (41) tends to be piece-wise constant: $\gamma(\xi) = \frac{1}{2}$ for $0 < \xi < 2$ and null otherwise. When ξ_2 tends to ∞ and α to 1, the distribution tends to be canonical. This distribution is reminiscent of one which is suitable for quantum systems though allowing in that case only a finite number of states. As is well known, for them, with appropriate care, a sudden transit from a distribution with α positive into one with α negative can be achieved experimentally.

(vi) Sinusoidal: Given a constant α less than $\frac{\pi^2}{4}$ take

$$\gamma(\xi) = 0\,, \quad \text{when} \quad \xi > 2\left(1 - \frac{4\alpha}{\pi^2}\right)^{-1},$$

$$\gamma(\xi) = \frac{1}{2}\left(1 - \frac{4\alpha}{\pi^2}\right)\left(1 + \alpha \cos\frac{\pi}{2}\left(1 - \frac{4\alpha}{\pi^2}\right)\xi\right). \tag{43}$$

The limit when α goes to zero coincides with the limit case (iii) when $\beta \to 0$. γ either decreases or increases with increasing ξ, depending on the sign of α. This distribution may be of interest when energy and numerosity are functions of an angle from a given direction.

(vii) Fermi and Bose. For β non-null

$$\gamma(\xi) = \left| e^{|\beta|\xi}(e^{\beta} - 1)^{-1} - 1 \right|^{-1} \tag{44}$$

satisfies the first normalization condition; now choose β so as to fulfill also the second one, which requires that

$$\beta^2 = \mathrm{Di}\log(e^{\beta} - 1)\,, \tag{45}$$

where

$$\mathrm{Di}\log y = \sum_{k=1}^{\infty} \frac{y^k}{k^2} = \int_y^0 \frac{\lg(1-t)}{t}\,dt\,. \tag{46}$$

There are two solutions, one with β negative (Bose-Einstein subcase) and the other with β positive (Fermi-Dirac subcase):

$$\beta = -0.814651\ldots, \qquad \beta = 1.405050\ldots \tag{47}$$

4.2. *The tensor case.*

As hinted repeatedly, a classification of mass points in families with specific energy is inadequate at times to cast satisfactory constitutive laws completing system (26) or (27). One can explore broader alternatives (see, e.g., [8]), in particular one can attempt the classification in tensorial terms; i.e., when φ_I vanishes, in terms of the Reynolds tensor. Precisely, to pursue here the latter (special, but most important) case, think of the linear space of symmetric tensors and, within it, the manifold $\mathcal{N}$ of all rank-1 tensors, i.e., of all tensors N of the type $v \otimes v$ with v

any vector. With γ a function of the tensor variable $H^{-1/2}NH^{-1/2}$, call now

$$\gamma(H^{-1/2}NH^{-1/2})(H^{-1}\cdot dN)$$

the number fraction of mass points with Reynolds tensor in the immediate neighborhood of N; imagine again the histogram of γ smoothed out to render it continuous and differentiable. It would also be integrable over $\mathcal{N}$ together with its product by $H^{-1}N$ and with the properties of normality

$$\int_{\mathcal{N}} \gamma(H^{-1/2}NH^{-1/2})\, H^{-1}\cdot dN = 1\,,$$

$$\int_{\mathcal{N}} (H^{-1}\cdot N)\gamma(H^{-1/2}NH^{-1/2})(H^{-1}\cdot dN) = 1\,.$$

Then, formally, one can proceed in analogy with the scalar case; in particular, one can introduce the extended canonical distribution, valid on $\mathcal{N}$,

$$\gamma = e^{-H^{-1}\cdot N}$$

(see, e.g., [9]) and explore also alternative distributions.

5. Granular temperature.

When the intimation at the end of Section 2 is mandatory, knowledge of the distribution γ becomes essential; then the need would appear, from the developments of Section 4, to seek another equation (a sort of Boltzmann equation) to describe the evolution of γ. Actually it often occurs that either the class of the accessible distributions is restricted on physical grounds and each distribution is then identified by few parameters, or, at least, only a few variables linked to the distribution are essential and suffice. Such is the granular temperature ϑ, which is defined below:

$$\vartheta = -\frac{d\xi}{d(\log\gamma)} = -\gamma\frac{d\xi}{d\gamma}\,. \tag{48}$$

It is a constant parameter in case (i). If the case (iii) is taken as the limit case (v) for $\alpha \to 0$, the associated temperature is infinite. In case (v), subcase $\xi_1 = 0$, then $\vartheta = \alpha^{-1}$; hence the graph of temperature against ξ_2 shows ϑ decreasing from 0 to $-\infty$ as ξ_2 ranges from 1 to 2, and then decreasing from $+\infty$ to 1 as ξ_2 grows to $+\infty$. It is noteworthy to remark that null temperature can be achieved only through negative values;

transition from positive to negative temperature can occur only through ∞, as is known experimentally.

In distributions different from exponential, as in case (ii), the derivative (48) is not a constant; one can declare that temperature is meaningless for such cases or be satisfied with an average value ϑ_w of the derivative over its support.

More precisely, suppose that, as required for invertibility, $\gamma(\xi)$ be strictly monotone and positive only over an interval $(\xi_1, \xi_2) \in (\xi_1, +\infty]$; then for the weaker definition ϑ_w of the temperature, one obtains

$$(49) \qquad \vartheta_w = (\gamma(\xi_1) - \gamma(\xi_2))^{-1} \int_{\gamma(\xi_1)}^{\gamma(\xi_2)} \frac{d\xi}{d(\log \gamma)} d\gamma = \\ = (\gamma(\xi_1) - \gamma(\xi_2))^{-1} \int_{\xi_1}^{\xi_2} \gamma d\xi = \frac{1}{\gamma(\xi_1) - \gamma(\xi_2)} .$$

Summing up, for the special distributions above, the temperature turns out to be

$$\text{(i)} \;\; \vartheta = 1 ; \quad \text{(ii)} \;\; \vartheta_w = \frac{3}{2} ; \quad \text{(iii)} \;\; \vartheta = \infty ;$$

$$\text{(iv)} \;\; \vartheta_w = \frac{1}{6} \frac{\beta^2}{\beta - 2} ; \quad \text{(vi)} \;\; \vartheta_w = \frac{\pi^2}{(\pi^2 - 4\alpha)\alpha} ; \quad \text{(vii)} \;\; \vartheta_w = \left| \frac{2 - e^\beta}{e^\beta - 1} \right| .$$

In case (v), subcase $\xi_1 = 0$, $\vartheta = \alpha^{-1}$, hence ϑ varies with the choice of ξ_2 as was described above.

As hinted at the end of Section 2, the temperature (or its reciprocal, the temperance), even when allowed to roam over the entire real axis, may be yet inadequate to allow closure of system (26), (28) for a sufficiently wide class of bodies. Then one can explore broader alternatives (see, e.g., [8]) and insinuate the idea that a tensor related to the distribution of shufflings may be of help. Precisely, one may think to the tensor case discussed in Section 4. Then, over the support of γ on $\mathcal{N}$ also $\log \gamma$ becomes meaningful and the following *temperature tensor* can be defined:

$$(50) \qquad - \frac{dN}{d(\log \gamma)} .$$

As already mentioned, by far-fetched analogy with standard cases, one may dream up occurrences when H, S, and Z are functions of the temperature tensor on physical grounds; then, the last equation (27) becomes an evolution equation for the temperature tensor. Naturally such dreams need by substantiated by offering some concrete cases where the fantasy bears fruits; for the moment, let us rest content to have drawn attention to a possible avenue which is wider than that opened up by the mere scalar temperature and hence perhaps more attuned to the study of granular materials.

6. Transition to a continuum model.

The system (27) is already written in such a way as to suggest the possible evolution equations for a continuum, where the image of the body is a fit region rather than a discrete set in Euclidean space.

Now mass density ϱ takes the defining rôle for mass; ϱ and the current place x, the current gross local shape G, the current tensor of moment of inertia Y, and the kinetic tensor H, are all fields.

The conservation equation for mass is the classical one

$$\dot{\varrho} + \varrho \operatorname{div} \dot{\mathrm{x}} = 0\,, \tag{51}$$

and its twin for tensor moment of inertia is still the third of (27):

$$\dot{Y} = YB^T + BY\,, \qquad B = \dot{G}G^{-1}. \tag{52}$$

The evolution equations for x, G and H can be formally adapted from the first, second and fourth of (27):

$$\begin{gathered} \varrho\ddot{x} = \widehat{f}\,, \\ \varrho(\dot{K} - BK - H) = \widehat{M} - \widehat{A}\,, \qquad K = YB^T, \\ \varrho(\dot{H} + BH + HB^T) = \widehat{S} - \widehat{Z}\,. \end{gathered} \tag{53}$$

The sources per unit volume of momentum, moment of momentum and stir need be still specified. The choice is most difficult because those sources might not be necessarily of purely local character; at least weakly non-local effects may be expected. Thus a vast field of inquiry is opened, possibly, even necessarily, involving concepts recalled in Section 5; below reference is made only to very special choices advanced in important contexts. They all presume that the gross local shape and orientation be invariant: $B = 0$; Y, constant. This presumption implies the irrelevance of equation (52) and the dropping of the second equation in system (41), thus implying that $A = \varrho H$; besides, for $\widehat{f}$, the standard Cauchy form is postulated

$$\widehat{f} = \varrho b + \operatorname{div} \Sigma \,,$$

requiring a volume action b and a Cauchy stress Σ; finally, for Σ, the special constitutive relation $\Sigma = \varrho H$ is accepted. The choices of $\widehat{S}$ and $\widehat{Z}$ remain open and again an extended Cauchy type Ansatz is called upon with a volume stir and a shuffle flux expressed with the help of a hyperstress; for both stir and hyperstress appropriate constitutive relations are finally chosen.

All these special choices seem to be satisfactory within the particular contexts where they are advanced. But perhaps some general rules for $\widehat{f}$, $\widehat{M}$, $\widehat{A}$, $\widehat{S}$ and $\widehat{Z}$ should rather be sought and corresponding fairly general subchapters of continuum mechanics exhaustively written.

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