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► **To cite this version:**

H. Herrmann. On the thermodynamics of granular media. Journal de Physique II, 1993, 3 (4), pp.427-433. 10.1051/jp2:1993141 . jpa-00247843

HAL Id: jpa-00247843

<https://hal.science/jpa-00247843>

Submitted on 4 Feb 2008

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Classification
Physics Abstracts
05.70 — 46.10

Short Communication

On the thermodynamics of granular media

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(Received 8 February 1993, accepted 16 February 1993)

Abstract. — A thermodynamic formulation for moving granular material is proposed. The fluctuations due to the constant flux and dissipation of energy are controlled in a “granular” ensemble by a pressure φ (“compression”) which is conjugate to a contact volume (“contactopy”). The corresponding response function (“dissipativity”) describes how dissipation increases with φ and should serve to identify the fluidization transition and $1/f$ noise. In the granular ensemble one can consider the granular medium as a gas of elastically colliding particles and define a “granular” temperature and other standard thermodynamic quantities.

Granular materials, like sand or powders, subjected to an external force will locally perform rather statistical motion due to the random nature of the size and shape of grains and their contacts. One example is the motion of sand on a vibrating plate, say a loudspeaker [1-6]. At sufficiently high frequency the individual grains chaotically jump up and down forming a gas-like cloud of colliding particles. Other examples are displacements inside a shear-cell [7-11] or flow down an inclined chute [11-15] where in addition to a laminar flow with a well defined (average) velocity profile one has Brownian-like motion of the particles perpendicular to the flow direction.

The above observations have inspired several authors to use thermodynamical concepts to describe granular media. On one hand a “granular temperature” T_{gr} has been defined [7, 16, 17] as $T_{gr} = \langle v^2 \rangle - \langle \mathbf{v} \rangle^2$, i.e. proportional to the kinetic energy surplus with respect to the global motion. This temperature has been determined numerically as a function of various external parameters and material constants and under certain conditions consistency with experimental measurements was confirmed [7]. The drawback of the above definition is that it is only thermodynamically justified if an equipartition theorem exists which is not the case for granular particles since they dissipate energy at collisions.

Edwards and collaborators [18-20] have put forward an entirely different, original idea: based on the important observation that granular materials do not conserve energy while the entropy S is well defined they proposed to consider the volume V to replace the internal energy in the

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usual thermodynamic formalism. In this way a temperature-like quantity $X = \partial V / \partial S$ which they called “compactivity” can be defined. Although formally correct, this formalism is not easy to justify from first principles. In particular, in many real situations like on the vibrating table or on an inclined plane, the volume is not well limited at large heights. While Edwards’s approach seems intuitively correct for dense packings and the definition of T_{gr} reasonable in the limit of strong internal motions or weak dissipation they fail in the corresponding opposite limit.

Purpose of the present note is to propose a different thermodynamic approach to granular materials founded on similar principles as equilibrium thermodynamics and which should at least partially incorporate the intuitive pictures of previous work.

As opposed to usual thermodynamics of molecular gases the elementary units of granular materials are mesoscopic grains consisting of many atoms each ($10^{15} - 10^{25}$). When these object interact (collide) the Lennard-Jones potentials of the individual atoms are unimportant and completely different mechanisms must be considered. It is important that on a microscopic scale the surface of the grains is rough. Solid friction is the immediate consequence: when two touching grains are at rest with respect to each other a finite force F_s is needed to trigger relative motion (*static friction*), while moving against each other a finite force F_d is needed to maintain the motion (*dynamic friction*). $F_d < F_s$ and both only depend on the normal force and neither on the velocity nor on the area of contact (*Coulomb law*). No doubt, this picture is idealized and an entire discipline, called tribology, has evolved to study solid friction in depth [21]. For our purpose it is, however, more convenient to remain on the simple text-book level. The solid friction has the crucial consequence that on the level of the elementary units, namely the grains, the system does *not* conserve energy as opposed to molecular thermodynamics. Another source of dissipation can be plastic deformation of grains due to the normal force acting at collisions.

If energy is not constantly pumped into a granular system it will stop moving and fall into one of its static configurations. Constant motion of the grains can only be produced when there is a steady state of energy flux. We are, however, not interested in this flux itself also because it is difficult to measure experimentally. We just want to describe the motion of the granular particles in a similar way as one describes the motion of molecules in a gas at a given temperature. The presence of the energy flux and the fact that on the level of the grains on which we want to formulate a thermodynamics the energy is locally dissipated (i.e. not conserved) will, however, force us to introduce concepts beyond that of usual equilibrium thermodynamics.

We will assume typical conditions for local “equilibrium”: most experiments have velocity and density gradients [1-15] and in those cases only a subsystem spatially small compared to the gradient should be considered. An eventual energy flux into the system should distribute the energy over it homogeneously. This constraint can also reduce the size of the subsystem. Outside this subsystem a generalized “heat bath” is assumed. Spatial and temporal averages should be exchangeable (“ergodicity”). We will in fact in the following consider *temporal* averaging for practical (numerical) purposes. The averaging procedure can even be complicated [4, 6] by the existence of density waves.

It is important to notice that the dissipated energy is of course only lost on the mesoscopic level - microscopically this energy will be transformed essentially into heat and blown away by the surrounding air. This gives us a reasonable starting point for the formulation of an analogy to usual thermodynamics. It seems natural to consider energy conservation as the first “thermodynamical principle”:

$$\Delta I = \Delta E_{int} + \Delta D \quad (1)$$

The internal energy E_{int} is like in traditional thermodynamics the kinetic and potential energy of all the degrees of freedom of the grains as elastic bodies (translation, rotation, elasticity, etc.). ΔD is the energy dissipated in a given time and ΔI is the energy that was pumped into the system while ΔD was dissipated in order to maintain the steady state ⁽¹⁾. Usually ΔI is some kind of work (gravity on the inclined plane, $\frac{1}{2}A\omega^2$ on the loudspeaker, etc.). If one allows for changes in the volume of the system then equation (1) will become $\Delta I = \Delta E_{\text{int}} + \Delta D + \Delta W$ where ΔW is the work done to change the volume.

Let us give to the excess dissipated energy $\Delta \mathcal{D} = \Delta D - \Delta I$ in the following the nick-name “dissipate”. We will deal with \mathcal{D} in a similar way as one treats in usual thermodynamics the heat. Like the heat, the dissipate is not a potential since it depends on the process by which a given state is reached. It does, however, not stem from the kinetic energy of the particles as the heat in a molecular gas but is due to collisions, i.e. two particles coming together, touching and separating again.

The dissipated energy is proportional to the sum of normal forces f_n^i that push the particles together during collision i . One can therefore express changes in \mathcal{D} as

$$\delta \mathcal{D} = \wp \delta C \quad (2)$$

where \wp is an internal pressure acting at collisions that we shall call “compression” ⁽²⁾. It can be defined as $\wp = \rho \langle f_n^i / A_i \rangle$ where f_n^i is the normal force and A_i the area of contact of collision i and the average is performed over all collisions. ρ is the density of collisions, defined as the number of collisions per unit volume and unit time. It is easy to determine \wp numerically. When the particles do not have collisions the compression is zero and no energy is dissipated. The quantity C , which we will in the following call “contactopy”, in analogy to the entropy, has the dimension of a volume (contact volume). It is defined as the conjugate variable to the compression \wp .

The contactopy has contributions due to plasticity and due to dynamic and static friction. Let us in the following argue for a geometrical interpretation of C and consider first the two contributions from friction. The dynamic (or better kinetic) part of the contactopy is proportional to $\sum_i A_i \ell_i$ where ℓ_i is the distance over which two solid grains slip during collision i . Since ℓ_i is given by the collision time multiplied by the velocity of the particles this part is proportional to the particle overlap volume V_{ov} that one has (for technical reasons) in molecular dynamic simulations [4, 6, 10, 15, 22]. Apart from geometrical prefactors the proportionality constant is the dimensionless dynamic friction coefficient μ_d , i.e. a material constant of the grains. The overlap volume V_{ov} can be defined more precisely as the sterically excluded volume that would arise if the centers of mass of the particles follow the real trajectories but one does not take into account the elasto-plastic deformation. The static (or potential) contribution of friction to the contactopy C only comes into play when the elastic (potential) energy of two unlocking particles that were sticking is released. It depends on the penetration depth d_i at collision i because this determines the amount of material that will be compressed (or fragmented). Therefore this second contribution is proportional to $\sum_i A_i d_i$, i.e. also proportional to V_{ov} . The proportionality factor contains the static friction coefficient μ_s and the Young modulus Y of the grains. The other contribution to the potential part of the contactopy comes from plasticity and is proportional to the size of the plastic zone, i.e. again to V_{ov} , when the

⁽¹⁾ In contrast to traditional thermodynamics we have an energy flux and the dissipated energy itself increases with time. Therefore one can formulate equation (1) alternatively as $J_I = \dot{E}_{\text{int}} + \dot{D}$ where J_I is the energy flux into the system. Although in some cases this description gives a more intuitive physical picture we will prefer in the following to argue only in terms of changes ΔD and ΔI during a fixed time interval.

⁽²⁾ In real collisions also shear forces can contribute to dissipation so that \wp would then be a like a stress tensor. For that reason we explicitly did not call it pressure.

material dependent plastic yield force F_p is reached. The complex stick-slip mechanism [10, 23] that is triggered between two rigid grains by the interplay of static and dynamic friction makes it difficult to determine precisely the resulting material dependent constant $\gamma(\mu_d, \mu_s, F_p, Y)$ that following the simple arguments given above relates via

$$C = \frac{\gamma}{\rho'} V_{ov} \quad (3)$$

the contactopy to the (average) overlap volume V_{ov} . The division by the number ρ' of collisions per unit volume in equation (3) assures that C is an extensive quantity. The proportionality of equation (3) can be checked numerically by measuring independently the input of energy and the average internal pressure to get C and summing up the overlap volumina of the collisions to get V_{ov} .

The contactopy plays a central rôle here and in similarity to the approach of Edwards [18] can be interpreted as a volume. But although it resembles the internal energy in having a kinetic and a potential contribution it is analogous in our thermodynamic formalism to the entropy. Because of equation (3) the contactopy represents a geometric characterization of the system. This makes it likely to be a total differential dC , i.e. independent on how the system was driven into its state, while in contrast, the dissipate depends on the work done on the system. Numerically this could be checked by monitoring V_{ov} but the ultimate test should be experimental in analogy to Carnot's experiments.

The idea to define a potential for a dissipative system actually dates back to Lord Rayleigh [24] ("dissipation function") and has been worked out in detail by Prigogine and collaborators [25]. The contactopy is on one hand a concrete example for such a potential on the other hand it does not only contain the statistical aspects of an "internal entropy production" [25] but has for physical reasons the dimension of a volume. It would in fact be important to work out a statistical interpretation of C in the (space-time) phase space of the collision events in analogy to Boltzmann's statistical definition of the entropy in the space of all configurations of positions and velocities.

The "equilibrium" - which is in fact a steady state driven by the energy flux - can now be defined as the ensemble *minimizing* at fixed E_{int} the contactopy (instead of maximizing the entropy). One can *postulate* an analog to the second law of thermodynamics that any change of state at constant internal energy E_{int} should decrease the contactopy

$$\Delta C \leq 0 \quad (4)$$

Physically such a behaviour seems naturally be driven by the elastic repulsion between colliding (overlapping) grains and the tendency of the system to prefer many smaller collisions to a few strong ones. The third law of thermodynamics, namely that at zero compression there is no overlap between grains, i.e. vanishing contactopy, is less evident. Numerical tests of the above statements should be performed taking into account that as mentioned before they are valid in (sub)systems into which the energy flow allows for homogeneous dissipation.

As in usual thermodynamics one can now work in different ensembles. One can fix either the compression φ which we shall call the "granular ensemble" or the contactopy (let's call it "atomistic ensemble"). Since in practice (experimentally and numerically), however, the later case is difficult to implement we will in the following usually consider the granular ensemble. On top of this we can build up the traditional body of thermodynamics as if the grains were a gas of particles interacting elastically. We can fix or free the number N of particles, define a "granular" temperature T_g and entropy S or impose to the system either an external volume V or an external pressure p . A novelty for granular media is that one could also impose an external shear τ or its "conjugate", the dilatancy V_d [26].

A granular potential G_r can be defined as

$$G_r = E_{\text{int}} + \wp C \quad (5)$$

which depends on \wp and the extensive variables N, V, S and V_d . An immediate consequence of equation (4) is that at constant compression \wp the equilibrium is given by the minimum of G_r . The analog to the specific heat might be called “dissipativity” κ defined as

$$\kappa = \frac{\partial \mathcal{D}}{\partial \wp} = \wp \frac{\partial C}{\partial \wp} \quad (6)$$

This is a new quantity characterizing the granular medium which measures how much more energy can be dissipated if the compression is increased. It could be measured directly by numerically evaluating the derivative of equation (6) or through the fluctuations of the energy in a thermally closed system, i.e. surrounded by (infinitely) heavy and stiff walls. The dissipativity κ should be positive and go to zero for $\wp \rightarrow 0$ and $\wp \rightarrow \infty$. Interesting for practical purposes is that κ contains through the γ of equation (3) the material dependent properties concerning friction, among others also the stick-slip mechanism between grains. If a fluctuation-dissipation theorem for the response function κ is valid then one might identify $1/f$ noise [23, 27] from its frequency dependence over time scales proportional to the size of the grains or even over larger time scales when collective phenomena like arching or bridge-collapsing [8, 9] come into play.

We know that there exists a “fluidization transition” in granular media between a regime of block motion at low energy flow to a gas-like collisional regime at high energy flow [3, 4]. This transition could be driven by changing \wp : for small \wp the potential part of C dominates (block motion) and for large \wp the kinetic part of C is relevant (collisional motion). It seems likely that the transition point is given by a singularity of the dissipativity κ . This could be checked experimentally and numerically.

In the granular ensemble a “dissipate” bath (instead of a heat bath) is coupled to the system and consequently the internal energy E_{int} of the granular material is a fluctuating quantity. In order to give Boltzmann’s statistical interpretation to the entropy S it is therefore conceptually better to work in the atomistic ensemble: a “state” is given by the positions, orientations, linear and angular velocities of the grains as rigid bodies. In fact the entropy is well-defined as noted already in reference [18]. A reasonable definition for a “granular” temperature T_g would then be:

$$T_g = \left(\frac{\partial G_r}{\partial S} \right)_{\wp} \quad (7)$$

Note that it is similar but not identical to the granular temperature defined by previous authors [7, 16, 17]. T_g is the variable that controls the granular canonical ensemble with the granular free energy F_g as potential, defined as the Legendre transformation of the granular potential: $F_g = G_r - T_g S$. In equilibrium F_g should have a minimum. The usual Boltzmann distribution determines the statistical weights of the states in this ensemble. As in the case of the usual temperature one can measure T_g by monitoring the exchange of internal energy between a subsystem and its heat bath which should obey this Boltzmann distribution. Also a direct measurement of T_g by changing an external pressure (see eg. (17.1) of Ref. [28]) should be possible. A specific heat can be defined as a derivation with respect to T_g .

Experimentally \wp and T_g are independent control parameters of the system: since T_g increases with the kinetic energy of the particles it is essentially controlled by the amount ΔI of energy that is fed into the system per unit time. The compression \wp or better the quantity \wp/T_g also depends on the density of collisions and can therefore increase by fragmenting the grains into smaller pieces. (Note that when a given grain is split into eight pieces, the cross

section of each individual piece decreases by a factor four, so that φ will increase by two.) One can therefore, by changing the grain diameters and ΔI modify φ/T_g and T_g independently and can therefore consider phase diagrams in the $\varphi/T_g - T_g$ plane.

As already mentioned one can also go to other ensembles by changing variables via further Legendre transformations. One can liberate the number of grains and introduce a granular grandcanonical potential controlled by a chemical potential. One can also fix an external pressure and calculate the average volume. The fact that both volume and contactopy will then be conjugate to the pressure could explain why in granular media one finds in equilibrium macroscopic density fluctuations [29] as opposed to usual fluids or gases. Of practical interest is also to fix an external shear and measure the average expansion, i.e. the dilatancy [8, 9, 26].

It is useful to note that in the case when friction and plasticity vanish the system does not dissipate energy anymore, the contactopy will be zero and $G_r = E_{\text{int}}$. In that case the atomistic and granular ensembles are identical and classical thermodynamics is immediately recovered. Our formalism is therefore a genuine generalization of equilibrium thermodynamics.

We have described within a thermodynamic formalism the fluctuations arising from the constant flux and dissipation of energy that drives a granular material's kinematic behaviour. By separating the dissipative degree's of freedom (friction and plasticity) from the conservative ones (translation, rotation, elasticity) we define a "granular ensemble" coupled to a "dissipate bath" which is in fact the one in which experimental and numerical measurements are usually performed. We introduce a potential that we call "contactopy" and argue that it is proportional to the steric overlap volume of the collisions which the particles would have had per time unit if while following the real trajectories they had no elasto-plastic deformation. It would be interesting to give also a statistical interpretation to the contactopy in order to define it as a dissipative potential [25]. The fluctuating internal energy is replaced by a granular potential controlled by an intensive variable that we call "compression", which is conjugate to the contactopy. Going into a granular canonical ensemble we define a "granular temperature" similar to the one defined previously [16, 17]. We propose various numerical and experimental tests for the assumptions that we have made in our theory and suggest that a frequency dependent "dissipativity" should characterize the stick-slip behaviour of the material and the transition to fluidization.

Acknowledgement.

I thank R. Balian, J. Kertész, M. Kiessling, J. Lebowitz, C. Moukarzel, S. Roux, D. Stauffer, D. Wolf, R.K.P. Zia and in particular H.G. Herrmann for encouraging discussions.

References

- [1] Faraday M., *Philos. Trans. R. Soc. London* **52** (1831) 299;
Walker J., *Sci. Am.* **247** (1982) 167;
Dinkelacker F., Hübler A. and Lüscher E., *Biol. Cybern.* **56** (1987) 51.
- [2] Evesque P. and Rajchenbach J., *Phys. Rev. Lett.* **62** (1989) 44; *C. R. Acad. Sci. Ser. 2* **307** (1988) 1; **307** (1988) 223;
Laroche C., Douady S., Fauve S., *J. Phys. France* **50** (1989) 699;
Evesque P., *J. Phys. France* **51** (1990) 697;
Rajchenbach J., *Europhys. Lett.* **16** (1991) 149;
Clément E., Duran J. and Rajchenbach J., *Phys. Rev. Lett.* **69** (1992) 1189.
- [3] Clément E. and Rajchenbach J., *Europhys. Lett.* **16** (1991) 133.
- [4] Gallas J.A.C., Herrmann H.J and Sokolowski S., *Physica A* **189** (1992) 437.

- [5] Zik O. and Stavans J., *Europhys. Lett.* **16** (1991) 255;
Mehta A. and Barker G.C., *Phys. Rev. Lett.* **67** (1991) 394.
- [6] Gallas J.A.C., Herrmann H.J and Sokolowski S., *Phys. Rev. Lett.* **69** (1992) 1371;
Tagushi Y.-h., *Phys. Rev. Lett.* **69** (1992) 1367.
- [7] Campbell C.S. and Brennen C.E., *J. Fluid Mech.* **151** (1985) 167;
Campbell C.S., *Ann. Rev. Fluid Mech.* **22** (1990) 57;
Hanes D. M. and Inman D. L., *J. Fluid Mech.* **150** (1985) 357;
Walton O.R. and Braun R.L., *J. Rheol.* **30** (1986) 949.
- [8] Bashir Y.M. and Goddard J.D., *J. Rheol.* **35** (1991) 849.
- [9] Bagnold R. A., *Proc. Roy. Soc. London A* **295** (1966) 219.
- [10] Thompson P. A. and Grest G. S., *Phys. Rev. Lett.* **67** (1991) 1751.
- [11] Jaeger H.M., Liu C.-H., Nagel S.R. and Witten T.A., *Europhys. Lett.* **11** (1990) 619.
- [12] Drake T. G., *J. Geophys. Res.* **95** (1990) 8681.
- [13] Johnson P. C. and Jackson R., *J. Fluid Mech.* **150** (1985) 67.
- [14] Savage S. B., *J. Fluid Mech.* **92** (1979) 53;
Savage S.B. and Hutter K., *J. Fluid Mech.* **199** (1989) 177;
Savage S.B., *Disorder and Granular Media*, D. Bideau Ed. (North-Holland, Amsterdam, 1992).
- [15] Pöschel T., *J. Phys. II France* **3** (1993) 27.
- [16] Ogawa S., Proc. of US-Japan Symp. on Continuum Mechanics and Statistical Approaches to the Mechanics of Granular Media, S.C. Cowin and M. Satake Eds. (Gakujutsu Bunken Fukyu-kai, 1978) p.208.
- [17] Jenkins J.T. and Savage S.B., *J. Fluid Mech.* **130** (1983) 186;
Jaeger H.M., Lui C.-h. and Nagel S.R., *Phys. Rev. Lett.* **62** (1989) 40;
Jaeger H.M. and Nagel S.R., *Science* **255** (1992) 1523.
- [18] Edwards S.F. and Oakeshott R.B.S., *Physica A* **157** (1989) 1080.
- [19] Edwards S. F., *J. Stat. Phys.* **62** (1991) 889.
- [20] Mehta A. and Edwards S. F., *Physica A* **157** (1989) 1091.
- [21] Johnson K.L., *Contact Mechanics* (Cambridge Univ. Press, 1989).
- [22] Haff P.K. and Werner B.T., *Powder Techn.* **48** (1986) 239;
Cundall P.A. and Strack O.D.L., *Géotechnique* **29** (1979) 47.
- [23] Chen K., Bak P. and Obukhov S.P., *Phys. Rev. A* **43** (1991) 625;
Thompson P.A. and Robbins M.O., *Science* **250** (1990) 792;
Feder H.J.S. and Feder J., *Phys. Rev. Lett.* **66** (1991) 2669;
Carlson J.M. and Langer J.S., *Phys. Rev. Lett.* **62** (1989) 2632.
- [24] Lord Rayleigh, *Proc. Lond. Math Soc.* **4** (1873) 357.
- [25] Prigogine I., *Bull. Acad. Roy. Belg. Cl. Sci.* **31** (1954) 600;
Glansdorff P. and Prigogine I., *Thermodynamic Theory of Structure, Stability and Fluctuations* (Wiley Interscience, New York, 1971).
- [26] Reynolds O., *Philos. Mag. S.* **20** (1885) 469.
- [27] Lui C.-h. and Jaeger S.R., *Phys. Rev. Lett.* **68** (1992) 2301;
Baxter G.W., PhD thesis.
- [28] Landau L.D. and Lifschitz E.M., *Statistical Physics* (Akademie Verlag, Berlin, 1987).
- [29] Baxter G. W., Behringer R. P., Fagert T. and Johnson G. A., *Phys. Rev. Lett.* **62** (1989) 2825;
Pöschel T., preprint.