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# On entropy estimates of contact forces in static granular assemblies

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## Abstract

As an extension of previous work by others, this articles deals with maximum-entropy estimates for the statistics of static contact forces in assemblies of nearly rigid grains. As found in the previous works, the constraint of mean stress leads provisionally to a distribution of contact force that is exponential at large force. This behavior, found in various experiments and numerical simulations, does not depend on special models of force propagation postulated in the contemporary physics literature.

Following K. Bagi [Behringer, R. Jenkins, J.T. (Eds.), Powders and Grains, Balkema, 1997, p. 251] consideration is also given to entropy maximization under the constraint of constant mean strain, which leads to a similar exponential tail in the distribution of particle displacements.

In contrast to the previous works, it is emphasized that the exact form of the probability density depends on the statistical weight (a priori probability) assigned to elementary volumes in the state-space of contact forces or displacements. This leads to the conclusion that the large-force exponential is a general representation of maximum-entropy statistics arising from global constraints, whereas the state-space measure is dictated by local mechanics. A few examples of state-space measure are considered, and the resulting distributions are compared to previous experiment and simulation. A striking analogy is revealed between the force distribution in a static sphere assembly and the Maxwell–Boltzmann velocity distribution for gases.

Based on the methods of statistical thermodynamics, a virtual-thermodynamic formalism is presented for complementary strain energies in granular statics. This involves no direct appeal to the concept of (static) granular temperature favored in certain statistical-physics literature. As a possible test of the general validity of the entropy principle in granular statics, the question is raised as to whether it can describe the heterogeneous two-phase structure found in photoelastic experiments and numerical simulations of granular assemblies.


*Keywords:* Static granular force distributions; Maximum entropy; Virtual thermodynamics

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## 1. Background

A major challenge in granular mechanics is the development of a reliable connection between continuum-level phenomenological models and more fundamental micromechanical models. As with other random heterogeneous media, this is essentially a problem in statistical mechanics.

In the case of systems dominated by random thermal motion, statistical thermodynamics represents a useful limit of statistical mechanics, as well known for molecular systems in states of thermodynamic equilibrium (Hill, 1960). This accounts in part for the long-standing efforts to apply similar ideas, in particular, the maximum-entropy principle, not only to granular dynamics with large kinetic energy, but also to granular statics (Shahinpoor, 1980; Backman et al., 1983; Bagi, 1997; Rothenburg, 1980; Kruyt and Rothenburg, 2002; Troadec et al., 2002; Bagi, 2003; Kruyt, 2003). Such efforts are problematic in several respects.

As a first difficulty, there is no physically obvious counterpart to temperature and the associated stochastic exploration of phase space. However, as recognized in most of the works cited above, the probabilistic interpretation of entropy still stands, e.g. as an information-theoretic Shannon entropy (Shannon and Weaver, 1964; Sloane and Wyner, 1993). The associated maximum-entropy principle then represents a maximum-likelihood estimate for the statistics of systems with prescribed macroscopic averages as global constraints.

Within the information-theoretic interpretation, the concept of temperature no longer is strictly necessary, not withstanding the intense search for a replacement in certain statistical-physics literature (see Blumenfeld and Edwards, 2003, and references therein). Unfortunately, in static random systems, subject to arbitrary methods of preparation, there is no compelling physical principle that would elevate information-theoretic entropy and various surrogate temperatures to the status enjoyed in classical thermodynamics.

With the above reservations as to its general validity, the intent of this brief article is to set down certain qualifications and ramifications of the entropy principle, after a brief review of recent literature overlooked in a related article (Goddard, 2002).

To begin with, we note that Bagi (1997), citing the ideas of Rothenburg (1980), derives maximum-entropy estimates for the statistics of particle displacements as well contact forces. For the latter, she finds the large-force exponential behavior observed in numerous experiments and numerical simulations (Liu et al., 1995; Mueth et al., 1998; Radjai et al., 1996, 1998, 1999; O'Hern et al., 2001; Erikson et al., 2002).

The findings of Bagi and the subsequent simulations of O'Hern et al. (2001) on "jammed" frictionless spheres, indicate that the exponential force distribution may be viewed as a robust statistical feature of static granular packings, independent of the precise details of force transmission. It follows that this exponential behavior cannot then be viewed as a confirmation of various load-diffusion models proposed in the soil-mechanics and physics literature (Harr, 1977; Coppersmith et al., 1997; Socolar, 1998; Snoeijer and van Leeuwen, 2002).

This view is further supported by the theoretical work of Kruyt and Rothenburg (2002) on contact forces in frictional granular assemblies, whose maximum-entropy estimate includes the Coulomb condition ($\mu f_n \geqslant |f_t|$) on particle contacts but still exhibits the large-force exponential. As shown below, such local mechanical constraints can be expressed as restrictions on state-space measure, without eliminating the exponential distribution of large forces.

In other recent work, Troadec et al. (2002) and Troadec (2003) apply the principle of maximum (Shannon) entropy to steric arrangement and local kinematics of particle clusters. As in the above works, there is an implicit assumption as to state-space measure with certain implications for local mechanics, a matter addressed in the following discussion.

## 2. Thermodynamic framework and elastic particle assemblies

We adopt the formalism of statistical thermodynamics (Hill, 1960) for mechanical systems having a large number of degrees of freedom. Following Goddard (2002), we let $\mathbf{z} \in \Omega$ denote a representative point in the relevant state (or phase) space $\Omega$, endowed with probability measure $P(\mathbf{z})\,\mathrm{d}\Omega(\mathbf{z})$, where $\mathrm{d}\Omega(\mathbf{z})$ is an elemental state-space measure which remains to be specified. While $P(\mathbf{z})$ may depend on time, we restrict attention here to spatially homogeneous systems, such that $P(\mathbf{z})$ and $\mathrm{d}\Omega(\mathbf{z})$ are independent of spatial position. The statistical average (expectation) of an arbitrary mechanical variable $A(\mathbf{z})$ is then given by

$$\langle A \rangle = \int_{\Omega} A(\mathbf{z}) P(\mathbf{z})\,\mathrm{d}\Omega(\mathbf{z}), \tag{1}$$

The standard statistical-thermodynamical estimate for the unknown probability distribution $P(\mathbf{z})$ is based on maximization of the entropy functional:

$$S[P] = -\langle \log P \rangle = -\int_{\Omega} P(\mathbf{z}) \log P(\mathbf{z})\,\mathrm{d}\Omega(\mathbf{z}) \tag{2}$$

subject to a discrete set of constraints of the form $\langle A(z) \rangle = \mathrm{const.}$ (Troadec et al., 2002; Troadec, 2003, admit a more general functional constraint on $P(\mathbf{z})$.)

Since the celebrated Boltzmann distribution $P(\mathbf{z}) \propto \exp\{-\beta E(\mathbf{z})\}$ arises from the constraint on internal energy $\langle E(\mathbf{z}) \rangle = \mathrm{const.}$ (Gibbs, 1902; Hill, 1960), one might expect it to apply to assemblies of elastic particles subject to constant elastic strain energy (Nguyen and Coppersmith, 1999; O'Hern et al., 2001; Goddard, 2002). For example, in static assemblies of nearly rigid, non-cohesive frictionless elastic spheres, having elastic contact energy given by normal compressive contact force $f \geqslant 0$ with $E \propto f^{\nu}$, the Boltzmann distribution takes on the form

$$P(f) = Z^{-1} \exp(-\beta f^{\nu}), \quad \text{where } Z = \int_{f=0}^{\infty} \exp(-\beta f^{\nu})\,\mathrm{d}\Omega(f), \tag{3}$$

where $\beta$ is a constant derivable from the mean elastic energy (*vide infra*). However, the actual probability density in $f$, say, $\rho(f)$, with

$$\rho(f)\,\mathrm{d}f = P(f)\,\mathrm{d}\Omega(f), \tag{4}$$

obviously depends on the measure $\mathrm{d}\Omega(f)$, that is on the *a priori* statistical weight assigned to the interval $\mathrm{d}f$ in the state-space of contact forces. For later purposes, we note that (4) is a special case of the general relation

$$\begin{aligned} &P(\mathbf{z})\,\mathrm{d}\Omega(\mathbf{z}) = \rho(\mathbf{z})\,\mathrm{d}V(\mathbf{z}) \quad \text{with } \mathrm{d}V(\mathbf{z}) := \mathrm{d}z_1 \mathrm{d}z_2, \ldots, \mathrm{d}z_n, \\ &\mathrm{d}\Omega(\mathbf{z}) = J(\mathbf{z})\,\mathrm{d}V(\mathbf{z}) \quad \text{and} \quad \rho(\mathbf{z}) = J(\mathbf{z}) P(\mathbf{z}), \end{aligned} \tag{5}$$

where the $\mathrm{d}z_k$ represent individual scalar components of $\mathbf{z}$. The importance of the a priori weight in state space, a paramount issue in statistical thermodynamics, has also been recognized in the theory of information (Shannon and Weaver, 1964, pp. 90–91).

For example, consider a Hamiltonian dynamical system with $\mathbf{z}$ representing generalized canonical coordinates and momenta $\{q_k, p_k\}$.The measure $\mathrm{d}\Omega$ in (2) is then chosen to be:

$$\mathrm{d}\Omega(\mathbf{z}) \propto \mathrm{d}V := \prod_k \mathrm{d}q_k \mathrm{d}p_k, \tag{6}$$

reflecting the assignment of equal a priori probability to dynamically invariant volume elements in phase space (Gibbs, 1902; Hill, 1960).

Static assemblies of elastic particles, e.g. nearly rigid, particles with localized contact elasticity, may be considered as a degenerate Hamiltonian systems with $p_k \equiv 0$, representing the zero-temperature limit of O'Hern et al. (2001). However, the use of particle positions as canonical variables would require a consideration of local mechanics involving both force and displacement. To avoid this, the present author (Goddard, 2002) has argued that, since local elastic energy is conserved in any admissible quasi-static rearrangement of elastic particles, it is appropriate to identify the state-space measure with elastic energy $E$, implying that

$$\mathrm{d}\Omega \propto \mathrm{d}E \propto f^{\nu-1}\,\mathrm{d}f, \tag{7}$$

for the power-law form considered above. For later reference, we note the values corresponding to various contact models (cf. O'Hern et al., 2001; Goddard, 2002, after typographical correction):

$$\nu = \begin{cases} 2, & \text{Hookean}, \\ 5/3, & \text{Hertzian}, \\ 3/2, & \text{empirical}, \end{cases} \tag{8}$$

where the empirical value is that inferred from the pressure dependence of elastic stiffness (Goddard, 1990), a dependence that may actually involve strain-induced variation in contact density.

Note that linear-elastic contacts give rise to a Gaussian distribution for $\rho(f)$ in (3). However, despite its relevance to harmonic (i.e. Hookean) lattices, a Gaussian having *zero mean* has not turned up in detailed numerical simulations based of nearly rigid non-cohesive particles (O'Hern et al., 2001). We recall that the Gaussian distribution found in the simulations of Makse et al. (2000):

$$\rho(f) \propto \exp\{-k^2(f - \langle f \rangle)^2\}, \tag{9}$$

also discussed by Kruyt and Rothenburg (2002) and in prior works cited by them, arises in the limit of large confining stress and involves force fluctuations about a large mean force $\langle f \rangle \approx k^{-1}$ that (while not precisely defined in Makse et al., 2000) presumably represents an effective Hookean stiffness. Although it is not clear that the Hertz–Mindlin contact law assumed by Makse et al. (2000) remains valid in this limit, one still might generally expect to obtain their incremental Hookean response at large force (Goddard, 1990), with Gaussian fluctuations arising solely from geometric disorder.

While instructive, the above elastic-energy model is inappropriate in several respects. Experiments and computer simulations are rarely if ever done under conditions of constant elastic strain energy. Moreover, the model is not strictly applicable to the interesting limit of rigid frictional particles. These considerations serve to motivate the past treatments of constant imposed stress or strain, treatments which are summarized and extended in the following discussion.

## 3. Constant stress and virtual thermodynamics

With the standard expression for (Cauchy) stress (Bagi, 1997; Kruyt and Rothenburg, 2002; Goddard, 2002)

$$\mathbf{T} = n_c\langle \mathbf{M}(\mathbf{f},\mathbf{l})\rangle \quad \text{with } \mathbf{M}(\mathbf{f},\mathbf{l}) := -\mathbf{f}\otimes\mathbf{l}, \tag{10}$$

where $n_c$ denotes contact number density, $\mathbf{f}$ the vectorial contact force, $\mathbf{l}$ the branch vector connecting centroids of adjacent grains, and $\mathbf{M}$ the associated force dipole. (The sign on $\mathbf{M}$ has been chosen to represent a compressive state of stress when $\mathbf{f}$ is parallel to $\mathbf{l}$.) The state space is now defined by $\mathbf{z} = \mathbf{f} \oplus \mathbf{l}$, and the minimization (2) of subject to stationarity of (10) yields the canonical distribution

$$P(\mathbf{f},\mathbf{l}) = Z^{-1}\exp\{\mathbf{\Lambda} : \mathbf{M}\} = Z^{-1}\exp\{-\mathbf{f}\cdot\mathbf{\Lambda}\cdot\mathbf{l}\}, \tag{11}$$

where the colon denotes contraction of a tensor product and $Z$ the *partition function*,

$$Z(\mathbf{\Lambda}) = \int_{\Omega} \exp\{-\mathbf{f} \cdot \mathbf{\Lambda} \cdot \mathbf{l}\} \mathrm{d}\Omega(\mathbf{f}, \mathbf{l}), \tag{12}$$

a function of the Lagrange multiplier (tensor) $\mathbf{\Lambda} = (\lambda_{ij})$.

To consolidate and extend existing works on the subject, we pursue the standard thermodynamic formalism (Hill, 1960), according to which all macroscopic properties are derivable from $Z$, most notably,

$$\mathbf{T} = \partial_{\mathbf{\Lambda}} \psi \quad \text{with } \psi(\mathbf{\Lambda}) = -n_c \log Z, \tag{13}$$

with $\psi$ and $\mathbf{\Lambda}$ assuming the respective roles of free energy and (infinitesimal) displacement gradient.

A scaling of $\mathbf{\Lambda}$ by some parameter having dimensions of energy obviously is required for the dimensional consistency of (13), but we see no compelling reason to elevate it to the role of temperature in classical thermodynamics. At any rate, we treat it as constant for the present purposes.

The extension of (13) to finite strain could in principle be accomplished by employing the Piola–Kirchhoff stress and the deformation gradient, respectively, in lieu of the Cauchy stress and the displacement gradient. However, this would require a description of the joint statistics of force and displacement, which will not be pursued here.

The relation (13) represents a "virtual" thermodynamics, which involves no explicit reference to temperature. In the limit of perfectly rigid particles the energy $\psi$ must be regarded as purely extrinsic in origin, arising from work done by the surroundings in the course of particle rearrangement. Moreover, for frictional sphere assemblies, the real (as opposed to virtual) thermodynamic validity of (13) appears to hinge on the possibility of an elastic–plastic decomposition of the type employed in well-known incremental plasticity theories, a matter which will be address further below.

With the restriction to infinitesimal strain adopted in recent works on the subject (Bagi, 1997; Kruyt and Rothenburg, 2002; Goddard, 2002; Kruyt, 2003), the statistics of the branch vector $\mathbf{l}$ can be considered known and given by an appropriate distribution $P_1(\mathbf{l})$, such that

$$P(\mathbf{f}, \mathbf{l}) = P_2(\mathbf{f}|\mathbf{l}) P_1(\mathbf{l}) \quad \text{with } \mathrm{d}\Omega(\mathbf{f}, \mathbf{l}) = \mathrm{d}\Omega_2(\mathbf{f}, \mathbf{l})\, \mathrm{d}\Omega_1(\mathbf{l}), \tag{14}$$

where $P_2$ represents conditional probability. As pointed out by Kruyt and Rothenburg (2002), the entropy principle now applies to $P_2$, and they give a detailed analysis of 2-d disks with contacts subject to the Coulomb condition. In a form also applicable to spheres, it can be written as

$$g(\mathbf{f}, \mathbf{l}) := |\mathbf{f}_t| - \mu f_n \leqslant 0, \quad \text{where } f_n = \mathbf{f} \cdot \mathbf{n},\ \ \mathbf{f}_t = \mathbf{f} - f_n \mathbf{n},\ \ \mathbf{n} = \mathbf{l}/|\mathbf{l}|, \tag{15}$$

where $\mu$ denotes the Coulomb coefficient.

We note that the unilateral constraint (15) represents a boundary in state space and that any number of such boundaries $g_k \leqslant 0$ can be expressed as the formal restriction on $\mathrm{d}\Omega$:

$$\mathrm{d}\Omega(\mathbf{f}, \mathbf{l}) = \mathrm{d}\Omega'(\mathbf{f}, \mathbf{l}) \prod_k H(-g_k), \tag{16}$$

where $\mathrm{d}\Omega'(\mathbf{f}, \mathbf{l})$ is free of boundary constraints, and where the product of Heaviside functions $H$ represents an indicator-function for the admissible region of state space. Thus, the mechanical constraints leading to such boundaries can be incorporated directly into the state-space measure.

To illustrate the salient points, we review certain results for isotropic monodisperse assemblies of frictionless spheres, given in a slightly different notation by Goddard (2002).

### 3.1. Frictionless sphere assemblies

For frictionless non-cohesive spheres, $\mathbf{f} = f_n\mathbf{n}$, with $f_n \geqslant 0$, where $\mathbf{n}$ is the unit branch vector of (15), and for monodisperse spheres of diameter $\sigma$, the distribution $P_1$ of (14) is given by

$$P_1(\mathbf{l}) = \frac{1}{4\pi\sigma^2}\delta(l-\sigma) \quad \text{with } \mathrm{d}\Omega_1(\mathbf{l}) = l^2\,\mathrm{d}l\,\mathrm{d}\Omega_0(\mathbf{n}), \;\; \mathrm{d}\Omega_0(\mathbf{n}) \equiv \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi, \tag{17}$$

with $\theta, \phi$ representing polar coordinates on the unit sphere and $\delta$ the Dirac delta. Hence, (11) reduces to the distribution for $f = f_n$, which we denote simply by $P$:

$$P(f) = Z^{-1}\int_{\Omega_0} \exp\{-\beta(\mathbf{n})f\}\,\mathrm{d}\Omega_0(\mathbf{n}), \tag{18}$$

with

$$Z(\mathbf{\Lambda}) = \int_0^\infty \int_{\Omega_0} \exp\{-\beta(\mathbf{n})f\}\,\mathrm{d}\Omega_0(\mathbf{n})\,\mathrm{d}\Omega(f), \tag{19}$$

where $\Omega_0$ denotes the surface of the unit sphere, and

$$\beta(\mathbf{n}) = \beta(\mathbf{n}, \mathbf{\Lambda}) = \sigma\,\mathbf{n}\cdot\mathbf{\Lambda}\cdot\mathbf{n}, \tag{20}$$

which involves only the symmetric part of $\mathbf{\Lambda}$, whose skew-symmetric part may now be ignored. Since $Z$ is an isotropic function of $\mathbf{\Lambda}$ (Goddard, 2002), so are $\psi$ and the stress $\mathbf{T}$ in (13).

For the power-law form (7), one obtains

$$Z \propto \int_{\Omega_0} \beta^{-\nu}(\mathbf{n})\,\mathrm{d}\Omega_0(\mathbf{n}). \tag{21}$$

As pointed out by Goddard (2002), it appears possible to obtain analytic expressions for $Z(\mathbf{\Lambda})$ in terms of the isotropic invariants of $\mathbf{\Lambda}$ for certain special values of $\nu$ or special symmetries of $\mathbf{\Lambda}$, the latter of which must be identical with those of $\mathbf{T}$. In particular, the symmetry of stress $\mathbf{T} = \mathbf{T}^{\mathrm{T}}$ and $\mathbf{\Lambda}$, allows one to reduce (20) to the simple form

$$\beta(\mathbf{n}) = \sigma\{(\lambda_1\cos^2\phi + \lambda_2\sin^2\phi)\sin^2\theta + \lambda_3\cos^2\theta\}, \tag{22}$$

where the polar angles $\theta, \phi$ are referred to orthogonal principal axes of $\mathbf{\Lambda}$, with eigenvalues denoted by $\lambda_i$.

In the case of isotropic confinement, all the $\lambda_i$ are equal and (18) reduces to (Goddard, 2002):

$$P(f) = Z^{-1}\exp\{-\beta f\}, \tag{23}$$

with

$$Z = \int_0^\infty \exp\{-\beta f\}\,\mathrm{d}\Omega(f), \tag{24}$$

from which $\beta$ is given by the confining pressure or mean force as

$$\langle f\rangle = \beta^{-1}\int_0^\infty \mathrm{e}^{-s}s\,\mathrm{d}\Omega(s\beta^{-1}) \Big/ \int_0^\infty \mathrm{e}^{-s}\,\mathrm{d}\Omega(s\beta^{-1}), \tag{25}$$

once $\mathrm{d}\Omega(f)$ is specified.

With the power-law $\mathrm{d}\Omega(f) \propto f^{\nu-1}\,\mathrm{d}f$, one readily finds that (Goddard, 2002) $\beta = \nu\langle f\rangle^{-1}$ and, hence, that (23) reduces to the gamma distribution in $F$:

$$\rho(F) = \nu \frac{(\nu F)^{\nu-1}}{\Gamma(\nu)} e^{-\nu F}, \quad \text{where } F = \frac{f}{\langle f \rangle}, \tag{26}$$

which is identical with a (mean-field) approximate solution for a special model of force propagation (Liu et al., 1995; Antony, 2001) referred to above in the introduction. We recall that the maximum-entropy estimate with $\nu = 1$ was employed by Backman et al. (1983) to derive mean elastic wave speeds based on the Hertzian contact model in (8), a procedure which can only provide an *a posteriori* accounting for contact elasticity.

Fig. 1 (from Goddard, 2002) presents a comparison of (26) with $\nu = 3/2$ to the empiricism

$$\rho(F) = \alpha(1 - \beta e^{-F^2}) \exp\{-\nu F\} \quad \text{with } F = f/\langle f \rangle, \tag{27}$$

employed by Mueth et al. (1998), with $\beta = 0.75, \nu = 1.5$, and by Radjai et al. (1998), with $\beta = 0.6, \nu = 1.35$, to fit their respective experiments and numerical simulations of sphere assemblies. The parameter $\alpha$ follows in principle from normalization of $\rho$.

Not shown is a related empiricism proposed by Antony (2001) nor the version of (27) employed by Silbert et al. (2002), with $\beta = 0.78$, $\nu = 1.55$ (and $\alpha = 3.1$, approximately equal to the value 3.32 required by normalization), to represent their numerical simulations for frictional-elastic sphere assemblies. Silbert et al. (2002) also consider a curve-fit based on the value $\nu = 1.35$ of Radjai et al. (1998), with discrepancies at large force like those in Fig. 1.

As regards the various curves in Fig. 1, we recall that the simulations of Radjai et al. (1998) are for 2D rigid discs, while those of Silbert et al. (2002) involve spheres, with either Hookean or Hertzian contact, corresponding to the two exponents $\nu \neq 1.5$ given above in (8). The relative insensitivity of all these results to the assumed form of elastic contact implies that the parameter $\nu$ governing the exponential tail cannot be attributed to contact elasticity as suggested by Goddard (2002).

Furthermore, as pointed out by Goddard (2002), no distribution of the form (26) with $\nu > 1$ can capture the behavior near $f = 0$ shown in Fig. 1, which reflects a substantial population of "dead" contacts with zero force. While one could choose $d\Omega(f)$ empirically to represent the state of affairs near $f = 0$, there is no obvious theoretical rationale for doing so. From a thermodynamic perspective, the situation recalls the classical "ultraviolet catastrophe" (i.e. the breakdown of Boltzmann statistics for blackbody radiation near

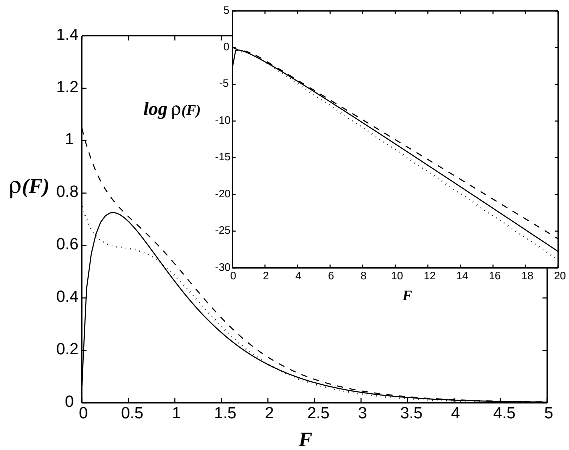


Fig. 1. Comparison of contact force distributions: (a) Dotted curve ···, empirical fit of experiments on spheres (Mueth et al., 1998), (b) dashed curve ----, numerical simulations on disks (Radjai et al., 1998), (c) solid curve –, Eq. (26) with $\nu = 3/2$. The inset semi-log plot shows the exponential tails.

zero wavelength. Tegmark and Wheeler (2001), provide an engaging contemporary perspective, and Hill, 1960, p. 463 ff., treats the alternative Bose–Einstein statistics underlying Planck's celebrated empirical resolution of the problem.)

To close here, we consider a somewhat more compelling thermodynamic analogy to the kinetic theory of gases, already alluded to by Kruyt and Rothenburg (2002, p. 4). To be more specific, note that the stress in an ideal gas is obtained from (10) by means of the correspondence:

$$\mathbf{l} \to m\mathbf{n}, \;\; \mathbf{f} \to v^2\mathbf{n} \quad \text{with } \mathbf{f}\otimes\mathbf{l} \to m\mathbf{v}\otimes\mathbf{v}, \tag{28}$$

where $m$ denotes mass, $\mathbf{v}$ velocity and $v = |\mathbf{v}|$ speed, of gaseous molecules. The Maxwell–Boltzmann distribution then arises from maximization of entropy subject to constant isotropic stress (pressure), with

$$\mathrm{d}\Omega \propto \mathrm{d}p_x\,\mathrm{d}p_y\,\mathrm{d}p_z \propto v^2\,\mathrm{d}v \propto E^{1/2}\,\mathrm{d}E, \tag{29}$$

and can be written in the alternative forms for density in velocity or energy:

$$\rho_v \propto \exp\{-\beta v^2\}v^2 \quad \text{or} \quad \rho_E \propto \exp\left\{-\frac{\beta E}{2m}\right\}E^{1/2}, \tag{30}$$

with the respective exponents $v = 3$ and 3/2. This analogy not only is valid for isotropic confinement but also carries over to the constraint of anisotropic (shear) stress, where it leads to anisotropic Maxwellian velocities for rapid granular flow (Jenkins and Richman, 1988; Chou and Richman, 1998) or for non-equilibrium flow of molecules and plasmas.

### *3.2. Kinematic constraint, complementary energy and uniqueness*

In the work cited above, Bagi (1997) also provides an entropy estimate for the statistics of particle displacements subject to a global constraint on displacement gradient. In the present notation, the latter is given

$$\mathbf{L} = n_c\langle\mathbf{u}\otimes\mathbf{a}\rangle,$$

where $\mathbf{u}$ denotes relative displacement between neighboring particle centroids and $\mathbf{a}$ the local area vector associated with Delaunay–Voronoi tessellation of the granular medium (Bagi, 1997). The preceding analysis carries over directly, by means of the correspondence:

$$\mathbf{f} \to -\mathbf{u}, \quad \mathbf{l} \to \mathbf{a}, \quad \mathbf{T} \to \mathbf{L},$$

leading to a canonical distribution analogous to (11). The Lagrange multiplier $\mathbf{\Lambda}$ now plays the role of stress $\mathbf{T}$ in the relations:

$$\mathbf{L} = \partial_{\mathbf{\Lambda}}\varphi, \;\; \varphi = -n_c\log Z \quad \text{with } Z = \int_\Omega \exp\{-\mathbf{u}\cdot\mathbf{\Lambda}\cdot\mathbf{a}\}\,\mathrm{d}\Omega(\mathbf{u},\mathbf{a}), \tag{31}$$

where $\varphi$ represents a complementary strain energy and where, as in (13), scaling is required by a parameter having dimensions of energy.

We note that the decomposition of relative displacement into elastic and dissipative (plastic) contributions

$$\mathbf{u} = \mathbf{u}^{\mathrm{E}} + \mathbf{u}^{\mathrm{P}} \tag{32}$$

leads directly to a similar decomposition of velocity gradient $\mathbf{L}$. Furthermore, it is an easy matter to show that the factorization of state-space measure

$$\mathrm{d}\Omega(\mathbf{u},\mathbf{a}) = \mathrm{d}\Omega^{\mathrm{P}}(\mathbf{u}^{\mathrm{P}},\mathbf{a})\,\mathrm{d}\Omega^{\mathrm{E}}(\mathbf{u}^{\mathrm{E}},\mathbf{a}), \tag{33}$$

leads to the decomposition

$$\phi(\mathbf{T}) = \phi^{\mathrm{E}}(\mathbf{T}) + \phi^{\mathrm{P}}(\mathbf{T}) \tag{34}$$

and, hence, to

$$\mathbf{L}^m = \partial_{\mathbf{T}}\phi^m \quad \text{for } m = \mathrm{E}, \mathrm{P} \tag{35}$$

Thus, the statistical independence required by (33) provides a sufficient condition for the existence of distinct elastic and dissipative potentials, of the type assumed in certain phenomenological treatments of plasticity and viscoelasticity (Collins and Houlsby, 1997; Grmela, 2003). A similar decomposition of the contact force **f** leads, via a factorization of the form (33), to a decomposition of the complementary energy $\psi$ like that of (34) and (35). Thus, the validity of relations like (33), which embody assumptions about particle-level statistical mechanics, appears worthy of further investigation.

A fully rigorous pursuit of the virtual-thermodynamic formalism would require that the measures $\mathrm{d}\Omega(\mathbf{f}, \mathbf{l})$ and $\mathrm{d}\Omega(\mathbf{u}, \mathbf{a})$ be chosen to satisfy the Legendre relation:

$$\psi(\mathbf{L}) + \varphi(\mathbf{T}) = \mathbf{T} : \mathbf{L} \tag{36}$$

In the same spirit, we should regard the eventual non-convexity of $\psi$ or $\varphi$, and the consequent non-unique relation between stress and kinematics, as tantamount to thermodynamic phase transition. We recall that an associated lack of uniqueness would allow for the possibility of the well-known strain localization or for its less familiar counterpart, stress localization (Goddard, 2002). The latter might provide a phenomenological mesoscale description of the ubiquitous force chains and the associated "two-phase" structure found in photoelastic experiments (Drescher and De-Josselin-de Jong, 1972) and computer simulations (Radjai et al., 1998).

## 4. Discussion

Previous studies suggest that the maximum-entropy principle provides a useful method for analyzing the statistical mechanics of static granular assemblies. The prior analyses of Bagi (1997), Kruyt and Rothenburg (2002) and Kruyt (2003) show that the ubiquitous exponential distribution of the largest contact forces arises as a statistical phenomena, largely independent of particle-scale mechanics. Hence, this feature does not represent a very stringent test of various force-propagation models proposed in the recent physics literature.

A previous paper (Goddard, 2002) and the present more detailed analysis emphasize the fact that the entropy principle depends on the state-space measure, whose exact form generally depends on certain details of the local mechanics. A theoretical picture thus emerges, in which some aspects of the statistical mechanics are dictated by externally imposed constraints, while others depend more on local mechanics, as reflected in a priori weights assigned to various regions in state space.

Although the information-theoretic interpretation of entropy is doubtless the most general, the formalism of statistical thermodynamics provides an attractive framework in which to discuss energetics. It remains. however, to be shown that the strain-energy functions arising from this "virtual thermodynamics" provide a physically tenable description of quasi-static granular mechanics. If so, it remains further to ascertain whether it can guide our understanding of phenomena such as dead contacts and force-chains in granular assemblies.

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