The classical granular temperature 
and slightly beyond

D. Serero\textsuperscript{a}, C. Goldenberg\textsuperscript{b}, S. H. Noskowicz\textsuperscript{a}, I. Goldhirsch\textsuperscript{a}

\textsuperscript{a}Department of Fluid Mechanics and Heat Transfer, Faculty of Engineering, 
Tel Aviv University, Ramat-Aviv, Tel Aviv 69978, Israel.

\textsuperscript{b}Laboratoire de Physique et Mécanique des Milieux Hétérogènes (CNRS UMR 7636), ESPCI, 10 rue Vauquelin, 75231 Paris Cedex 05, France.

Abstract

One goal of this paper is to discuss the classical definition of granular temperature as an extension of its thermodynamic equivalent and a useful concept which provides an important characterization of fluidized granular matter. Following a review of some basic concepts and techniques (with emphasis on fundamental issues) we present new results for a system that can exhibit strong violations of equipartition, yet is amenable to description by classical granular hydrodynamics, namely a binary granular gas mixture. A second goal of this article is to present a result that pertains to dense granular and molecular solids alike, namely the existence of a correction to the elastic energy which is related to the heat flux in the equations of continuum mechanics. The latter is of the same (second) order in the strain as the elastic energy. Although recent definitions of temperatures for granular matter, glasses and other disordered many-body systems are not within the scope of this article we do make several general comments on this subject in the closing section.

Key words: Temperature, granular matter, elasticity, kinetic theory

PACS: 05.20.Dd, 47.45.Ab, 45.70.Mg, 83.80.Fg, 62.20.Dc

Email addresses: serero@eng.tau.ac.il (D. Serero), chayg@pmmh.espci.fr (C. Goldenberg), henri@eng.tau.ac.il (S. H. Noskowicz), isaac@eng.tau.ac.il (I. Goldhirsch).

\textsuperscript{1} I. G. gratefully acknowledges support from the Israel Science Foundation (ISF), grant. no. 689/04, the German Israel Science Foundation (GIF), grant no. 795/2003 and the US-Israel Binational Science Foundation (BSF), grant no. 2004391. CG gratefully acknowledge support from a European Community FP6 Marie Curie Action (MEIF-CT2006-024970).
1 Introduction

The axiomatic formulation of thermodynamics provides a precise definition of temperature. Nearly any textbook on thermodynamics shows this definition to be compatible with common experience. Equilibrium statistical mechanics endows temperature with a microscopic meaning but invokes a few assumptions (e.g., ergodicity). The physical relevance and usefulness of both of these theories is beyond debate.

As there are practically no equilibrium systems in nature there is clearly a need to describe non-equilibrium systems. The most successful theories that treat such systems are those devoted to near-equilibrium states, namely states in which the macroscopic fields vary sufficiently slowly in space and time so that (near) local equilibrium distributions can establish themselves everywhere while the state of the system hardly changes. That this should occur is not entirely obvious. It helps to note that e.g., in gases local equilibration occurs within a few collisions per particle, i.e. on time scales that are much smaller than macroscopic times. In other words, these approaches are effective when there is significant scale separation between the spatial and temporal micro- and-macroscales. In the latter case one can justify hydrodynamics, elasticity and other macroscopic theories, and the transport coefficients are given by Green-Kubo expressions derived using linear (and non-linear) response theories (1) or projection operator approaches (2; 3), a similar statement holding for fluctuation dissipation ‘theorems’ e.g., for Brownian motion (4).

The macroscopic fields that represent the states of systems that possess scale separation are usually taken to be the densities of the conserved entities, namely the (mass or number) density, the momentum density and the energy density. These fields are “slow” since any change in their local values necessitates motion to (non-locally) transport an amount of the entity represented by the field. It is usually assumed that on macroscopic time scales the system ‘remembers’ only the slow fields, the other degrees of freedom rapidly accommodating themselves to those fields and becoming “noise” whose statistics is determined by the slow fields. The description of far-from-equilibrium systems, such as turbulent fluids and glasses, is not as intuitively founded as that of near-equilibrium systems; in particular, since many of these systems lack scale separation it is a-priori unclear which fields are sufficient to provide a closed description for them (nor is the nature of a relevant statistical ensemble for the unresolved degrees of freedom obvious).

The BBGKY hierarchy (see e.g., (5)) is an exact formulation for many-body systems that does not require them to be reversible (6) on the microscopic (particle scale) level or characterized by ‘slow’ or hydrodynamic fields. However, without approximations that truncate it to a manageable size it is nearly
useless. A truncation which is valid at low densities (gases) begets the Boltzmann equation (5; 7). Like the BBGKY hierarchy, the Boltzmann equation is well defined without the introduction of the concept of temperature or other macroscopic fields and it resolves near-microscopic scales. However it is a nontrivial integrodifferential equation that can be directly solved in very few cases. One of the important uses of the Boltzmann equation is the derivation of hydrodynamic constitutive relations. The form of the hydrodynamic equations (i.e., the equations of continuum mechanics) is very general and holds for single realizations (see Appendix A). They also follow from the Boltzmann equation (whose unknown is a distribution function). A gradient (Chapman-Enskog) expansion of the solution of the Boltzmann equation begets explicit expressions for the hydrodynamic fluxes in terms of gradients of the hydrodynamic fields (constitutive relations). This expansion is formally valid when there is scale separation (see more below) although the resulting hydrodynamic equations have been successfully employed when scale separation is weak or non-existent, such as in the case of weak shocks or granular matter (8).

Granular systems are different from molecular systems not only in the respective sizes of their constituents but (more importantly) the fact that the grains interact in a dissipative way (e.g., collide inelastically in the granular gas). Therefore all granular states are of non-equilibrium nature. An important consequence of this fact (9) is that granular systems do not possess strong scale separation except in the near-elastic case. In addition, typical granular systems comprise much fewer than (say) an Avogadro number of grains, therefore they are very small by molecular standards. Therefore granular systems are basically mesoscopic (9): they are expected to exhibit strong fluctuations within any reasonably defined ensemble and realizations may not be representative of these ensembles, see e.g., (10; 11), even in the fluidized phase.

Imagine a granular gas which so close to being elastic that the percentage of the energy lost in a collision is minute. Since local equilibration is established in a matter of a few collisions per particle the main effect of the weak inelasticity is to cause the decay of the kinetic energy on long time scales (of course, if the system is forced this ‘lost’ energy can be replenished). Therefore near-elastic granular gases are expected to behave in a way that is close to that of elastic gases, as detailed calculations show (8). In other words, the elastic limit is not singular (for finite times) and one expects the temperature to be a relevant field with properties that are similar to those encountered in elastic systems. It is a-priori unclear whether a similar statement holds for strongly inelastic granular gases. It is interesting to note that even in the realm of near-elastic granular gases there is no known equivalent of Boltzmann’s H-theorem.

Granular solids are jammed in static positions with no possibility to explore phase space. They are athermal. Furthermore, their states are typically metastable (the ground state of a sand-pile is one in which all grains reside
on the ground). Although the concept of temperature seems to be a-priori irrelevant to these systems, there have been interesting suggestions to define effective (configurational) temperatures for them as properties of appropriate ensembles, e.g., \((12; 13)\). Slow or quasistatic flows of dense granular matter are clearly athermal as well. Here possible dynamic applications of the above mentioned effective temperatures, such as fluctuation-dissipation (FD) relations have been proposed, and tested, see e.g., \((14; 15)\), indicating a possible dynamical relevance of these temperatures. Unlike the FD relations for granular gases \((16; 17; 18)\) (which are not trivial but can be derived by means borrowed from near-equilibrium statistical mechanics), the FD relations for dense and quasistatic granular flows (or glasses) have been conjectured (see, though \((19)\)). Still the above mentioned as well as other findings are interesting and suggestive of a possible underlying theoretical framework. Such a framework is probably not going to enjoy the generality of the near-equilibrium formulations and may necessitate an increase in the number of variables that characterize the considered systems (as is often the case in non-equilibrium situations). A proposal for defining non-equilibrium temperatures which has attracted considerable attention is due to Tsallis \((20)\). Whether this definition is relevant to granular matter is unclear as yet, see though \((21)\).

In old theories of granular matter (gases included) the granular temperature was not accounted for (as it does not correspond to a conserved entity) \((22)\). Even in some modern studies the granular temperature is (used but) eliminated from the equations of motion [e.g., for length scales for which heat conduction is subdominant to heat production and dissipation \((23)\)]; in these cases the temperature is claimed to be enslaved to the other fields (but it still plays a useful role as a state characterizing field). Systematic derivations of hydrodynamic equations for granular gases \((24; 25)\) invariably account for the granular temperature as a relevant field. These equations have been validated against simulations and experiments \((8)\), even when scale separation is weak.

The present paper has three major goals. The first is to show that the temperature field is needed for the description of granular gases as a characterizing field, if not a quasi-thermodynamic entity. This is done in Section 2, where the concept of granular temperature is explained in the context of the CE expansion. The goal of Section 3 is to provide an example of a kinetic theory (for binary granular gases) in which the temperature field is one of the hydrodynamic fields and which does produce sensible results even when equipartition is strongly violated (here a novel method for carrying out the CE expansion is presented and applied). The third goal, taken up in Section 4, is to show the existence of a correction to the classical formula for the elastic energy of granular and molecular matter alike; this correction is shown to be related to the heat flux in the equations of continuum mechanics. Section 5 concludes this paper and briefly discusses some issues concerning non-thermodynamic temperatures. Some technical details are relegated to Appendices.
Granular Gases and the Chapman-Enskog expansion

As mentioned in the Introduction, the equations of continuum mechanics are very general and in particular, they hold for practically all single realizations of many body systems (see Appendix A). These equations comprise the equation of continuity (for the density, \( \rho \)), Eq. (A.2), the momentum density, \( p \), equation, Eq. (A.10), and the equation for the energy density, \( e \), Eq. (A.15), in which (in the dissipative/inelastic case) an energy sink term, \( \rho \Gamma \), arises. An equation for the internal specific energy easily follows from the above, see Eq. (A.20). Note that the derivation in Appendix A produces also explicit expressions for the relevant fields and fluxes in terms of the microscopic degrees of freedom. In particular, note that the expression for the stress tensor is not precisely the same as the commonly used Voigt or Born or Kirkwood expression; the latter are limits of Eq. (A.9) when the coarse-graining volume (or width of the coarse-graining function) is very large and do not satisfy the equations of continuum mechanics unless there is scale separation or one considers homogeneous deformations of lattice configurations.

In the realm of molecular or granular gases, when the internal potential energy is negligible (for dilute systems) or when a model of hard spheres is employed one can replace the specific internal energy by the (granular) temperature, \( T \). In this case Eq. (A.20) can be rewritten as:

\[
\rho(r,t) \frac{DT(r,t)}{Dt} = \frac{\partial V_\beta(r,t)}{\partial r_\alpha} \sigma_{\beta\alpha}(r,t) - \text{div} Q(r,t) - \rho(r,t)\Gamma(r,t) \tag{1}
\]

with notation that is defined in Appendix A. Following Eq. (A.19) the (granular) temperature field is given by the following intuitive expression:

\[
T(r,t) = \frac{\frac{1}{2} \sum_i m_i v_i^2(t) \phi[\mathbf{r} - \mathbf{r}_i(t)]}{\sum_j m_j \phi[\mathbf{r} - \mathbf{r}_j(t)]} \tag{2}
\]

Note that when scale separation does not exist, the temperature, much like other fields, may be resolution dependent (i.e. it depends on the width of the coarse graining function \( \phi \))(26).

The hydrodynamic description of a fluid, granular or otherwise, is complete when constitutive relations express \( \sigma \), \( Q \) and \( \Gamma \) in terms of the hydrodynamic fields. It is \textit{a-priori} unclear whether such a closure exists for granular fluids. Extended Chapman-Enskog (CE) expansions provide explicit constitutive relations for granular gases, as further detailed below.

The Boltzmann equation is a non-trivial integrodifferential equation for the single-particle velocity distribution, \( f(\mathbf{v},\mathbf{r},t) \), whose integral over the (parti-
cle) velocities, \( \mathbf{v} \), is the number density, \( n(r, t) \). The ratio \( f(v, r, t)/n(r, t) \) is the probability density for a particle to have velocity \( \mathbf{v} \) when it is found (or more accurately its center of mass is found) at point \( r \) at time \( t \). In the relatively simple case of a dilute monodisperse collection of smooth hard spheres of unit mass and diameter \( d \) whose collisions are characterized by a fixed coefficient of normal restitution, \( \alpha \), the Boltzmann equation reads (24; 25; 27):

\[
\frac{\partial f(v_1)}{\partial t} + \mathbf{v}_1 \cdot \nabla f(v_1) = \frac{d^2}{\mathbf{k} \cdot \mathbf{v}_{12} > 0} \int d\mathbf{v}_2 d\mathbf{k} (\mathbf{k} \cdot \mathbf{v}_{12}) \left( \frac{1}{\alpha^2} f(v'_1)f(v'_2) - f(v_1)f(v_2) \right)
\]

where \( \nabla \) is a spatial gradient. The unit vector \( \mathbf{k} \) points from the center of particle ‘1’ to the center of particle ‘2’. The relation between the precollisional (primed) and postcollisional velocities is given by: \( \mathbf{v}_1 = \mathbf{v}'_1 - \frac{1 + \alpha}{2} (\mathbf{k} \cdot \mathbf{v}_{ij}) \mathbf{k} \) where \( \mathbf{v}'_j \equiv \mathbf{v}'_i - \mathbf{v}'_j \). The dependence of \( f \) on the spatial coordinates and time is not explicitly spelled out in Eq. (3). Notice that in addition to the explicit dependence of Eq. (3) on \( \alpha \), it also implicitly depends on \( \alpha \) through the relation between the postcollisional and precollisional velocities. The condition \( \mathbf{k} \cdot \mathbf{v}_{12} > 0 \) represents the fact that only particles whose relative velocity is such that they approach each other, can collide.

In the derivation of the Boltzmann equation (5; 7) it is assumed that the velocities and positions of colliding particles are not correlated. This assumption of “molecular chaos” is justified for dilute gases but not for dense gases or strongly inelastic granular gases (9; 28; 29; 30). This fact is related to the reduction in the normal component of the relative velocity of colliding particles. In relatively dense gases particles heading towards each other may not collide as they are ‘stopped’ by collisions with other particles. This phenomenon is modeled in the Enskog-corrected Boltzmann equation (7).

The Chapman-Enskog expansion is a method to perturbatively solve the Boltzmann equation. Scale separation is formally necessary for its implementation. When all gradients vanish, a local Maxwellian distribution, corresponding to the values of the hydrodynamic fields at each point, solves the Boltzmann equation in the elastic case. A gradient expansion (formally, an expansion in the Knudsen number) around this solution automatically yields the result that the distribution function depends on space and time only through its dependence on the fields (which is quasi-local since \( f(r, t) \) depends on the values of the fields and their spatial derivatives at \( (r, t) \)). The often made statement that within the CE expansion \( f \) is assumed to depend on space and time only through its dependence on the hydrodynamic fields is not precise: this assumption is made only for the zeroth order of the expansion.
In the case of granular gases, the (kinetic) energy density is not strictly conserved, and this led to questions whether it should be included in the set of hydrodynamic fields \((8; 23; 31; 32)\). Following the discussion in the introduction, when the degree of inelasticity is sufficiently small, it is justified to include the granular temperature in the set of hydrodynamic fields. An extension of the Chapman Enskog expansion based on this approach has been proposed and implemented in \((24)\). There, the small parameters used to expand the Boltzmann equation were the Knudsen number, \(K \equiv \frac{\ell}{L}\), where \(\ell\) is the mean free path given by \(\ell = \frac{1}{\pi n d^2}\), and \(L\) is a macroscopic length scale (i.e., the length scale which is resolved by hydrodynamics, not necessarily the system size) and the degree of inelasticity, defined by \(\epsilon \equiv 1 - \alpha^2\). In another approach \((25)\) to the problem only the Knudsen number is the small parameter and the temperature is assumed to comprise a relevant hydrodynamic field for all values of the degree of inelasticity. This method does not seem to lead to contradictions for any value of \(\alpha\); as a matter of fact it has recently been used to obtain accurate values for the linear transport coefficients for all physically allowed values of \(\alpha\) \((33)\). Whether the results are indeed relevant to strongly inelastic granular gases, where scale separation does not hold and precollisional correlations may be prominent, remains to be seen.

3 Binary granular gases: extreme violations of equipartition

Consider a mixture of smooth hard spheres, composed of species \(A\) and \(B\), of masses \(m_A\) and \(m_B\), and diameters \(\sigma_A\) and \(\sigma_B\), respectively. The coefficient of normal restitution (assumed to be fixed) for a collision of a particle of species \(\alpha \in \{A, B\}\) with a particle of species \(\beta \in \{A, B\}\) is denoted by \(e_{\alpha\beta}\) (hence, \(e_{\alpha\beta} \in \{e_{AA}, e_{BB}, e_{AB}\}\)). The transformation of velocities due to a collision of a sphere of species \(\alpha\) with a sphere of species \(\beta\) is given by:

\[v_1 = v'_1 - (1 + e_{\alpha\beta}) M^{\alpha\beta} \left( v'_{12} \cdot \hat{k} \right) \hat{k}\]

\[v_2 = v'_2 + (1 + e_{\alpha\beta}) M^{\alpha\beta} \left( v'_{12} \cdot \hat{k} \right) \hat{k}\]

where \(\{v'_1, v'_2\}\) denote the precollisional velocities of the spheres (the index ‘1’ refers here to species \(\alpha\)), and \(\{v_1, v_2\}\) are the corresponding postcollisional velocities; \(\hat{k}\) is a unit vector pointing from the center of sphere \(\alpha\) to that of sphere \(\beta\), and \(M^{\alpha\beta} \equiv \frac{m_\beta}{m_\alpha + m_\beta}\), \(v_{12} \equiv v_1 - v_2\), a similar definition holding for the primed (precollisional) velocities. Obvious kinematic constraints require that \(v'_{12} \cdot \hat{k} \geq 0\). Define the degrees of inelasticity as: \(\varepsilon_{\alpha\beta} \equiv 1 - e_{\alpha\beta}^2\).

The kinetic description of a binary granular gas mixture involves two Boltz-
mann equations, one for each species \((34; 35)\):

\[
Df_\alpha \equiv \frac{\partial f_\alpha}{\partial t} + v_1 \cdot \nabla f_\alpha = \mathcal{B}(f_\alpha, f_\alpha, e_{\alpha\alpha}) + \mathcal{B}(f_\alpha, f_\beta, e_{\alpha\beta}) \quad \alpha \neq \beta, \tag{6}
\]

where \(f_\alpha(v)\) is the distribution function for particles of species \(\alpha\), and

\[
\mathcal{B}(f_\alpha, f_\beta, e_{\alpha\beta}) = \sigma_{\alpha\beta}^2 \int \int_{v_{12} \cdot k > 0} \left[ \frac{f_\alpha(v_1')}f_\alpha(v_2') - f_\alpha(v_1)f_\beta(v_2) \right] (v_{12} \cdot k) \, dv_2 \, dk, \tag{7}
\]

where \(\sigma_{\alpha\beta} \equiv \frac{\sigma_\alpha + \sigma_\beta}{2}\). Here \(v_1\) and \(v_1'\) pertain to species \(\alpha\), and \(v_2\) and \(v_2'\) pertain to \(\beta\). Notice that \(\mathcal{B}(f_\alpha, f_\beta, e_{\alpha\beta})\) depends on the coefficients of normal restitution both explicitly, as shown in Eq. (7), and implicitly through the collision law.

The hydrodynamic fields in the present case comprise the two number densities, \(n_A\) and \(n_B\) (or the mass densities \(\rho_A = n_A m_A\) and \(\rho_B = n_B m_B\)), the mixture’s velocity field, \(V\), and the temperature field, \(T\), defined (differently from the monodisperse case) as twice the mean fluctuating kinetic energy of a particle (these are the only slow fields in the elastic limit), as explicitly defined below. The continuum equations of motion follow from the pertinent Boltzmann equation directly (using the standard procedure of computing velocity moments of the equation). Their validity is general since they are based on the underlying conservation laws. The equation of motion for the number density, \(n_\alpha\), with \(\alpha \in \{A, B\}\), is:

\[
\frac{Dn_\alpha}{Dt} = -\text{div } J_\alpha - n_\alpha \text{ div } V \tag{8}
\]

where \(\frac{D}{Dt}\) is the material derivative and \(J_\alpha = n_\alpha (V_\alpha - V)\) is the particle flux density of species \(\alpha\). As \(V_\alpha\), the velocity field of species \(\alpha\) (or the flux \(J_\alpha\)) is not a hydrodynamic field, it must be given by an appropriate constitutive relation. The velocity field obeys (as expected): \(\rho \frac{DV_i}{Dt} = -\frac{\partial \sigma_{ij}}{\partial x_j} + \rho g\), where the summation convention is used, and \(\sigma_{ij}\) is the stress tensor. The granular temperature field obeys: \(n \frac{dT}{Dt} = T \text{ div } J - \text{ div } Q - 2\sigma_{ij} \frac{\partial V_i}{\partial x_j} - \Gamma\), where \(J \equiv J_A + J_B\) is the total particle flux, and \(Q\) is the heat flux.

The form of the constitutive relations can be easily determined from tensorial (and symmetry) considerations, the result being (to linear order in the gradients, or Navier-Stokes order): \(\sigma_{ij} = p\delta_{ij} - 2\mu D_{ij} - \delta_{ij} \eta_0 \text{ div } V\), where

\[
D_{ij} = \frac{1}{2} \left( \frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \text{ div } V \right) \text{ is the traceless rate of strain tensor, } \mu \text{ is}
\]

\[
\text{and } \eta_0 \text{ is the coefficient of shear viscosity.}
\]
the shear viscosity, \( \eta_B \) is the bulk viscosity (which vanishes in the dilute limit) and \( p \) is the pressure. The diffusion flux can be rewritten as

\[
\mathbf{J}_\alpha = \frac{n_\alpha}{n_\alpha} \frac{1}{\sigma_{AB}^2} \sqrt{\frac{T}{m_\alpha}} \left( -\kappa_A^T \nabla \ln T - \kappa_A^n \nabla \ln n - \kappa_{\alpha}^c \nabla \ln c \right),
\]

where \( \kappa_A^T, \kappa_A^n \) and \( \kappa_{\alpha}^c \) are non-trivial functions of the parameters

\[
S \equiv \{ \{ \varepsilon_{\alpha\beta} \}, \, M_A \equiv \frac{m_A}{m_A + m_B}, \, \frac{\sigma_A}{\sigma_A + \sigma_B}, \, c \},
\]

where the concentration field, \( c \), is defined as \( c \equiv \frac{n_A}{n} = \frac{n_A}{n_A + n_B} \). Similarly, the heat flux can be rewritten as

\[
Q = \frac{1}{\sigma_{AB}^2} \sqrt{\frac{T}{m_0}} \left( -\lambda_T \nabla \ln T - \lambda^n \nabla \ln n - \lambda^c \nabla \ln c \right)
\]

where \( m_0 \equiv m_A + m_B \). In the dilute limit the equation of state is the same as that for an ideal gas: \( p = \frac{nT}{3} \). Much like in the monodisperse case the number density for species \( \alpha \) is given by: \( n_\alpha = \int f_\alpha(\mathbf{v}) \, d\mathbf{v} \), the corresponding mass density being \( \rho_\alpha = m_\alpha n_\alpha \); the overall number density is \( n \equiv n_A + n_B \), and the overall mass density is \( \rho \equiv \rho_A + \rho_B \). The velocity field of species \( \alpha \) is given by: \( \mathbf{V}_\alpha = \frac{1}{n_\alpha} \int f_\alpha(\mathbf{v}) \, \mathbf{v} \, d\mathbf{v} \). As mentioned, \( \mathbf{V}_\alpha \) is not a hydrodynamic field, and needs to be expressed as a functional of the hydrodynamic fields. The mixture’s velocity field is: \( \mathbf{V} = \frac{1}{\rho} (\rho_A \mathbf{V}_A + \rho_B \mathbf{V}_B) \). The granular temperature of species \( \alpha \) is defined by: \( T_\alpha = \frac{1}{n_\alpha} \int f_\alpha(\mathbf{v}) \, m_\alpha \, (\mathbf{v} - \mathbf{V})^2 \, d\mathbf{v} \) (not a hydrodynamic field). The velocity fluctuations of each of the species are measured with respect to the (hydrodynamic) mixture’s velocity field, not the species’ velocity fields. The mixture’s granular temperature is defined as: \( T = \frac{1}{n} (n_A T_A + n_B T_B) \). The kinetic expression for the stress tensor (7) is: \( \sigma_{ij} = m_A \int f_A(\mathbf{v}) \, u_i u_j \, d\mathbf{v} + m_B \int f_B(\mathbf{v}) \, u_i u_j \, d\mathbf{v}, \) where \( \mathbf{u} \equiv \mathbf{v} - \mathbf{V} \) is the peculiar (fluctuating) velocity of a particle (irrespective of the species). Similarly, the heat flux is composed of two contributions, for obvious reasons: \( Q = \int f_A(\mathbf{v}) \, m_A u^2 \mathbf{u} \, d\mathbf{v} + \int f_B(\mathbf{v}) \, m_B u^2 \mathbf{u} \, d\mathbf{v} \). Our definition of the heat flux may differ by a factor of 2 from some other definitions. The sink term is given by \( \Gamma = \Gamma_A + \Gamma_B + \Gamma_{AB} \), where:

\[
\Gamma_\alpha \equiv \varepsilon_{\alpha\alpha} \frac{m_\alpha \pi \sigma_{\alpha}^2}{8} \int \int f_\alpha(\mathbf{v}_1) f_\alpha(\mathbf{v}_2) |v_{12}|^3 \, d\mathbf{v}_1 \, d\mathbf{v}_2,
\]

and

\[
\Gamma_{AB} \equiv \varepsilon_{AB} \frac{m_{AB} \pi \sigma_{AB}^2}{2} \int \int f_A(\mathbf{v}_1) f_B(\mathbf{v}_2) |v_{12}|^3 \, d\mathbf{v}_1 \, d\mathbf{v}_2.
\]
The HCS distributions for binary granular gas mixtures (much like in the monodisperse case) are scaling solutions, in which the distribution functions are rendered time independent when the velocities are scaled by the respective (decaying) thermal speeds of the species comprising the mixture. It serves as a zeroth order in the extended Chapman-Enskog expansion of (34). The lhs of the Boltzmann equations for the HCS can be rewritten in this case as:

\[ \frac{\partial f^{\text{HCS}}_\alpha}{\partial t} = \frac{\partial f^{\text{HCS}}_\alpha}{\partial T} \]

and the two Boltzmann equations become:

\[ -\frac{\Gamma}{n} \frac{\partial f^{\text{HCS}}_\alpha}{\partial T} = B \left( f^{\text{HCS}}_\alpha, f^{\text{HCS}}_\alpha, e^{\alpha\alpha} \right) + B \left( f^{\text{HCS}}_\alpha, f^{\text{HCS}}_\beta, e^{\alpha\beta} \right) \quad \alpha \neq \beta \quad (13) \]

These equations need to be solved subject to the following ‘constraints’ which fix the values of the hydrodynamic fields:

\[ \int f^{\text{HCS}}_A \, du = n_A, \quad \int f^{\text{HCS}}_B \, du = n_B \]

and \( \int f^{\text{HCS}}_A m_A u^2 \, du + \int f^{\text{HCS}}_B m_B u^2 \, du = n_T \). The common way of solving Eqs. (13) is to represent the functions, \( f^{\text{HCS}}_\alpha \), by Sonine polynomial series times Maxwellians in the respective non-dimensionalized (peculiar) velocities. However, it can be shown (33) that due to the exponential tails of the HCS distributions these expansions are not convergent yet they are asymptotic and Borel resummable. To overcome this difficulty, consider the modified expansion:

\[ f^{\text{HCS}}_\alpha = f^{M,\eta}_\alpha \phi_\alpha \equiv n_\alpha \left( \frac{n_\alpha}{\pi} \right)^{\frac{3}{2}} e^{-\eta u^2_\alpha} \phi_\alpha \quad (14) \]

where \( \gamma_\alpha = \frac{3m_\alpha}{2T} \), \( \phi_\alpha \equiv \sum_{p=0}^{\infty} h^p_\alpha \left( u^2_\alpha \right) \), and \( \eta > 0 \) is a constant, i.e. \( f_\alpha \) is represented by a truncated Sonine polynomial series (whose coefficients are denoted by \{h^p_\alpha\}) times a Maxwellian in which the temperature is replaced by a “wrong” temperature \( \frac{T}{\eta} \). It can be shown (33) that this method produces convergent series when \( \eta < 0.5 \). Upon substituting the form (14) in Eq. (13) and projecting on the Nth order Sonine polynomial \( S^N_{\frac{3}{2}} \left( u^2_\alpha \right) \), one obtains the following non linear algebraic system for the coefficients \( h^p_\alpha \):

\[ \frac{n_\alpha \Gamma}{n_T} \sum_p h^p_\alpha R_{pN} = \frac{M_\alpha^3 n_\alpha^2 \sigma^2_\alpha}{\pi^3} \sqrt{\frac{2T}{3m_0}} \sum_{p,q} B^{pqN}_{\alpha\alpha} h^p_\alpha h^q_\alpha \]

\[ + \chi_{\alpha\beta} \left( \frac{M_\beta M_\alpha}{M_\alpha + M_\beta} \right)^{\frac{3}{2}} n_\alpha n_\beta \sigma^2_{\alpha\beta} \sqrt{\frac{2T}{3m_0}} \sum_{p,q} B^{pqN}_{\alpha\beta} h^p_\alpha h^q_\beta \quad (15) \]

where \( m_0 \equiv m_A + m_B \), \( M_\alpha \equiv \frac{m_\alpha}{n_\alpha} \), and \( R_{pN} \) is defined as follows:

\[ R_{pN} = \frac{1}{\pi^\frac{3}{2}} \int e^{-\eta u^2_\alpha} S^N_{\frac{3}{2}} \left( u^2_\alpha \right) \]

\[ \times \left[ \frac{3}{2} S^p_{\frac{3}{2}} \left( u^2_\alpha \right) - u^2 \left( \eta S^p_{\frac{3}{2}} \left( u^2_\alpha \right) - \frac{\partial}{\partial u^2_\alpha} S^p_{\frac{3}{2}} \left( u^2_\alpha \right) \right) \right] \, du_\alpha \quad (16) \]
where \( u_\alpha \equiv \sqrt{T_0} u \), and the coefficients (or coupling constants), \( B_{\alpha \beta}^{pqN} \), are defined, in terms of the rescaled velocities \( \tilde{u} \equiv \frac{\sqrt{3m_0^2}}{2T} u \), by:

\[
B_{\alpha \beta}^{pqN} = \int S_{\frac{1}{2}}^N \left( M_\alpha \tilde{u}_1^2 \right) \int \int \left[ \frac{1}{e_{\alpha \beta}} e^{-\eta M_\alpha \tilde{u}_1^2 - \eta M_\beta \tilde{u}_2^2} S_{\frac{1}{2}}^p \left( M_\alpha \tilde{u}_1^2 \right) S_{\frac{1}{2}}^q \left( M_\beta \tilde{u}_2^2 \right) - e^{-\eta M_\alpha \tilde{u}_1^2 - \eta M_\beta \tilde{u}_2^2} S_{\frac{1}{2}}^p \left( M_\alpha \tilde{u}_1^2 \right) S_{\frac{1}{2}}^q \left( M_\beta \tilde{u}_2^2 \right) \right] (\tilde{u}_1 \cdot \mathbf{k}) d\tilde{u}_1 d\tilde{u}_2 d\mathbf{k}
\]  

(17)

Though straightforward in principle, the computation of these coefficients turns out to be forbiddingly tedious as the order of the Sonine expansions is increased. In order to be able to carry out high order expansions, we made use of a computer-aided method exploiting the fact that the Sonine polynomials can be derived from their respective generating functions, \( G_m(s, x) \):

\[
G_m(s, x) = (1 - s)^{m-1} e^{-\frac{s}{1-s}} \sum_{p=0}^{\infty} s^p S^p_m(x)
\]  

(18)

This fact enables one to define generating functions for the integrals (16) and (17): \( R(s, w) \equiv \sum_{p,N} s^p w^N R_{pN} \) and \( B_{\alpha \beta}(w, s, t) \equiv \sum_{p,q,N} s^p t^q w^N B_{\alpha \beta}^{pqN} \) of the coefficients, \( B_{\alpha \beta}^{pqN} \), and \( R_{pN} \), respectively (where all sums here and below range from zero to infinity). The latter can then be computed (using a symbolic processor such as MAPLE\textsuperscript{TM}) to any desired order by taking successive derivatives of \( R(s, w) \) and \( B_{\alpha \beta}(w, s, t) \). These generating functions are given by:

\[
R(s, w) = \frac{3}{2} \frac{(1 - s) w}{(1 - w s + (\eta - 1)(1 - w)(1 - s))^{\frac{3}{2}}}
\]  

(19)

and using Eq. (17)

\[
B_{\alpha \beta} = (1 - s)^{-\frac{3}{2}} (1 - t)^{-\frac{3}{2}} (1 - w)^{-\frac{3}{2}}
\times \left[ \frac{1}{e_{\alpha \beta}} I_{\alpha \beta} \left( \frac{M_\alpha w}{1 - w}, 0, \left( \frac{s}{1 - s} + \eta \right) M_\alpha, \left( \frac{t}{1 - t} + \eta \right) M_\beta \right) - I_{\alpha \beta} \left( M_\alpha \left( \eta + \frac{w}{1 - w} + \frac{s}{1 - s} \right), \left( \frac{t}{1 - t} + \eta \right) M_\beta \right) \right]
\]

where \( I_{\alpha \beta}(a, b, c, d, x, y, z) \) is the integral defined by:

\[
I_{\alpha \beta}(a, b, c, d, x, y, z) \equiv \int_{u_{12} \cdot \mathbf{k} > 0} d\mathbf{u}_1 d\mathbf{u}_2 d\mathbf{k} (\mathbf{u}_{12} \cdot \mathbf{k}) e^{-F}
\]  

(20)
where \( F = au^2 + bu^2 + cu' + du'^2 + \frac{v}{2}(u_1 + u_1')^2 + \frac{v}{2}(u_1 + u_2)^2 + \frac{v}{2}(u_1 + u_2')^2 \) and \( I_{\alpha\beta}(a, b) \equiv I_{\alpha\beta}(a, b, 0, 0) \). It is easy to calculate \( I_{\alpha\beta} \), the result being:

\[
I_{\alpha\beta} = \frac{2\pi^2}{\lambda^2} \frac{1}{\mu_{\alpha\beta}(\nu_{\alpha\beta} + \mu_{\alpha\beta})}
\]  

(21)

where \( \lambda = a + b + c + d + 2x + 2y + 2z \), \( \mu_{\alpha\beta} = R_{\alpha\beta} - \frac{K^2_{\alpha\beta}}{\lambda} \), \( \nu_{\alpha\beta} = S_{\alpha\beta} \)

\[-\frac{t^\alpha\beta}{\lambda} \left( (d+y) M^{\alpha\beta} - (c+x) M^{\beta\alpha} \right) \left( 2K_{\alpha\beta} + t^\alpha\beta \left((d+y) M^{\alpha\beta} - (c+x) M^{\beta\alpha}\right) \right),
\]

\[R_{\alpha\beta} = (a+c+2x) \left( M^{\beta\alpha}\right)^2 + (b+d) \left( M^{\alpha\beta}\right)^2 + \frac{1}{2} \left( M^{\alpha\beta} - M^{\beta\alpha} \right)^2 \left(y+z\right),
\]

\[S_{\alpha\beta} = \frac{1}{2} t^\alpha\beta \left[ \left(t^\alpha\beta - 2\right) \left(2c+x\right) \left(M^{\alpha\beta}\right)^2 + \left(M^{\alpha\beta}\right)^2 \left(2d+y\right) + 2M^{\alpha\beta} M^{\beta\alpha} \left(y+z\right) \right],
\]

\[-2 \left( M^{\alpha\beta}\right)^2 \left,(\alpha\beta) = (a+c+2x+y+z) - M^{\alpha\beta} (b+d+y+z) \right),
\]

\[t^\alpha\beta \equiv \frac{1+e_{\alpha\beta}}{e_{\alpha\beta}}. \]

Next, using Eq. (14) for \( f_a \) in Eq. (11) and (12), multiplying the result by \( s^p t^q \) and summing over \( p \) and \( q \), one obtains: \( \Gamma = \frac{\sqrt{\pi} \sqrt{2 \pi^2 \sigma^2 \mu^2}}{\sqrt{m_0 T^2}} \), where

\[
\bar{\Gamma} \equiv \varepsilon_{AA} n_A^2 \sigma_A^2 M_A^4 \sum_p \sum_p \Gamma_{AA} h_A^p h_A^q + 4 \varepsilon_{AB} \frac{n_A n_B}{n^2} M_A^2 M_B^2 \sum_p \sum_q \Gamma_{AB} h_A^p h_B^q
\]

\[\Gamma_{AB} = \chi_{BB} \varepsilon_{BB} \frac{n_B^2 \sigma_B^2 M_B^4}{n^2} \sum_p \sum_q \Gamma_{BB} h_B^p h_B^q,
\]

\[
\Gamma_{\alpha\beta} = 1_{\rho_{\alpha\beta}} \sqrt{\partial^{\rho_{\alpha\beta}} \Phi^\alpha} \bigg|_{s=0,t=0}, \]

the generating function \( G_{\alpha\beta}(s, t) \) being given by:

\[
G_{\alpha\beta}(s, t) = \left( \frac{(1-s)M_{\alpha\beta}}{(s+\eta(1-s))} + \frac{(1-s)M_{\alpha\beta}}{(s+\eta(1-s))} \right) \frac{2}{(s+\eta(1-s))^\eta} \frac{(s+\eta(1-s))^\eta}{(s+\eta(1-s))^\eta}
\]

\[
M_{\alpha\beta}^3
\]  

(23)

With the coupling constants calculated, the algebraic equations, Eq. (15), are now solved to produce the distribution functions, from which one can easily calculate the temperature ratio, \( T_A/T_B \). Fig. 1(a) shows a plot of the temperature ratio as a function of \( \frac{m_A}{m_A + m_B} \) for a system of particles of equal mass density, \( c = 0.5 \) and \( \varepsilon_{AA} = \varepsilon_{BB} = \varepsilon_{AB} = 0.8 \). Note that the temperature ratio can “violate” equipartition quite strongly. In order to compute the heat conductivity and the thermal diffusion coefficient, we now turn to solve the Boltzmann equation, carrying out the Chapman-Enskog expansion to first order in gradients of the hydrodynamic fields, with the homogeneous cooling state distribution function serving as a zeroth order solution. The distribution functions are expressed as \( f_a = f_a^{MCS} + f_a^K \), where \( f_a^K \) is the first order perturbation in a gradient expansion, written for convenience as \( f_a^K = f_a^M \Phi^K \).
cf. Eq. (14), where the value of \( \nu \) may be taken to be different from that of \( \eta \). To first order in the gradients of the hydrodynamic fields, the two coupled Boltzmann equations for the perturbations \( \Phi^K_\alpha \) read:

\[
D^K f_A = \left( L^{(1)}_{AA} + L^{(2)}_{AA} + L^{(1)}_{AB} \right) \Phi^K_A + L^{(2)}_{AB} \Phi^K_B
\]

\[
D^K f_B = L^{(2)}_{BA} \Phi^K_A + \left( L^{(1)}_{BB} + L^{(2)}_{BB} + L^{(1)}_{BA} \right) \Phi^K_B
\]

where

\[
L^{(1)}_{\alpha\beta} \Phi^K_\alpha \equiv B \left( f^{M,\nu}_\alpha \Phi^K_\alpha, f^{(HCS)}_{\beta,\nu}, e_{\alpha\beta} \right) \quad \alpha \neq \beta
\]

\[
L^{(2)}_{\alpha\beta} \Phi^K_\beta \equiv B \left( f^{(HCS)}_\alpha, f^{M,\nu}_\beta \Phi^K_\beta, e_{\alpha\beta} \right) \quad \alpha \neq \beta
\]

are the linearized Boltzmann operators, and \( D^K f_\alpha \) denotes the first order term in the expansion of \( Df_\alpha \). Following the definition of the operator, \( D \):

\[
Df_\alpha = f^{M,\eta}_\alpha \left[ \phi_\alpha D \ln n_\alpha + 2 \gamma_\alpha u_i \left( \eta \phi_\alpha - \phi'_\alpha \right) DV_i 
+ \left( \gamma_\alpha u^2 \left( \eta \phi_\alpha - \phi'_\alpha \right) - \frac{3}{2} \phi_\alpha \right) D \ln T + c \frac{\partial \phi_\alpha}{\partial c} D \ln c \right] 
+ f^{M,\nu}_\alpha D \Phi^K + \Phi^K f^{M,\nu}_\alpha \left[ D \ln n_\alpha + 2 \gamma_\alpha u_i \nu DV_i + \left( \gamma_\alpha u^2 \nu - \frac{3}{2} \right) D \ln T \right]
\]

where a prime superscript of a function denotes a derivative with respect to its argument. Carrying out the expansion to first order in gradients leads, on the basis of tensorial considerations, to the following form for the function \( \Phi^K_\alpha \):

\[
\Phi^K_\alpha = \Phi^K_{\alpha,T} \left( \gamma_\alpha u^2 \right) \sqrt{\gamma_\alpha u_j} \frac{\partial \ln T}{\partial x_j} 
+ \Phi^K_{\alpha,n} \left( \gamma_\alpha u \right) \sqrt{\gamma_\alpha u_j} \frac{\partial \ln n}{\partial x_j} 
+ \Phi^K_{\alpha,c} \left( \gamma_\alpha u \right) \sqrt{\gamma_\alpha u_j} \frac{\partial \ln c}{\partial x_j} 
+ \Phi^K_{\alpha,V} \left( \gamma_\alpha u \right) \gamma^{\frac{4}{3}} u_i u_j \frac{\partial V_i}{\partial x_j}
\]

(24)

where for any tensor \( A_{ij}, \overline{A}_{ij} \equiv \frac{1}{2} \left( A_{ij} + A_{ji} - \frac{2}{3} \delta_{ij} A_{kk} \right) \). \( D^K f_\alpha \) is given by:

\[
D^K f_\alpha = \frac{\Gamma}{nT} f^{M,\nu}_\alpha \left[ \left( \gamma_\alpha u^2 \left( \Phi^K_{\alpha,c} \right)' - \left( \gamma_\alpha u^2 \nu - \frac{2}{3} \right) \Phi^K_{\alpha,c} \right) \frac{\partial \ln \tilde{\Gamma}}{\partial c} \Phi^K_{\alpha,T} + \left( \gamma_\alpha u^2 \left( \Phi^K_{\alpha,n} \right)' - \left( \gamma_\alpha u^2 \nu - \frac{2}{3} \right) \Phi^K_{\alpha,n} - \Phi^K_{\alpha,T} \right) \sqrt{\gamma_\alpha u_j} \frac{\partial \ln n}{\partial x_j} \right]
\]
Using $(\ref{24})$ in the definition of $Q$ and $J_A$, one obtains:

\[
\kappa_A^T = -\frac{1}{3} Tr \left[ \int f_{\alpha A}^{M,\nu} \left[ \Phi_{\alpha A}^{K,T} (\gamma_A u^2) \sqrt{\gamma_A u} \right] u_i d\mathbf{u} \right] \\
\lambda^T = -\frac{1}{3} Tr \left[ \int \left( m_{AB} f_{MB}^{M,\nu} \Phi_{\alpha B}^{K,T} (\gamma_B u^2) \sqrt{\gamma_B} \right) u^2 u_i u_j d\mathbf{u} \right]
\]

where $\Phi_{\alpha}^{K,T}$ obey (with $\beta \neq \alpha$):

\[
\left( L_{\alpha\alpha}^{(1)} + L_{\alpha\beta}^{(2)} + L_{\alpha\beta}^{(1)} \right) \left( \Phi_{\alpha}^{K,T} (\gamma_A u^2) \sqrt{\gamma_A u} \right) + \left( L_{\alpha\beta}^{(2)} \right) \left( \Phi_{\beta}^{K,T} (\gamma_A u^2) \sqrt{\gamma_B} \right) \\
- \frac{\sqrt{\gamma_A}}{9} \frac{n s_{\alpha}^2}{\sqrt{m_0}} \sqrt{T} \left( \Phi_{\alpha}^{K,T} (\gamma_A u^2) \sqrt{\gamma_A u} \right) = R_{\alpha}^T
\]

where $H_{\alpha}^T \left( \Phi_{\alpha}^{K,T} \sqrt{\gamma_A u} \right) = f_{\alpha}^{M,\nu} \left( \gamma_A u^2 \left( \Phi_{\alpha}^{K,T} \right)' - \left( \gamma_A u^2 \nu - \frac{3}{2} \right) \Phi_{\alpha}^{K,T} \right) \sqrt{\gamma_A u}$ and $R_{\alpha}^T = f_{\alpha}^{M,\nu} \left( (\gamma_A u^2 - n m_\alpha) (\eta \phi_\alpha - \phi_\alpha) - \frac{3}{2} \phi_\alpha \right) \mathbf{u}$. The equations (26) are solved subject to the constraint $\int f_k^A m_A \mathbf{u} d\mathbf{u} + \int f_k^B m_B \mathbf{u} d\mathbf{u} = 0$ using the same computer aided method applied to the solution of the HCS. The functions $\Phi_{\alpha}^{K,T}$ are represented by series of Sonine polynomials $\Phi_{\alpha}^{K,T} = \sum_{p=0}^{\infty} \hat{\lambda}_{\alpha A}^{K,T,p} S_n^N \left( \gamma_A u^2 \right)$ (the factor $\nu < 1$ in the function $f_{\alpha}^{M,\nu}$ ensuring the convergence of the series), which is substituted in (26). The resulting equation is then projected on $S_n^N \left( \gamma_A u^2 \right) \sqrt{\gamma_A u}$ to yield a linear system of equations for the coefficients $\hat{\lambda}_{\alpha A}^{K,T,p}$. The system of equations is then solved (after evaluating the coupling constants using the generating function method explained above). The resulting perturbations are then used to calculate the transport coefficients. Results for the thermal diffusion constant, $\kappa_A^T$, and the heat conductivity, $\lambda^T$, are presented in Fig. 1(b,c). Note the nontrivial dependence of these transport coefficients on $m_{\alpha}$. Although clearly equipartition is strongly broken, these transport coefficients are well behaved (as are those not shown here).
4 Elastic energy and “heat flux”

Consider a set of particles whose binary interaction potential is harmonic (or approximated by): 

\[ U(r_{ij}(t)) = \frac{1}{2} K_{ij} (|r_{ij}| - l_{ij})^2, \]

where \( l_{ij} \) is the equilibrium separation of particles \( i \) and \( j \) and \( r_{ij} \equiv r_i - r_j \). The force on particle \( i \) exerted by particle \( j \) is given by 

\[ f_{i/j} = -\nabla_i U(r_{ij}) = -K_{ij} (|r_{ij}| - l_{ij}) \hat{r}_{ij}, \]

where \( \hat{r}_{ij} \equiv r_{ij} / |r_{ij}| \) is a unit vector. Consider, for simplicity, an unstressed reference configuration, in which all particle pairs are at their equilibrium separation \( (|r_{ij}^0| = l_{ij}) \), where the superscript 0 denotes the reference configuration. The relative displacement of particles \( i \) and \( j \) is defined by: 

\[ u_{ij} \equiv r_{ij} - r_{ij}^0. \]

To linear order in the displacements the corresponding force can be approximated by:

\[
\begin{align*}
    f_{i/j} &= -K_{ij} (|r_{ij}| - l_{ij}) \hat{r}_{ij} = -K_{ij} (|r_{ij}^0 + u_{ij}| - |r_{ij}^0|) \hat{r}_{ij} \\
    &= -K_{ij} (\hat{r}_{ij}^0 \cdot u_{ij}) \hat{r}_{ij}^0.
\end{align*}
\]

For atomic systems, the harmonic approximation is obtained from a Taylor expansion of the (effective) interatomic potential around its minimum. For granular materials, the contact interactions among the particles are typically described using contact mechanics (36; 37) (force models used in simulations of granular materials are reviewed in (38; 39; 40; 41; 42)). For the present discussion, it is assumed that the interparticle forces can be linearized for small deformations with respect to a reference configuration.

Consider the contact stress, see Eq. (A.8). Upon substituting the formula for the force to linear order in the displacements, Eq. (27), in Eq. (A.8) one obtains an expression for the linear elastic stress tensor:

\[
\sigma_{\alpha\beta}^{lin}(\mathbf{r}, t) = \frac{1}{2} \sum_{ij} K_{ij} \hat{r}_{ij}^0 \hat{r}_{ij}^{\alpha} \hat{r}_{ij}^{\beta} u_{ij}, \quad \int_0^1 ds \phi[\mathbf{r} - \mathbf{r}_{ij}^0 + s \hat{r}_{ij}^0].
\]
It is interesting to examine the potential energy density as read off Eq. (A.1) and compare it to the relation used in continuum linear elasticity. In the quasistatic limit, the energy density reduces to the potential energy density [in this limit, the time of deformation goes to infinity \((t_f \rightarrow \infty)\) and the velocities go to zero \((v_i \rightarrow 0)\), so that the kinetic energy is zero while the displacement \(u_i \sim v_i t_f\), is kept finite]. To lowest nonvanishing order in the strain, the potential energy is given by \(\frac{1}{2} K_{ij} \left( \dot{r}_{ij}^0 \cdot u_{ij} \right)^2\). Hence, at this order:

\[
e^{el}(\mathbf{r}, t) = \frac{1}{4} \sum_{ij} K_{ij} \left( \dot{r}_{ij}^0 \cdot u_{ij} \right)^2 \phi[\mathbf{r} - \mathbf{r}_i(t)].
\] (29)

Classical linear elasticity identifies the elastic energy as \(e^{el} = \frac{1}{2} \sigma^{lin} : \epsilon^{lin}\), where \(e^{lin}\) is defined in Eq. (B.7). Since the stress is symmetric for central forces (it is easily verified that Eq. (28) is invariant to the exchange of \(\alpha\) and \(\beta\)), we can calculate \(\frac{1}{2} \sigma^{lin}_{\alpha\beta} \frac{\partial u^{lin}_{\alpha}}{\partial r_{\beta}} = \frac{1}{2} \frac{\partial}{\partial r_{\beta}} \left( \sigma^{lin}_{\alpha\beta} u^{lin}_{\alpha} \right)\) instead, the second equality following from the static equilibrium relation \(\frac{\partial \sigma^{lin}_{\alpha\beta}}{\partial r_{\beta}} = 0\), see also Eq. (B.3). It follows, using Eq. (A.8) and definition (B.6) that:

\[
\frac{1}{2} \sigma^{lin}_{\alpha\beta} \epsilon^{lin}_{\alpha\beta} = - \frac{1}{4} \frac{\partial}{\partial r_{\beta}} \sum_{ij} u^{lin}_{\alpha} f_{i/j} u^{lin}_{ij\beta} \int_0^1 ds \phi[\mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0]
\]

Next, using Eq. (B.15) one obtains:

\[
\frac{1}{2} \sigma^{lin}_{\alpha\beta} \epsilon^{lin}_{\alpha\beta} = - \frac{1}{4} \frac{\partial}{\partial r_{\beta}} \sum_{ij} [u_{i\alpha} - u'_{i\alpha}] f_{i/j} \int_0^1 ds \phi[\mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0]
\]

\[
= - \frac{1}{4} \sum_{ij} u_{i\alpha} f_{i/j} \int_0^1 ds \phi[\mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0]
\]

\[
= \frac{1}{4} \sum_{ij} u_{i\alpha} f_{i/j} \int_0^1 ds \phi[\mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0]
\]

In equilibrium \(\sum_j f_{i/j} = 0\), hence \(\sum_j f_{i/j} \phi(\mathbf{r} - \mathbf{r}_i(t)) = 0\) and it can be
replaced by $-\sum_j f_{i/j} \phi (\mathbf{r} - \mathbf{r}_i(t))$. Therefore

$$\frac{1}{2} \sigma_{\alpha\beta}^{\text{lin}} \varepsilon_{\alpha\beta}^{\text{lin}} = - \frac{1}{4} \sum_{ij} u_{i\alpha} f_{i/j} \left( \phi [\mathbf{r} - \mathbf{r}_i(t)] + \phi [\mathbf{r} - \mathbf{r}_j(t)] \right)$$

$$+ \frac{1}{4} \frac{\partial}{\partial r_\beta} \sum_{ij} u'_{i\alpha} f_{i/j} \phi \left[ \mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0 \right]$$

$$= - \frac{1}{4} \sum_{ij} u_{i\alpha} f_{i/j} \phi [\mathbf{r} - \mathbf{r}_i(t)] + \frac{1}{4} \frac{\partial}{\partial r_\beta} \sum_{ij} u'_{i\alpha} f_{i/j} \phi \left[ \mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0 \right]$$

Next, substituting the expression for the force, Eq. (27), one obtains:

$$\frac{1}{2} \sigma_{\alpha\beta}^{\text{lin}} \varepsilon_{\alpha\beta}^{\text{lin}} = \frac{1}{4} \sum_{ij} K_{ij} \left( \mathbf{r}_{ij}^0 \cdot \mathbf{u}_{ij} \right)^2 \phi [\mathbf{r} - \mathbf{r}_i(t)]$$

$$+ \frac{1}{4} \frac{\partial}{\partial r_\beta} \sum_{ij} f_{i/j} u'_{i\alpha} r_{ij}^0 \phi \left[ \mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0 \right]$$

$$= \epsilon^\text{el}(\mathbf{r}, t) + \frac{1}{4} \frac{\partial}{\partial r_\beta} \sum_{ij} f_{i/j} u'_{i\alpha} r_{ij}^0 \phi \left[ \mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0 \right]$$

$$= \epsilon^\text{el}(\mathbf{r}, t) + \frac{1}{8} \frac{\partial}{\partial r_\beta} \sum_{ij} f_{i/j} \left( u'_{i\alpha} + u'_{j\alpha} \right) r_{ij}^0 \phi \left[ \mathbf{r} - \mathbf{r}_i^0 + s \mathbf{r}_{ij}^0 \right]$$

(30)

This result is identical to that obtained on the basis of dynamical considerations in Appendix B, cf. Eqs. (B.12,B.14).

It follows that the coarse grained elastic energy density is not precisely given by the classical expression $\frac{1}{2} \sigma^{\text{lin}} : \varepsilon^{\text{lin}}$; the above additional term provides a correction to the classical expression. The correction represents the adiabatic limit of the divergence of the (time integral of) the heat flux or, in physical terms, the divergence of the fluctuating part of the work of the interparticle forces, i.e. the work done on the fluctuating parts of the displacements or the work which is unresolved by macroscopic elasticity. As this term is a divergence of a flux, its average over a volume, $\Omega$, whose linear dimension is $W$, is proportional to $W^{D-1}$, while the average over the first term is proportional to $W^D$. Therefore their ratio tends to zero as $1/W$, i.e., the average of $\frac{1}{2} \sigma^{\text{lin}} : \varepsilon^{\text{lin}}$ over a sufficiently large volume (not its ‘local value’) begets the standard elastic energy density. It should be emphasized that both contributions to the elastic energy density are of the same (second) order in the displacements (or
strain), i.e. the additional term is not a “higher order” correction but rather a correction that appears when the deformation is not affine (i.e., when $u_i' \neq 0$).

4.1 Numerical results: 2D disordered harmonic networks

In order to examine the correction to the classical elastic energy numerically, we use disordered harmonic networks in 2D, obtained as follows: “particles” (of equal mass) are placed at the nodes of a triangular lattice, of lattice constant $d$. The system is square shaped. Nearest neighbors are connected by springs (with rest lengths equal to the lattice constant, ensuring a stress-free reference state). We introduce disorder in two ways: first, the spring network is diluted by randomly removing a fraction $c$ of the springs. Second, we employ spring constants which are uniformly distributed in the range $[K - \delta K, K + \delta K]$. The particle positions are the same as in the triangular lattice, hence the density remains uniform. We use periodic boundary conditions in both axes, and apply a specified global strain to the system by imposing a change in the period as well as (for shear deformation) Lees-Edwards boundary conditions.

The (linear) static equilibrium equations are solved (by inversion of the dynamical matrix) for a given applied global strain, $\epsilon_{\alpha \beta}^{app}$, yielding a set of corresponding displacements $\{u_i\}$. The latter are used for calculating the CG linear strain field, $\epsilon_{\alpha \beta}^{lin}$ [using Eq. (B.7)], the CG linear stress, $\sigma_{\alpha \beta}^{lin}$ [Eq. (28)], the CG potential energy density, $\epsilon_{el}$ [Eq. (29)], and the fluctuating energy flux, $\frac{1}{2} Q_{force,rev,1}$ [Eq. (B.14)]. The coarse graining function used (43) is a 2D Gaussian, $\phi(r) = \frac{1}{\pi w^2} e^{-|r|^2/w^2}$.

We verified that for a lattice with uniform spring constants (i.e., $c = \delta K = 0$), the strain components are uniform and equal to the applied global strain for $w \gg d$, as expected, since in for this system, under homogeneous deformation, the particle displacements are affine. The resulting stress components are uniform as well, and are consistent with the continuum isotropic elastic moduli for a triangular lattice (Lamé constants $\lambda = \mu = \frac{\sqrt{3} K}{4}$). As expected, in this case the CG energy density conforms to the classical expression, $\epsilon_{el} = \frac{1}{2} \sigma_{lin} : \epsilon_{lin}$.

For disordered systems, even under a “homogeneous applied strain” as described above, there is a correction to the classical expression for the energy density, as detailed above. Fig. 2(a) presents a contour plot of the relative energy difference $\Delta \tilde{e} \equiv 2 \frac{\epsilon_{el}^{app}}{\sigma_{lin}^{app} \epsilon_{lin}^{app}} - 1 = -\frac{\text{div} Q_{force,rev,1}}{\sigma_{lin}^{app} \epsilon_{lin}^{app}}$, for a system of $30 \times 30$ particles, with $c = 2\%$ and $\delta K/K = 25\%$ subject to an applied strain $\epsilon_{xx}^{app} = -\epsilon_{yy}^{app} = 5 \cdot 10^{-3}$, $\epsilon_{xy}^{app} = 0$, calculated with a CG width, $w = 4d$. The deviation from the classical expression is non-negligible ($\Delta \tilde{e} \simeq 1\%$), even thought the present system has a relatively small disorder [we verified that in the same system, a linear stress-strain relation holds to within $4\%$ (43)]. It is interesting
to try to relate the fluctuating energy flux to a local measure of the disorder in the particle displacements. A possible field for characterizing the fluctuating displacements is the “noise” field \( \eta(\mathbf{r}) \equiv \sum_i m_i |\mathbf{u}'(\mathbf{r})|^2 \phi(|\mathbf{r} - \mathbf{r}_i(t)|) \), defined in an analogous way to the kinetic temperature. In Fig. 2(b) we compare the fluctuating energy flux with the gradient of the noise field. It appears that their magnitude (but not their directions) exhibits quite a strong correlation, suggesting that the fluctuating energy flux may indeed be related to gradients of the noise, but the corresponding “conductivity” may be anisotropic. This is to be expected, since the system is locally anisotropic [as the local elastic tensor has been checked to be anisotropic (43)]. It is possible that a tensorial, rather than scalar, characterization of the displacement fluctuations is required, analogous to an “anisotropic temperature”.

5 Conclusion

We have shown that the classical definition of granular temperature as a measure of the fluctuating kinetic energy is useful for the description of granular gases even when this temperature is not the (inverse of the) thermodynamic conjugate potential of the energy, as in (local) equilibrium. An analysis of the case of a near-elastic granular gas shows that indeed one can venture into the nonequilibrium domain starting from local equilibrium (for the near elastic case). The example of a binary granular gas mixture in which the temperatures of the components can be very different from each other and still the Chapman-Enskog method produces sensible results, is a compelling case in favor of the use of the granular temperature field for far-from-equilibrium sys-
tems, at least in the fluidized phase. In the ‘opposite’ limit of a granular solid we have shown that the heat flux (which is always present, even in athermal system, as shown in Appendix A) is not ‘lost’ when one performs a deformation of an elastic solid: its effect appears in the form of a correction to the classical elastic energy density. This correction is strongly correlated with the gradient of an ‘elastic temperature’ which is a measure of the degree of non-affinity induced by the randomness of the system. Note that the system considered is not pre-stressed whereas many granular systems are. This fact does not change the fundamental conclusion that in elastic solids there is an accumulation of energy as a result of work done on the non-affine (or fluctuating) degrees of freedom. As the physics of this finding is very general we believe it applies (with a proper modification) to granular solids beyond the elastic regime. Indeed a strong correlation of the displacement ‘noise’ with the appearance of localized plastic events has been suggested in (44). Another connection of this kind has been proposed in (45). At this stage we do not know whether there is a direct link between this ‘new’ contribution that stems from the heat flux and (gradients of) ‘configurational temperatures’. However, since there is an obvious link between diffusion and non-affinity (see e.g., (46)) and a seemingly established link between diffusion and a ‘configurational temperature’ (through an FD relation) it comes to reason that the ‘extra’ term in the elastic energy is related to a configurational measure of disorder. Following the spirit of a suggestion by Savage (47) one may perhaps conjecture that an effective temperature which combines the configurational and kinetic contributions (perhaps just as a sum) can serve as a generalized granular temperature valid for all granular phases (with appropriate extensions to other systems). At this stage it seems that much more research is necessary to establish whether this or similar conjectures are of any physical value. As a final comment we would like to mention the rather well known fact that (even relatively simple) non-equilibrium systems exhibit rich behavior and cannot usually be characterized by the same number of macroscopic variables or fields as (near) equilibrium systems. Therefore, even if it turns out that many properties of granular matter can be correlated with a generalized temperature or temperatures there is a good chance that more characterizations will be needed for this class of systems to fully describe or explain their behavior.

A Continuum Mechanics: a microscopic derivation

The equations of continuum mechanics are derived below from microscopic considerations. For sake of simplicity it is assumed that the constituents experience binary interactions whose reversible part is determined by a potential. The derivation below is a slight extension of what can be found in (26; 48) but unlike in (26) we do not invoke temporal coarse graining, for simplicity.
Consider a set of particles of mass \(m_i\), whose (center of mass) positions and velocities are \(\mathbf{r}_i(t)\) and \(\mathbf{v}_i(t) \equiv \dot{\mathbf{r}}_i(t)\), respectively. Let the binary interaction potential be denoted by \(U(\mathbf{r}_{ij})\), where \(\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j\). It is assumed that \(U = 0\) for \(i = j\). In addition, let \(\phi(\mathbf{r})\) denote a spatial coarse graining function, i.e. \(\phi\) is normalized (its integral over space equals unity), it is positive semidefinite and has a single maximum at \(\mathbf{r} = 0\). It is often convenient to employ a Gaussian distribution for \(\phi\). The width of \(\phi\) is the “coarse graining scale”.

The coarse-grained (CG) mass density, \(\rho(\mathbf{r}, t)\), at position \(\mathbf{r}\) and time \(t\) is given by: \(\rho(\mathbf{r}, t) \equiv \sum_i m_i \phi[\mathbf{r} - \mathbf{r}_i(t)]\). Note that while \(\mathbf{r}_i(t)\) is the position of particle \(i\) at time \(t\), \(\mathbf{r}\) is merely a considered position in space. Similarly, define the CG momentum density, \(\mathbf{p}(\mathbf{r}, t)\), by: \(\mathbf{p}(\mathbf{r}, t) \equiv \sum_i m_i \mathbf{v}_i(t) \phi[\mathbf{r} - \mathbf{r}_i(t)]\). The CG energy density, \(e(\mathbf{r}, t)\) is given by:

\[
e(\mathbf{r}, t) \equiv \sum_i \frac{1}{2} m_i v_i^2 \phi[\mathbf{r} - \mathbf{r}_i(t)] + \frac{1}{2} \sum_{i,j} U(\mathbf{r}_{ij}(t)) \phi[\mathbf{r} - \mathbf{r}_i(t)] \tag{A.1}
\]

By taking the time derivative of the density one obtains:

\[
\dot{\rho}(\mathbf{r}, t) = -\frac{\partial}{\partial \mathbf{r}_\alpha} \sum_i m_i v_{i\alpha}(t) \phi[\mathbf{r} - \mathbf{r}_i(t)] = -\text{div} \mathbf{p}(\mathbf{r}, t) \tag{A.2}
\]

where the summation convention has been invoked and Greek letters denote Cartesian coordinates. Defining the velocity field, \(\mathbf{V}(\mathbf{r}, t)\), as: \(\mathbf{V}(\mathbf{r}, t) \equiv \frac{\mathbf{p}(\mathbf{r}, t)}{\rho(\mathbf{r}, t)}\), one obtains from Eq. (A.2) the equation of continuity: \(\dot{\rho} = -\text{div} (\rho \mathbf{V})\). Next, upon taking the derivative of the momentum field one obtains:

\[
\dot{p}_\alpha(\mathbf{r}, t) = -\frac{\partial}{\partial \mathbf{r}_\beta} \sum_i m_i v_{i\alpha}(t) v_{i\beta}(t) \phi[\mathbf{r} - \mathbf{r}_i(t)] + \sum_i m_i \dot{v}_{i\alpha} \phi[\mathbf{r} - \mathbf{r}_i(t)] \tag{A.3}
\]

Denote by \(\mathbf{f}_i(t)\) the force experienced by particle \(i\) and by \(\mathbf{f}_{i/j}(t)\) the force exerted by particle \(j\) on \(i\). Using Newton’s second and third laws one obtains:

\[
\sum_i m_i \dot{v}_{i\alpha}(t) \phi[\mathbf{r} - \mathbf{r}_i(t)] = \sum_i \mathbf{f}_{i/j\alpha}(t) \phi[\mathbf{r} - \mathbf{r}_i(t)] = \sum_i \mathbf{f}_{j/i\alpha}(t) \phi[\mathbf{r} - \mathbf{r}_j(t)] = -\sum_{i,j} \mathbf{f}_{i/j\alpha}(t) \phi[\mathbf{r} - \mathbf{r}_j(t)].
\]

It follows that:

\[
\sum_i m_i \dot{v}_{i\alpha}(t) \phi[\mathbf{r} - \mathbf{r}_i(t)] = -\frac{1}{2} \sum_{ij} \mathbf{f}_{i/j\alpha}(t) \left( \phi[\mathbf{r} - \mathbf{r}_i(t)] - \phi[\mathbf{r} - \mathbf{r}_j(t)] \right)
\]

\[
= -\frac{1}{2} \sum_{ij} \mathbf{f}_{i/j\alpha}(t) \int_0^1 ds \frac{\partial}{\partial s} \phi[\mathbf{r} - \mathbf{r}_i(t) + s \mathbf{r}_{ij}(t)]
\]
\[
\dot{p}_\alpha(r, t) = -\frac{\partial}{\partial r_\beta} \frac{1}{2} \sum_i m_i f_{i/j\alpha} r_{ij\beta}(t) \int_0^1 ds \phi[r - r_i(t) + sr_{ij}(t)]
\] (A.4)

Substituting the latter result in Eq. (A.3) one obtains:  
\[
P_{\alpha\beta}(r, t) = \sum_i m_i v_{i\alpha}(t) v_{i\beta}(t) \phi[r - r_i(t)]
\] 
\[
+ \frac{1}{2} \sum_{ij} f_{i/j\alpha}(r, t) r_{ij\beta}(r, t) \int_0^1 ds \phi[r - r_i(t) + sr_{ij}(t)]
\] (A.5)

Next, define the fluctuating part of the velocity of a particle (when coarse graining is around the position \(r\) at time \(t\)) as: 
\[
v'_i(r, t) \equiv v_i(t) - V(r, t)
\]
Substituting this definition in Eq. (A.5) and performing straightforward algebra (using \(\sum_i v'_i(r, t) \phi(r - r_i(t)) = 0\), following the definitions of \(v'\) and the velocity field \(V\)), one obtains:
\[
P_{\alpha\beta}(r, t) = \rho(r, t) V_{\alpha}(r, t) V_{\beta}(r, t) + \sum_i m_i v'_{i\alpha}(r, t) v'_{i\beta}(r, t) \phi[r - r_i(t)]
\] 
\[
+ \frac{1}{2} \sum_{ij} f_{i/j\alpha}(r, t) r_{ij\beta}(r, t) \int_0^1 ds \phi[r - r_i(t) + sr_{ij}(t)]
\] (A.6)

Identifying
\[
\sigma^{\text{kin}}_{\alpha\beta}(r, t) = -\sum_i m_i v'_{i\alpha}(r, t) v'_{i\beta}(r, t) \phi[r - r_i(t)]
\] (A.7)
as the “kinetic stress” and
\[
\sigma^{\text{cont}}_{\alpha\beta}(r, t) = -\frac{1}{2} \sum_{ij} f_{i/j\alpha}(r, t) r_{ij\beta}(r, t) \int_0^1 ds \phi[r - r_i(t) + sr_{ij}(t)]
\] (A.8)
as the “contact stress”, the stress tensor, \(\sigma\), is given by:
\[
\sigma_{\alpha\beta}(r, t) = -\sum_i m_i v'_{i\alpha}(r, t) v'_{i\beta}(r, t) \phi[r - r_i(t)]
\] 
\[- \frac{1}{2} \sum_{ij} f_{i/j\alpha}(r, t) r_{ij\beta}(r, t) \int_0^1 ds \phi[r - r_i(t) + sr_{ij}(t)]
\] (A.9)
Note that an opposite convention for the sign of the stress tensor is often employed in the field of granular matter. It follows from Eq. (A.9) (employing \( p = \rho V \) and invoking the equation of continuity) that:

\[
\frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \rho \nabla \cdot \mathbf{V} = \frac{\partial \rho}{\partial t} + \rho \phi_{\beta} \nabla V = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial t} \frac{\partial}{\partial \rho} \nabla V = \frac{\partial \rho}{\partial t} \frac{\partial}{\partial \rho} \nabla V
\]

(A.10)

where \( \frac{D\rho}{Dt} = \frac{\partial \rho}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \) denotes the material derivative.

Next, consider the energy density. Taking the derivative of Eq. (A.1) one obtains after some simple algebra and the use of Newton’s second law:

\[
\dot{e}(\mathbf{r}, t) = -\frac{\partial}{\partial r_{\alpha}} \sum_i \left[ \frac{1}{2} m_i v_i^2(t) + \frac{1}{2} \sum_j U(\mathbf{r}_{ij}(t)) \right] v_{i\alpha}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
+ \sum_i \mathbf{f}_i(t) \cdot \mathbf{v}_i(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] - \frac{1}{2} \sum_i \mathbf{f}_{i,j}^{rev}(t) \cdot \mathbf{v}_{ij}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
+ \sum_i \frac{1}{2} m_i v_i^2(t) v_{i\alpha}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] + \frac{1}{2} \sum_{ij} U(\mathbf{r}_{ij}(t)) v_{i\alpha}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
- \mathbf{V}_\beta(\mathbf{r}, t) \mathbf{\sigma}^\text{kin}_{\alpha\beta}(\mathbf{r}, t) + \frac{1}{2} \sum_{ij} U(\mathbf{r}_{ij}(t)) v_{i\alpha}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
(A.11)

where the reversible part of the force \( \mathbf{f}_{i,j} \) is given by \( \mathbf{f}_{i,j}^{rev}(t) = -\frac{\partial U(\mathbf{r}_{ij}(t))}{\partial \mathbf{r}_{ij}(t)} \). Using the above decomposition of the velocity, \( \mathbf{v}_i(t) = \mathbf{v}_i'(\mathbf{r}, t) + \mathbf{V}(\mathbf{r}, t) + \mathbf{V}(\mathbf{r}, t) \), one obtains that the term whose divergence appears in Eq. (A.11) can be rewritten as:

\[
\sum_i \frac{1}{2} m_i v_i^2(t) v_{i\alpha}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] + \frac{1}{2} \sum_{ij} U(\mathbf{r}_{ij}(t)) v_{i\alpha}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
= e(\mathbf{r}, t) \mathbf{V}_\alpha(\mathbf{r}, t) + \frac{1}{2} \sum_i m_i v_i^2(t) v_{i\alpha}'(\mathbf{r}, t) v_{i\alpha}(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
- \mathbf{V}_\beta(\mathbf{r}, t) \mathbf{\sigma}^\text{kin}_{\alpha\beta}(\mathbf{r}, t) + \frac{1}{2} \sum_{ij} U(\mathbf{r}_{ij}(t)) v_{i\alpha}'(\mathbf{r}, t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
(A.12)

Next, note that

\[
\sum_i \mathbf{f}_i(t) \cdot \mathbf{v}_i(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] = \sum_{ij} \mathbf{f}_{i,j}(t) \cdot \mathbf{v}_i(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
= -\sum_{ij} \mathbf{f}_{i,j}(t) \cdot \mathbf{v}_j(t) \phi [\mathbf{r} - \mathbf{r}_j(t)] \\
= \frac{1}{2} \sum_{ij} \mathbf{f}_{i,j}(t) \cdot \mathbf{v}_j(t) \phi [\mathbf{r} - \mathbf{r}_i(t)] \\
+ \frac{1}{4} \sum_{ij} \mathbf{f}_{i,j}(t) \cdot (\mathbf{v}_i(t) + \mathbf{v}_j(t)) (\phi [\mathbf{r} - \mathbf{r}_i(t)] - \phi [\mathbf{r} - \mathbf{r}_j(t)])
\]
\[ \frac{1}{2} \sum_{ij} f_{ij}(t) \cdot v_{ij}(t) \phi \lfloor r - r_i(t) \rfloor \]

\[- \frac{\partial}{\partial r_\alpha} \frac{1}{4} \sum_{ij} f_{ij}(t) \cdot \lfloor v_i(t) + v_j(t) \rfloor r_{ij\alpha}(t) \int_0^1 ds \phi \lfloor r - r_i(t) + sr_{ij}(t) \rfloor \]

(A.13)

Using velocity decomposition and Eq. (A.8) one obtains from Eq. (A.13):

\[ \sum_i f_i(t) \cdot v_i(t) \phi \lfloor r - r_i(t) \rfloor = \frac{1}{2} \sum_{ij} f_{ij}(t) \cdot v_{ij}(t) \phi \lfloor r - r_j(t) \rfloor \]

\[- \frac{1}{4} \frac{\partial}{\partial r_\alpha} \sum_{ij} f_{ij}(t) \cdot \lfloor v'_i(r, t) + v'_j(r, t) \rfloor r_{ija}(t) \int_0^1 ds \phi \lfloor r - r_i(t) + sr_{ij}(t) \rfloor \]

\[ + \frac{\partial}{\partial r_\alpha} \left( V_\beta(r, t) \sigma_{\beta\alpha}^\text{cont}(r, t) \right) \]

(A.14)

Next, combining Eqs. (A.9, A.11, A.14) one obtains:

\[ \dot{e}(r, t) = - \frac{\partial}{\partial r_\alpha} \left( e(r, t) V_\alpha(r, t) - V_\beta(r, t) \sigma_{\beta\alpha}(r, t) + Q_\alpha(r, t) \right) - \rho(r, t) \Gamma(r, t) \]

(A.15)

where \( Q \) is identified as the heat flux and is given by:

\[ Q_\alpha = \frac{1}{2} \sum_{ij} \left( U(r_{ij}(t)) + m_i v_i^2 v_{i\alpha}' \right) v'_{i\alpha}(r, t) \phi \lfloor r - r_i(t) \rfloor \]

\[ + \frac{1}{4} \sum_{ij} f_{ij}(t) \cdot \lfloor v'_i(r, t) + v'_j(r, t) \rfloor r_{ija}(t) \int_0^1 ds \phi \lfloor r - r_i(t) + sr_{ij}(t) \rfloor \]

(A.16)

and the sink term, \(-\rho \Gamma\) is given by:

\[ -\rho(r, t) \Gamma(r, t) = \frac{1}{2} \sum_{ij} \left( f_{ij}(r, t) - f_{ij}^{\text{rev}}(r, t) \right) \cdot v_{ij}(r, t) \phi \lfloor r - r_i(t) \rfloor \]

\[ = \frac{1}{2} \sum_{ij} f_{ij}^{\text{irrev}}(r, t) \cdot v_{ij}(r, t) \phi \lfloor r - r_i(t) \rfloor \]

(A.17)

where the dissipative part of the force, \( f_{ij}^{\text{irrev}} \), is given by \( f_{ij} - f_{ij}^{\text{rev}} \). Note that the heat flux represents the transport of energy by the fluctuating velocity and the power related to the fluctuating velocities. The energy sink term is entirely due to the power associated with the dissipative part of the forces.
The energy density can be rewritten as follows:

\[
\begin{align*}
e(r, t) & \equiv \frac{1}{2} \sum_i m_i v_i^2 \phi [r - r_i(t)] \\
+ \frac{1}{2} \rho(r) V^2(r, t) + \frac{1}{2} \sum_{i,j} U(r_{ij}(t)) \phi [r - r_i(t)]
\end{align*}
\] (A.18)

Denote the internal specific energy by \(\bar{\rho} \). The latter is given by

\[
\rho(r, t) \bar{\rho}(r, t) \equiv \frac{1}{2} \sum_i m_i v_i^2 \phi [r - r_i(t)] + \frac{1}{2} \sum_{i,j} U(r_{ij}(t)) \phi [r - r_i(t)]
\] (A.19)

and the energy density therefore equals \(\frac{1}{2} \rho V^2 + \rho \bar{\rho}\). Substituting this decomposition into Eq. (A.15) and using Eqs. (A.2, A.10) one obtains:

\[
\rho(r, t) \frac{D\bar{\rho}(r, t)}{Dt} = \frac{\partial V_{\beta}(r, t)}{\partial r_\alpha} \sigma_{\beta\alpha}(r, t) - \text{div } Q(r, t) - \rho(r, t) \Gamma(r, t)
\] (A.20)

B  The quasistatic limit of Continuum Mechanics

Consider the case of slow deformations of a near-static assembly of particles. To this end, let the particle velocities be denoted by \(\mathbf{v}_i(t) = \delta \tilde{\mathbf{v}}_i(t)\), where \(\delta\) is a small parameter and \(\tilde{A}\) is considered to be \(O(1)\) for any dynamical variable, \(A\). The velocity field, \(\mathbf{V}\), as well as all other fields are rescaled in a similar way. Furthermore, let time be expressed as \(\tilde{t} = \frac{t}{\delta}\), hence \(\frac{\partial}{\partial t} = \delta \frac{\partial}{\partial \tilde{t}}\). With this rescaling the equations of continuum mechanics, Eqs. (A.2, A.10, A.15) become:

\[
\begin{align*}
\delta \frac{\partial \rho}{\partial \tilde{t}} &= -\delta \text{div } (\rho \mathbf{\tilde{V}}) \\
\delta^2 \rho \frac{D\mathbf{\tilde{V}}_\alpha}{Dt} &= \delta^2 \frac{\partial \sigma^{\text{kin}}_{\alpha\beta}}{\partial r_\beta} + \frac{\partial \sigma^{\text{cont}}_{\alpha\beta}}{\partial r_\beta} \\
\delta^3 \frac{\partial \tilde{e}^{\text{kin}}}{\partial \tilde{t}} + \delta \frac{\partial \tilde{e}^{\text{pot}}}{\partial \tilde{t}} &= -\frac{\partial}{\partial r_\alpha} \left( \delta^3 \tilde{e}^{\text{kin}}_\alpha + \delta \tilde{e}^{\text{pot}}_\alpha + \delta^3 \mathbf{\tilde{V}}_\beta \sigma^{\text{kin}}_{\beta\alpha} \\
- \delta^4 \tilde{e}^{\text{cont}}_\alpha \right) - \delta \rho \tilde{\Gamma}
\end{align*}
\] (B.1)

where the superscript ‘kin’ refers to the kinetic part, the superscript ‘pot’ refers to the potential part (involving the potential \(U\)) and the superscript
force refers to the fluctuating power contribution to the heat flux. To linear order in \( \delta \) the above equations reduce to:

\[
\frac{\partial \rho}{\partial t} = -\text{div} (\rho \vec{V}) \quad (B.2)
\]

\[
\frac{\partial \sigma_{\alpha\beta}^{\text{cont}}}{\partial r_\beta} = 0 \quad (B.3)
\]

\[
\frac{\partial \bar{e}_{\text{pot}}}{\partial t} = -\frac{\partial}{\partial r_\alpha} \left( e_{\text{pot}} \vec{V}_\alpha - \vec{V}_\beta \sigma_{\beta\alpha}^{\text{cont}} + Q_\alpha^{\text{pot}} + Q_\alpha^{\text{force}} \right) - \rho \bar{\Gamma} \quad (B.4)
\]

Using Eq. (B.3), the equation for the energy density becomes to linear order in the ‘slowness’, \( \delta \) (and after reverting to the original time variable):

\[
\frac{\partial e_{\text{pot}}}{\partial t} = -\frac{\partial}{\partial r_\alpha} \left( e_{\text{pot}} \vec{V}_\alpha + Q_\alpha^{\text{pot}} + Q_\alpha^{\text{force}} \right) + \frac{\partial \vec{V}_\beta}{\partial r_\alpha} \sigma_{\beta\alpha}^{\text{cont}} - \rho \Gamma \quad (B.5)
\]

We further specialize to the case when the particle relative displacements are small and the potential is quadratic in the relative displacements (to leading order). Let \( u_i(t) \) be the displacement of particle \( i \): \( \dot{u}_i(t) = v_i \). Also, define the displacement field \( u(r, t) \) via the Lagrangian relation:

\[
\frac{\partial u_{\text{La}}(R, t)}{\partial t} = V_{\text{La}}(R, t),
\]

where \( R \) is the initial position of a pathline and the superscript ‘La’ denotes the fact that one is employing Lagrangian coordinates. As shown in (43)

\[
u^\text{lin}(r, t) = \frac{\sum_i m_i u_i(t) \phi [r - r_i(t)]}{\sum_j m_j \phi [r - r_j(t)]} \quad (B.6)
\]

where the superscript ‘lin’ denotes the linear order in the displacements. To this order the (linear) strain field, \( \epsilon_{\alpha\beta}^{\text{lin}} \) is given by:

\[
\epsilon_{\alpha\beta}^{\text{lin}}(r, t) = \frac{1}{2} \left( \frac{\partial u_{\text{lin}}^{\alpha}(r, t)}{\partial r_\beta} + \frac{\partial u_{\text{lin}}^{\beta}(r, t)}{\partial r_\alpha} \right) \quad (B.7)
\]

Keeping in Eq. (B.5) only terms that are quadratic in the displacements one obtains (note that the potential is of second order in the displacements):

\[
\frac{\partial e_{\text{pot}}}{\partial t} = -\text{div} Q^{\text{force}} + \frac{\partial \vec{V}_\beta}{\partial r_\alpha} \sigma_{\beta\alpha}^{\text{cont}} - \rho \bar{\Gamma} \quad (B.8)
\]

Since for quadratic potentials \( \sigma_{\text{cont}}^{\text{lin}} \) is symmetric (as is easy to check, see also Eq. (28)) one can rewrite Eq. (B.8) as follows:

\[
\frac{\partial e_{\text{pot}}}{\partial t} = -\text{div} Q^{\text{force}} + \frac{1}{2} \left( \frac{\partial \vec{V}_\beta}{\partial r_\alpha} + \frac{\partial \vec{V}_\alpha}{\partial r_\beta} \right) \sigma_{\beta\alpha}^{\text{cont}} - \rho \bar{\Gamma} \quad (B.9)
\]
hence (to quadratic order in the displacements)

$$\frac{\partial e^{\text{bot}}}{\partial t} = -\text{div} \mathbf{Q}_{\text{force}} + \frac{\partial e^{\text{lin}}}{\partial t} \sigma^{\text{cont}, \alpha} - \rho \Gamma$$  \hspace{1cm} (B.10)

Consider next the following virtual dynamical evolution from a force free initial state to a final state at time $t_f$: $\mathbf{u}_i(t) = \mathbf{u}_i(t_f) \frac{t_f}{t}$. Assume that the reversible part of the force, $f^{\text{rev}}_{ij}$ is linear in the displacement difference $\mathbf{u}_{ij}$ and the irreversible part of the force is linear in the velocity difference $\mathbf{v}_{ij}$. In this dynamics the velocities are constant, the strain field satisfies $e^{\text{lin}}(\mathbf{r}, t) = e^{\text{lin}}(\mathbf{r}, t_f) \frac{t_f}{t}$, the reversible part of the contact stress, $\sigma^{\text{cont}, \text{rev}}$ (in which the force is replaced by the reversible part of the force) satisfies $\sigma^{\text{cont}, \text{rev}}(\mathbf{r}, t) = \sigma^{\text{cont}, \text{rev}}(\mathbf{r}, t_f) \frac{t_f}{t}$, the irreversible part of the contact stress, $\sigma^{\text{cont}, \text{irrev}}(\mathbf{r}, t)$, is constant in time, and similarly the part of the heat flux which corresponds to the reversible parts of the forces satisfies $Q^{\text{force}, \text{rev}}(\mathbf{r}, t) = Q^{\text{force}, \text{rev}}(\mathbf{r}, t_f) \frac{t_f}{t}$ and $Q^{\text{force}, \text{irrev}}(\mathbf{r}, t)$ is constant in time. In addition, $\rho \Gamma(\mathbf{r}, t)$ is constant in time. Note that within the approximation in which only the lowest nonvanishing order in the displacement is retained, $\mathbf{r}_{ij}(t)$ is replaced by $\mathbf{r}_{ij}(0)$. Upon substituting these expressions in Eq. (B.10) and integrating Eq. (B.10) over time from zero to $t_f$ one obtains:

$$e(\mathbf{r}, t_f) = \frac{1}{2} \epsilon^{\text{lin}}_{\alpha \beta}(\mathbf{r}, t_f) \sigma^{\text{cont}, \text{rev}}_{\beta \alpha}(\mathbf{r}, t_f) + \epsilon^{\text{lin}}_{\alpha \beta}(\mathbf{r}, t_f) \sigma^{\text{cont}, \text{irrev}}_{\beta \alpha}(\mathbf{r}, t_f)$$

$$- \frac{1}{2} \text{div} Q^{\text{force}, \text{rev}}(\mathbf{r}, t_f) t_f - \text{div} Q^{\text{force}, \text{irrev}}(\mathbf{r}, t_f) t_f - \rho(\mathbf{r}, t_f) \Gamma(\mathbf{r}, t_f) t_f \hspace{1cm} (B.11)$$

In order to keep the displacements fixed we replace the velocities that appear in the expressions for the various fields by $1/t_f$ times the corresponding displacements. A field in which the velocities have been replaced by the corresponding displacements is marked by a superscript I. It follows that at $t = t_f$: $\sigma^{\text{cont}, \text{rev}, \text{I}} = \sigma^{\text{cont}, \text{rev}}$, $\sigma^{\text{cont}, \text{irrev}, \text{I}} = t_f \sigma^{\text{cont}, \text{rev}}$, $Q^{\text{force}, \text{rev}, \text{I}} = t_f Q^{\text{force}, \text{rev}}$, $Q^{\text{force}, \text{irrev}, \text{I}} = t_f^2 Q^{\text{force}, \text{irrev}}$ (recall the assumption that $f^{\text{irrev}}_{ij}$ is linear in the particle velocities), and $(\rho \Gamma)^I = t_f^2 \rho \Gamma$. Substituting these expressions in Eq. (B.11), keeping the displacements fixed and letting $t_f$ go to infinity, one obtains:

$$e(\mathbf{r}, t_f) = \frac{1}{2} \epsilon^{\text{lin}}_{\alpha \beta}(\mathbf{r}, t_f) \sigma^{\text{cont}, \text{rev}}_{\beta \alpha}(\mathbf{r}, t_f) - \frac{1}{2} \text{div} Q^{\text{force}, \text{rev}, \text{I}}(\mathbf{r}, t_f) \hspace{1cm} (B.12)$$

where (changing $t_f$ to $t$) if follows from the expression for the heat flux, Eq (A.16) and the above definitions that

$$Q^{\text{force}, \text{rev}, \text{I}}_{\alpha} = \frac{1}{4} \sum_{i j} f^{\text{rev}}_{ij}(t) \cdot \left( \mathbf{u}'_i(\mathbf{r}, t) + \mathbf{u}'_j(\mathbf{r}, t) \right) r_{ij \alpha}(0) \hspace{1cm} (B.13)$$

27
\[
\times \int_0^1 ds \phi [r - r_i(t) + s r_{ij}(t)]
\]

where

\[
u'_i(r, t) \equiv u_i(t) - u^\text{lin}(r, t)
\]

is the displacement fluctuation of particle \(i\). We have thus obtained a correction to the classical formula for the elastic energy which represents the fluctuating work and stems from the integral of the heat flux over time. This result can be directly obtained from an analysis of the elastic energy, cf. Eq. (30).

References

[1] I. Oppenheim, Nonlinear response theory, in: J. W. Halley (Ed.), Correlation functions and quasiparticle interactions in condensed matter, Plenum, NY, 1998, pp. 235–258.
[2] H. Mori, Time-correlation functions in the statistical mechanics of transport processes, Phys. Rev. 111 (1958) 694–706.
[3] H. Mori, Statistical mechanical theory for transport in fluids, Phys. Rev. 112 (1958) 1829–1842.
[4] N. G. van Kampen, I. Oppenheim, Brownian motion as a problem of eliminating fast variables, Physica A 138 (1986) 231–248.
[5] S. Harris, An Introduction to the theory of the Boltzmann equation, Holt, Rinehart and Winston, New-York, 1971.
[6] I. Goldhirsch, A. S. Peletminskii, S. V. Peletminskii, A. I. Sokolovsky, Application of Bogolyubov’s approach to the derivation of kinetic equations for dissipative fluids, preprint (2007).
[7] S. Chapman, T. G. Cowling, The mathematical theory of nonuniform gases, Cambridge University Press, Cambridge, 1970.
[8] I. Goldhirsch, Rapid granular flows, Annu. Rev. Fluid Mech. 35 (2003) 267–293.
[9] M.-L. Tan, I. Goldhirsch, Rapid granular flows as mesoscopic systems, Phys. Rev. Lett. 81 (1998) 3022–3025.
[10] C. Goldenberg, I. Goldhirsch, Force chains, microelasticity, and macroelasticity, Phys. Rev. Lett. 89 (2002) 084302.
[11] C. Goldenberg, A. P. F. Atman, P. Claudin, G. Combe, I. Goldhirsch, Scale separation in granular packings: stress plateaus and fluctuations, Phys. Rev. Lett. 96 (2006) 168001.
[12] A. Mehta, S. F. Edwards, Statistical mechanics of powder mixtures, Physica A 157 (1989) 1091–1097.
[13] S. F. Edwards, The rheology of powders, Rheologica Acta 29 (1990) 493–499.
[14] H. A. Makse, J. Kurchan, Testing the thermodynamic approach to granular matter with a numerical model of a decisive experiment, Nature 415 (2002) 614–617.
[15] P. Mayor, G. D’Anna, A. Barrat, V. Loreto, Observing Brownian motion and measuring temperatures in vibration-fluidized granular matter, New J. Phys. 7 (2005) 1–16.
[16] I. Goldhirsch, T. P. C. van Noije, Green-Kubo relations for granular fluids, Phys. Rev. E 61 (2000) 3241–3244.
[17] N. V. Brilliantov, T. Pöschel, Self-diffusion in granular gases: Green-Kubo versus Chapman-Enskog, Chaos 15 (2005) 026108.
[18] A. B. J. Dufty, J. J. Brey, Linear response for granular fluids, J. Stat. Mech. Theor. and Expt. (2006) L08002.
[19] A. Puglisi, A. Baldassarri, V. Loreto, Fluctuation-dissipation relations in driven granular gases, Phys. Rev. E (2002) 061305.
[20] C. Tsallis, Possible generalization of Boltzmann-Gibbs statistics, J. Stat. Phys. 52 (1988) 479–487.
[21] C. Beck, Stretched exponentials from superstatistics, Physica A 365 (2006) 96–101.
[22] K. Hutter, K. R. Rajagopal, On flows of granular materials, Continuum Mechanics and Thermodynamics 6 (1994) 81–139.
[23] V. Kumaran, The constitutive relation for the granular flow of rough particles, J. Fluid Mech. 561 (2006) 1–42.
[24] N. Sela, I. Goldhirsch, Hydrodynamic equations for rapid flows of smooth inelastic spheres, to Burnett order, J. Fluid Mech. 361 (1998) 41–74.
[25] J. J. Brey, J. W. Dufty, C. S. Kim, A. Santos, Hydrodynamics of granular flow at low density, Phys. Rev. E 58 (1998) 4638–4653.
[26] B. J. Glasser, I. Goldhirsch, Scale dependence, correlations, and fluctuations of stresses in rapid granular flows, Phys. Fluids 13 (2001) 407–420.
[27] A. Goldshtein, M. Shapira, Mechanics of collisional motion of granular materials, part I: General hydrodynamic equations, J. Fluid Mech. 282 (1995) 75–114.
[28] I. Goldhirsch, M.-L. Tan, G. Zanetti, A molecular dynamical study of granular fluids: the unforced granular gas, J. Sci. Comp. 8 (1993) 1–40.
[29] R. Soto, M. Mareschal, Statistical mechanics of fluidized granular media: short-range velocity correlations, Phys. Rev. E 63 (2001) 041303.
[30] S. Luding, On the relevance of “molecular chaos” for granular flows, ZAMM. 80 (2000) S9–S12.
[31] T. P. C. van Noije, M. H. Ernst, Cahn-Hilliard theory for unstable granular fluids, Phys. Rev. E 61 (1997) 1765–1982.
[32] J. Wakou, R. Brito, M. H. Ernst, Towards a Landau-Ginzburg type theory for granular fluids, J. Stat. Phys 107 (2002) 3–22.
[33] S. H. Noskowicz, O. Bar-Lev, D. Serero, I. Goldhirsch, Strongly inelastic granular gases, cond-mat/0612694.
[34] V. Garzo, J. W. Dufty, Hydrodynamics of a granular binary mixture at low density, Phys. Fluids 14 (2002) 1476–1490.
[35] D. Serero, I. Goldhirsch, S. H. Noskowicz, M.-L. Tan, Hydrodynamics of granular gases and granular gas mixtures, J. Fluid Mech. 554 (2006) 237–258.

[36] G. M. L. Gladwell, Contact Problems in the Classical Theory of Elasticity, Sijthoff & Noordhoff, The Netherlands, 1980.

[37] K. L. Johnson, Contact Mechanics, Cambridge University Press, Cambridge, 1985.

[38] M. H. Sadd, Q. Tai, A. Shukla, Contact law effects on wave propagation in particulate materials using distinct element modeling, Int. J. Non-Linear Mech. 28 (1993) 251–265.

[39] O. R. Walton, Force models for particle-dynamics simulations of granular materials, in: E. Guazzelli, L. Oger (Eds.), Mobile Particulate Systems, Kluwer, Dordrecht, 1995, pp. 367–380.

[40] J. Schäfer, S. Dippel, D. E. Wolf, Force schemes in simulations of granular materials, J. de Physique I 6 (1996) 5–20.

[41] D. E. Wolf, Modeling and computer simulation of granular media, in: K. H. Hoffmann, M. Schreiber (Eds.), Computational Physics, Springer, Heidelberg, 1996, pp. 64–94.

[42] H. J. Herrmann, S. Luding, Review article: Modeling granular media on the computer, Cont. Mech. and Thermodynamics 10 (1998) 189–231.

[43] I. Goldhirsch, C. Goldenberg, On the microscopic foundations of elasticity, Eur. Phys. J. E 9 (2002) 245–251.

[44] C. Goldenberg, A. Tanguy, J.-L. Barrat, Particle displacements in the deformation of amorphous materials: local fluctuations vs. the non-affine field, cond-mat/0610518.

[45] A. Lemaitre, Rearrangements and dilatancy for sheared dense materials, Phys. Rev. Lett. 89 (2002) 195503.

[46] B. Utter, R. P. Behringer, Experimental measures of affine and non-affine deformation in granular shear, cond-mat/0702334.

[47] S. B. Savage, Analyses of slow high-concentration flows of granular materials, J. Fluid Mech. 377 (1998) 1–26.

[48] M. Babic, Average balance equations for granular materials, Int. J. Eng. Sci. 35 (1997) 523–548.