

Green–Kubo Expressions for a Granular Gas

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Received January 8, 2002; accepted June 10, 2002

The transport coefficients for a gas of smooth, inelastic hard spheres are obtained from the Boltzmann equation in the form of Green–Kubo relations. The associated time correlation functions are not simply those constructed from the fluxes of conserved densities. Instead, fluxes constructed from the reference local homogeneous distribution occur as well. The analysis exposes some complexities to be expected in the application of linear response methods to granular systems.

KEY WORDS: Granular flow; kinetic theory; Green–Kubo; hydrodynamics.

1. INTRODUCTION

The derivation of macroscopic equations (e.g., hydrodynamics) and associated transport coefficients from kinetic theory is limited in practice to weakly coupled systems (low density gases, ideal plasmas, anharmonic crystals). The application of formal methods from nonequilibrium statistical mechanics to this problem forty years ago provided the generality missing in kinetic theory.⁽¹⁾ These methods lead to the expected macroscopic dynamics with formally exact expressions for the transport coefficients known as Green–Kubo (GK) expressions. The latter are time integrals of equilibrium time correlation functions for the fluxes associated with conserved densities. The simplest example is the diffusion coefficient D for an impurity in a simple fluid

$$D = \lim_{t \rightarrow \infty} \frac{1}{d} \int_0^t dt' \langle \mathbf{v}(t) \cdot \mathbf{v} \rangle, \quad (1)$$

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where d is the dimension of the system, v is the impurity velocity, and the brackets denote an equilibrium ensemble average. Similar expressions apply for the viscosities, in terms of the autocorrelation function for the momentum flux, and the thermal conductivity, in terms of the autocorrelation function for the energy flux. The GK expressions provide an exact starting point for analysis and modeling of strongly coupled systems. In particular, they have stimulated extensive studies of transport via molecular dynamics simulation of these equilibrium time correlation functions. Much of the present knowledge about transport in strongly coupled systems (dense gases, liquids, plasmas, solids) derives from analysis of appropriate GK expressions.

Currently, there is great interest in the foundations of a fluid dynamics for granular media. Kinetic theory and statistical mechanical methods have been applied to idealized granular fluids comprised of smooth hard spheres interacting with inelastic collisions.⁽²⁻⁶⁾ The derivation of the corresponding Navier–Stokes level equations from kinetic theory at low and moderate densities has been given recently, with transport coefficients expressed as functions of the restitution coefficient.⁽⁷⁻⁹⁾ The results are in good agreement with selected tests using molecular dynamics and Monte Carlo simulations.⁽⁴⁾ It is tempting to expect that some form of the more general GK expressions should apply for granular media as well.^(3,10) The primary difference from normal fluids is the absence of a reference stable, stationary Gibbs state in terms of which the time correlation functions would be defined. Instead, the corresponding homogeneous state for an undriven system has a time dependence due to loss of energy on collisions (“cooling”). This is referred to as the homogeneous cooling state (HCS).^(11,12) Recently, analysis of impurity diffusion in a granular fluid has led to a GK expression similar to (1) with the velocity autocorrelation function defined in the HCS.^(3,13) A related analysis of impurity mobility also gives a GK expression for the mobility coefficient,⁽¹⁴⁾ although not simply in terms of the velocity autocorrelation function as is the case for normal fluids. The difference is due to the replacement of the Gibbs state by the HCS. Similar differences in the time correlation functions for other transport coefficients are found here as well. This is an indication that translation of linear response methods for normal fluids to granular fluids requires some care.

The objective here is to derive GK expressions for a granular gas based on the Boltzmann equation. This is accomplished by solving the Boltzmann equation by a method paralleling that used to derive the GK expressions from the Liouville equation. This may seem redundant since the transport coefficients are already known by other methods.⁽⁷⁾ However, the interest here is not so much in the transport coefficients themselves as

in their equivalent representation in terms of time integrals of appropriate correlation functions. It is not a priori clear that such a representation should exist since the reference homogeneous state is neither Gibbs-like nor stationary. What is the distribution over which the correlation functions should be defined? In what sense can these correlation functions be considered stationary when there is continual collisional cooling? What are the relevant fluxes being correlated and how is their time dependence generated? The answers to these questions are all known for the case of elastic collisions, but it is not obvious how they should be generalized to inelastic collisions. The analysis here provides this generalization in detail. Although limited to low density, it provides the necessary guidance and caution for a more general derivation based on the Liouville equation. The correlation functions are defined over a local HCS. When velocities are scaled with respect to the time dependent thermal velocity, and time is measured in terms of collision number, this state becomes stationary. As with the mobility, it is found that the time correlation functions involve fluxes generated from the local HCS rather than from the local Gibbs state. Furthermore, the time dependence is not simply determined from the linearized Boltzmann operator but includes additional time dependence of the temperature depending on the dimensions of the transport coefficient being considered. Of course, the results obtained agree with those from the Chapman-Enskog procedure and the time correlation functions reduce to those for the GK expressions in the elastic limit.

Although the changes found for a granular gas are significant, the representation of transport coefficients as time integrals of stationary correlation function remains and so we retain the terminology GK expressions. The new complications might seem to limit the utility of such expressions noted above for normal fluids. In particular, the Gibbs state is known analytically while the HCS is only known approximately. Such complications are associated with almost any nonequilibrium state and appear in both the GK and Chapman-Enskog representations. Nevertheless, the representation in terms of a stationary dynamics allows straightforward application of kinetic theory methods and molecular dynamics simulation. The suitability of the GK representation for these tools has been demonstrated recently for the self-diffusion coefficient.⁽¹⁵⁾ Excellent agreement between simulation and Boltzmann-Enskog kinetic theory is observed at moderate densities over a wide range of dissipation. Evaluation of GK expressions for other transport coefficients given here by direct simulation Monte Carlo is in progress.

It is a pleasure to dedicate this work to Bob Dorfman, colleague and mentor, who has taught us all so much about hard sphere transport (among many other subjects).

2. BOLTZMANN EQUATION AND HYDRODYNAMICS

The simplest model for a granular fluid is a system of N smooth hard spheres or disks at low density interacting via inelastic collisions. The collisions are characterized by a normal restitution coefficient $\alpha \leq 1$, where $\alpha = 1$ is the elastic limit. An accurate description of this gas can be obtained from a formal density expansion of the BBGKY hierarchy, just as for normal gases.^(6, 16) To leading order in the density, the single particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ obeys the Boltzmann equation, with collisions modified to account for the inelasticity,

$$(\partial_t + \mathbf{v} \cdot \nabla) f = J[f, f]. \quad (2)$$

The detailed form of the inelastic collision operator J is not required for the discussion here, beyond the properties required for the macroscopic balance equations:

$$\int d\mathbf{v} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2} m v^2 \end{pmatrix} J[f, f] = \begin{pmatrix} 0 \\ \mathbf{0} \\ -\frac{dp}{2} \zeta[f] \end{pmatrix}. \quad (3)$$

Here $p = nT$ is the low density pressure, n being the number density and T the granular temperature (with Boltzmann's constant set equal to unity). The functional $\zeta[f]$ is the "cooling rate," as will become apparent below. The number density and temperature, as well as the flow velocity \mathbf{u} are defined in the usual way

$$\begin{pmatrix} n \\ n\mathbf{u} \\ \frac{d}{2} nT \end{pmatrix} = \int d\mathbf{v} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2} mV^2 \end{pmatrix} f, \quad (4)$$

with $\mathbf{V} = \mathbf{v} - \mathbf{u}$, the velocity relative to the local flow. The balance equations for these fields follow directly from moments of the Boltzmann equation using Eq. (3),

$$D_t n + n \nabla \cdot \mathbf{U} = 0, \quad (5)$$

$$D_t u_i + (mn)^{-1} \nabla_j P_{ij} = 0, \quad (6)$$

$$D_t T + \frac{2}{dn} (P_{ij} \nabla_j u_i + \nabla \cdot \mathbf{q}) + T \zeta = 0, \quad (7)$$

where $D_t = \partial_t + \mathbf{u} \cdot \nabla$ is the material derivative. The pressure tensor P_{ij} and heat flux \mathbf{q} are linear functionals of f given by

$$P_{ij}[\mathbf{r}, t | f] = p(\mathbf{r}, t) \delta_{ij} + \int d\mathbf{v} D_{ij}(\mathbf{V}) f(\mathbf{r}, \mathbf{v}, t), \quad (8)$$

$$\mathbf{q}[\mathbf{r}, t | f] = \int d\mathbf{v} \mathbf{S}(\mathbf{V}) f(\mathbf{r}, \mathbf{v}, t). \quad (9)$$

Finally, the functions $D_{ij}(\mathbf{V})$ and $\mathbf{S}(\mathbf{V})$ characterizing the irreversible parts of the fluxes are

$$D_{ij}(\mathbf{V}) \equiv m \left(V_i V_j - \frac{1}{d} V^2 \delta_{ij} \right), \quad \mathbf{S}(\mathbf{V}) \equiv \left(\frac{m}{2} V^2 - \frac{d+2}{2} T \right) \mathbf{V}. \quad (10)$$

Clearly, the balance equations are not closed until the fluxes are expressed as functionals of the hydrodynamic fields n , \mathbf{u} , and T . This can be accomplished if a solution to the Boltzmann equation can be obtained in “normal form,”

$$f(\mathbf{r}, \mathbf{v}, t) = f(\mathbf{v} | \{y_\beta\}), \quad (11)$$

$$\{y_\beta(\mathbf{r}, t)\} \leftrightarrow \{n(\mathbf{r}, t), \mathbf{u}(\mathbf{r}, t), T(\mathbf{r}, t)\}. \quad (12)$$

The notation $f(\mathbf{v} | \{y_\beta\})$ means that the distribution is a functional of the hydrodynamic fields $y_\beta(\mathbf{r}, t)$, and that its space and time dependence occurs only through that of these fields. If such a solution can be found, its use in Eqs. (8) and (9) gives the fluxes as functionals of the fields. Such fluxes are then referred to as constitutive equations. The constitutive equations together with the exact macroscopic balance equations become a closed set of hydrodynamic equations. The origin of a hydrodynamic description in this context therefore is traced directly to the existence of a normal solution to the Boltzmann equation on some length and time scales. In practice, the functional form of this solution is constructed in some well-defined approximation, leading to corresponding approximate constitutive and hydrodynamic equations. The approximation of interest here is small spatial variations of the hydrodynamic fields over distances of the order of the mean free path. For gases with elastic collisions, the Chapman-Enskog method generates the normal solution perturbatively, and to leading order the constitutive equations are Newton's viscosity law and Fourier's heat law.^(1,17) The hydrodynamic equations become the Navier-Stokes equations. Application of this method to granular gases leads to similar results.⁽⁷⁾ The analysis is modified here to obtain the same results in an equivalent form with the transport coefficients represented by GK expressions.

3. SMALL GRADIENT SOLUTION

The first step in constructing the desired solution to the Boltzmann equation is to express it in terms of a reference distribution $f^{(0)}$,

$$f(\mathbf{r}, \mathbf{v}, t) = f^{(0)}(\mathbf{v} | \{y_\beta\}) + f^{(1)}(\mathbf{r}, \mathbf{v}, t). \quad (13)$$

The reference distribution is restricted to be normal and to give the exact moments of Eq. (4), i.e.,

$$\begin{pmatrix} n \\ n\mathbf{u} \\ \frac{d}{2}nT \end{pmatrix} = \int d\mathbf{v} \begin{pmatrix} 1 \\ \mathbf{v} \\ \frac{1}{2}mv^2 \end{pmatrix} f^{(0)}. \quad (14)$$

The Boltzmann equation then becomes

$$(\partial_t + \mathbf{v} \cdot \nabla + \bar{L}) f^{(1)} - J[f^{(1)}, f^{(1)}] = J[f^{(0)}, f^{(0)}] - (D_t + \mathbf{V} \cdot \nabla) f^{(0)}, \quad (15)$$

with the definition

$$\bar{L}f^{(1)} = -J[f^{(1)}, f^{(0)}] - J[f^{(0)}, f^{(1)}]. \quad (16)$$

The left side of Eq. (15) generates the dynamics of $f^{(1)}$. The solution of interest is such that $f^{(1)}$ should be proportional to the gradients of the hydrodynamic fields, since $f^{(0)}$ provides their local values through the constraint (14). This requires that the right side of (15) be proportional to the gradients of the fields. Evaluation of $(D_t + \mathbf{V} \cdot \nabla) f^{(0)}$ using the macroscopic balance equations gives terms proportional to the gradients, except for the contribution from the cooling rate in (7). In addition, the nonvanishing contribution $J[f^{(0)}, f^{(0)}]$ also is not of first order in the gradients. Therefore, the reference distribution is finally characterized by the condition that these non-gradient terms should vanish

$$J[f^{(0)}, f^{(0)}] + T\zeta^{(0)} \frac{\partial f^{(0)}}{\partial T} = 0, \quad \zeta^{(0)} = \zeta[f^{(0)}]. \quad (17)$$

This is an essential point in the analysis, and it is the origin of differences from the case of elastic collisions, as is discussed below. The distribution function $f^{(0)}$ is the analogue of the local Maxwellian for the case of elastic collisions, but the solution to Eq. (17) for $\alpha < 1$ is not the Maxwellian. Symmetry and dimensional analysis requires that $f^{(0)}$ have the scaling form

$$f^{(0)}(\mathbf{v} | \{y_\beta\}) = nv_0^{-d}(t) f^{(0)*}(\mathbf{V}^*), \quad \mathbf{V}^* = \mathbf{V}/v_0(t), \quad (18)$$

where $v_0(t) = [2T(t)/m]^{1/2}$ is the "thermal" velocity and $f^{(0)}$ is an isotropic function of \mathbf{V}^* . Then Eq. (17) is equivalent to

$$J[f^{(0)}, f^{(0)}] - \frac{1}{2} \zeta^{(0)} \frac{\partial}{\partial \mathbf{V}} \cdot (\mathbf{V} f^{(0)}) = 0. \quad (19)$$

Consider the initial condition $f^{(1)}(0) = 0$. This is a physically interesting case for hydrodynamics since $f^{(1)}(0)$ does not contribute to the initial value of the hydrodynamic fields, due to (14), and $f^{(0)}(0)$ is entirely determined by the hydrodynamic initial values. In this case, $f^{(1)}$ is manifestly proportional to the gradients of the fields. Retaining only terms of first order in these gradients, the Boltzmann equation becomes

$$(\partial_t + \bar{L}) f^{(1)} = -f^{(0)} \Phi_\beta \cdot \nabla y_\beta, \quad (20)$$

with the definitions

$$\Phi_1 = \frac{1}{n} \left(\mathbf{V} + \frac{T}{m} \frac{\partial}{\partial \mathbf{V}} \ln f^{(0)} \right), \quad (21)$$

$$\Phi_{2,ij} = \left(\frac{1}{d} \delta_{ij} \mathbf{V} \cdot \frac{\partial}{\partial \mathbf{V}} - V_i \frac{\partial}{\partial V_j} \right) \ln f^{(0)}, \quad (22)$$

$$\Phi_3 = m^{-1} \frac{\partial}{\partial \mathbf{V}} \ln f^{(0)} - \frac{\mathbf{V}}{2T} \left(d + \mathbf{V} \cdot \frac{\partial}{\partial \mathbf{V}} \ln f^{(0)} \right). \quad (23)$$

A term from $\zeta[f]$ to first order in the gradients does not occur since it vanishes. This follows from the fact that ζ is a scalar and can only be proportional to $\nabla \cdot \mathbf{u}$ at this order. Since $\Phi_{2,ij}(\mathbf{V})$ is traceless, there is no such contribution. The solution to Eq. (20) can be written in the form

$$f^{(1)} = -\mathbf{F}_\beta \cdot \nabla y_\beta. \quad (24)$$

When Eq. (24) is substituted into Eq. (20), the terms from $\partial_t \nabla y_\beta$ are higher order in the gradients, except for $\beta = 3$ which gives a contribution proportional to the cooling rate. The coefficients of the gradients are then found to obey the equations

$$(\partial_t + \bar{L}) \mathbf{F}_1 - \frac{T \zeta^{(0)}}{n} \mathbf{F}_3 = f^{(0)} \Phi_1, \quad (25)$$

$$(\partial_t + \bar{L}) F_{2,ij} = f^{(0)} \Phi_{2,ij}, \quad (26)$$

$$(\partial_t + \bar{L} - \frac{3}{2} \zeta^{(0)}) \mathbf{F}_3 = f^{(0)} \Phi_3. \quad (27)$$

4. SCALING

The apparent simplicity of Eqs. (25)–(27) is misleading since \bar{L} , $\zeta^{(0)}$, and Φ_α are functions of time through their dependence on the hydrodynamic fields. This dependence occurs as well for a gas with elastic collisions, but it can be neglected in that case when solving the equations since it is proportional to higher order gradients. For inelastic collisions, the temperature gives a time dependence that is of zeroth order in the gradients and cannot be neglected. However, it can be removed by a change of variables to dimensionless forms. A characteristic length scale is given by the mean free path ℓ and a dimensionless time s is defined accordingly by

$$ds = \frac{v_0(t)}{\ell} dt. \quad (28)$$

For simplicity we will take here $\ell = (n\sigma^{d-1})^{-1}$, where σ is the diameter of the particles, omitting a factor that depends on the dimension of the system. Integrating over an interval t shows that s is an average number of collisions during that time. Moreover, introduce dimensionless functions Φ_β^* and F_β^* as

$$\Phi_1 = \frac{2v_0(t)}{n} \Phi_1^*(\mathbf{V}^*), \quad \Phi_{2,ij} = 2\Phi_{2,ij}^*(\mathbf{V}^*), \quad \Phi_3 = \frac{2}{mv_0(t)} \Phi_3^*(\mathbf{V}^*), \quad (29)$$

$$\mathbf{F}_1 = \frac{2\ell}{v_0^d(t)} \mathbf{F}_1^*(\mathbf{V}^*, s), \quad F_{2,ij} = \frac{2n\ell}{v_0^{d+1}(t)} F_{2,ij}^*(\mathbf{V}^*, s), \quad \mathbf{F}_3 = \frac{2n\ell}{mv_0^{d+2}(t)} \mathbf{F}_3^*(\mathbf{V}^*, s). \quad (30)$$

In dimensionless form Eqs. (25)–(27) become

$$(\partial_s + \bar{\mathcal{L}}^*)(\mathbf{F}_1^* - \mathbf{F}_3^*) = f^{(0)*}(\Phi_1^* - \Phi_3^*), \quad (31)$$

$$(\partial_s + \bar{\mathcal{L}}^* + \frac{1}{2}\zeta^*) F_{2,ij}^* = f^{(0)*}\Phi_{2,ij}^*, \quad (32)$$

$$(\partial_s + \bar{\mathcal{L}}^* - \frac{1}{2}\zeta^*) \mathbf{F}_3^* = f^{(0)*}\Phi_3^*. \quad (33)$$

with the definitions

$$\bar{\mathcal{L}}^* = \bar{L}^* + \frac{1}{2}\zeta^* \frac{\partial}{\partial \mathbf{V}^*} \cdot \mathbf{V}^*, \quad (34)$$

$$\bar{L}^* = \frac{\ell}{v_0(t)} \bar{L}, \quad \zeta^* = \frac{\ell\zeta^{(0)}}{v_0(t)}. \quad (35)$$

The right sides of Eqs. (31)–(33) are independent of s , as are $\bar{\mathcal{L}}^*$ and ζ^* . The integration is now trivial

$$\mathbf{F}_1^*(\mathbf{V}^*, s) = \mathbf{F}_3^*(\mathbf{V}^*, s) + \int_0^s ds' e^{-s'\bar{\mathcal{L}}^*} f^{(0)*}(\Phi_1^* - \Phi_3^*), \quad (36)$$

$$F_{2,ij}^*(\mathbf{V}^*, s) = \int_0^s ds' e^{-s'(\bar{\mathcal{L}}^* + \frac{1}{2}\zeta^*)} f^{(0)*}\Phi_{2,ij}^*, \quad (37)$$

$$\mathbf{F}_3^*(\mathbf{V}^*, s) = \int_0^s ds' e^{-s'(\bar{\mathcal{L}}^* - \frac{1}{2}\zeta^*)} f^{(0)*}\Phi_3^*. \quad (38)$$

In the derivation of the above expressions, the assumed initial condition, implying that all the \mathbf{F}_β^* vanish for $s = 0$, has been used.

5. CONSTITUTIVE EQUATIONS

The pressure tensor and heat flux are determined from their definitions in Eqs. (8) and (9). Substitution of Eqs. (13) and (24) leads to results valid to first order in the gradients,

$$P_{ij}[\mathbf{r}, t | f] = p(\mathbf{r}, t) \delta_{ij} - \int d\mathbf{v} D_{ij}(\mathbf{V}) \mathbf{F}_\beta \cdot \nabla y_\beta, \quad (39)$$

$$\mathbf{q}[\mathbf{r}, t | f] = - \int d\mathbf{v} \mathbf{S}(\mathbf{V}) \mathbf{F}_\beta \cdot \nabla y_\beta. \quad (40)$$

Using fluid symmetry, these expressions reduce to

$$P_{ij} = p\delta_{ij} - \eta \left(\nabla_j u_i + \nabla_i u_j - \frac{2}{d} \delta_{ij} \nabla \cdot \mathbf{u} \right), \quad (41)$$

$$\mathbf{q} = -\kappa \nabla T - \mu \nabla n. \quad (42)$$

These are the expected Navier–Stokes constitutive equations, except for the additional term in the heat flux proportional to ∇n . It will be seen below that this new term is due entirely to the deviation of $f^{(0)}$ from the Maxwellian. The expressions for the transport coefficients are identified as

$$\eta = \frac{2nmlv_0(t)}{d^2 + d - 2} \int d\mathbf{V}^* D_{ij}^*(\mathbf{V}^*) F_{2,ij}^*(\mathbf{V}^*, s), \quad (43)$$

$$\kappa = \frac{nlv_0(t)}{d} \int d\mathbf{V}^* \mathbf{S}^*(\mathbf{V}^*) \cdot \mathbf{F}_3^*(\mathbf{V}^*, s), \quad (44)$$

$$\mu = \frac{mlv_0^3(t)}{d} \int d\mathbf{V}^* \mathbf{S}^*(\mathbf{V}^*) \cdot \mathbf{F}_1^*(\mathbf{V}^*, s). \quad (45)$$

The dimensionless forms of \mathbf{S} and D_{ij} are

$$\mathbf{S}^* \equiv \left(V^{*2} - \frac{d+2}{2} \right) \mathbf{V}^*, \quad D_{ij}^* = V_i^* V_j^* - \frac{1}{d} V^{*2} \delta_{ij}.$$

To put these expressions in the desired Green–Kubo form, define the adjoint operators L^* and \mathcal{L}^* by

$$\int d\mathbf{V}^* X(\mathbf{V}^*) \begin{pmatrix} \bar{L}^* \\ \bar{\mathcal{L}}^* \end{pmatrix} Y(\mathbf{V}^*) = - \int d\mathbf{V}^* Y(\mathbf{V}^*) \begin{pmatrix} L^* \\ \mathcal{L}^* \end{pmatrix} X(\mathbf{V}^*), \quad (46)$$

for arbitrary functions X and Y . From Eq. (34) it is trivially seen that

$$\mathcal{L}^* = L^* + \frac{1}{2} \zeta^* \mathbf{V}^* \cdot \frac{\partial}{\partial \mathbf{V}^*}. \quad (47)$$

The expression of L^* can be obtained by using the properties of the Boltzmann collision operator, but it will be not needed here.

Also, define “correlation functions” by

$$\langle XY \rangle = \int d\mathbf{V}^* f^{(0)*}(\mathbf{V}^*) X(\mathbf{V}^*) Y(\mathbf{V}^*). \quad (48)$$

Then, with these definitions and Eqs. (36)–(38), the transport coefficients given by Eqs. (43)–(45) can be rewritten as

$$\eta = \frac{2nm\ell v_0(t)}{d^2 + d - 2} \int_0^s ds' \langle D_{ij}^*(s') \Phi_{2,ij}^* \rangle e^{-\frac{1}{2}s'\zeta^*}, \quad (49)$$

$$\kappa = \frac{n\ell v_0(t)}{d} \int_0^s ds' \langle \mathbf{S}^*(s') \cdot \Phi_3^* \rangle e^{\frac{1}{2}s'\zeta^*}, \quad (50)$$

$$\mu = \frac{2T\kappa}{n} + \frac{m\ell v_0^3(t)}{d} \int_0^s ds' \langle \mathbf{S}^*(s') \cdot (\Phi_1^* - \Phi_3^*) \rangle. \quad (51)$$

The time dependence of the correlation functions is given by

$$X(s) = e^{s\mathcal{L}^*} X(\mathbf{V}^*). \quad (52)$$

Equations (49)–(51) are the Green–Kubo expressions for the transport coefficients of a low density granular gas. It is expected that the spectrum of \mathcal{L}^* assures that the correlation functions decay to zero for $s \gg 1$. This expectation is confirmed by low order matrix representations for \mathcal{L}^* ,⁽¹³⁾

kinetic model representations,⁽¹⁸⁾ and molecular dynamics simulations.⁽¹⁵⁾ In this limit, the above expressions agree with those obtained by the Chapman-Enskog method.⁽⁷⁾

6. DISCUSSION

To discuss the GK expressions for a granular gas it is instructive to write the corresponding results for elastic collisions ($\alpha = 1$). In that case, $f^{(0)}$ is the local Maxwellian and

$$\Phi_1^* \rightarrow 0, \quad \Phi_{2,ij}^* \rightarrow D_{ij}^*, \quad \Phi_3^* \rightarrow \mathbf{S}^*(\mathbf{V}). \quad (53)$$

Then $\mu \rightarrow \mu_0 = 0$, and

$$\eta \rightarrow \eta_0 = \frac{2nlv_0m}{d^2+d-2} \int_0^s ds' \langle D_{ij}^*(s') D_{ij}^* \rangle, \quad \kappa \rightarrow \kappa_0 = \frac{nlv_0}{d} \int_0^s ds' \langle \mathbf{S}^*(s') \cdot \mathbf{S}^* \rangle. \quad (54)$$

Since the temperature is constant to leading order in the gradients for $\alpha = 1$, the variable $s = (v_0/\ell)t$ is simply proportional to time. These are the standard forms for the GK expressions in terms of the autocorrelation functions composed from the “microscopic” fluxes \mathbf{S}^* and D_{ij}^* . There are several differences that occur for granular gases:

- The correlation functions are defined as averages over $f^{(0)}$. This local HCS distribution is determined from (19) and differs from the Maxwellian for all $\alpha < 1$.
- The correlation functions are not constructed from \mathbf{S}^* and D_{ij}^* alone. Each is paired with another function from the set Φ_β^* .
- The time integration is replaced by an integration over the average collision number, s . The correlation functions have approximate exponential decay in the variable s rather than t .
- The integrals over s are not controlled solely by the correlation functions. In addition there are time dependent factors arising from the change of the temperature over the duration of the integral.

The most surprising among these differences is the replacement of one of the “microscopic” fluxes \mathbf{S}^* or D_{ij}^* by one of the new variables Φ_β^* determined from $f^{(0)}$ through Eqs. (21)–(23). If $f^{(0)}$ were replaced by the local Maxwellian $f_M^{(0)*}$ in the above analysis, the correlation functions $\langle \mathbf{S}^*(s') \cdot \mathbf{S}^* \rangle$ and $\langle D_{ij}^*(s') D_{ij}^* \rangle$ would appear in Eqs. (49)–(51). However, this would not be a consistent solution to the Boltzmann equation and the

transport coefficients would not have the correct dependence on α (e.g., μ would vanish for all α). The role of $f^{(0)}$ is more than just a local reference state with the exact moments for n , T , and \mathbf{u} . In addition, it must be an approximate solution for the dynamics. In dimensionless form, $f^{(0)*}$ is a universal function of V^* determined from the equation

$$J^*[f^{(0)*}, f^{(0)*}] - \frac{1}{2} \zeta^* \frac{\partial}{\partial V^*} \cdot (\mathbf{V}^* f^{(0)*}) = 0, \quad \zeta^* = \zeta^*[f^{(0)*}], \quad (55)$$

without reference to any particular hydrodynamic state. The above analysis shows that (55) is necessary for a consistent ordering of the solution in terms of gradients. The local reference distribution for a given hydrodynamic state follows from this solution according to

$$f^{(0)} = n(\mathbf{r}, t) \left(\frac{m}{2T(\mathbf{r}, t)} \right)^{d/2} f^{(0)*} \left[\left(\frac{m}{2T(\mathbf{r}, t)} \right)^{1/2} (\mathbf{v} - \mathbf{u}(\mathbf{r}, t)) \right]. \quad (56)$$

Its dependence on the hydrodynamic variables is determined by the solution to (55).

An estimate for the Φ_β^* can be obtained from an approximation to $f^{(0)*}$ obtained by a polynomial expansion,^(11, 12) which to leading order is

$$f^{(0)*} = f_M^{(0)*} \left[1 + \frac{1}{4} c^*(\alpha) \left(V^{*4} - 5V^{*2} + \frac{15}{4} \right) \right], \quad (57)$$

$$c^*(\alpha) = \frac{32(1-\alpha)(1-2\alpha^2)}{81-17\alpha+30\alpha^2(1-\alpha)}. \quad (58)$$

This is known to be accurate to within a few percent for all α and $V^* \leq 1$. In this approximation the variables Φ_β^* become (for $d = 3$)

$$\Phi_1^* = \frac{1}{4} c^*(\alpha) \mathbf{S}^*, \quad (59)$$

$$\Phi_{2,ij}^* = D_{ij}^* \left[1 - \frac{1}{2} c^*(\alpha) (V^{*2} - \frac{5}{2}) \right], \quad (60)$$

$$\Phi_3^*(\mathbf{V}^*) = \mathbf{S}^* \left[1 - \frac{1}{2} c^*(\alpha) (V^{*2} - 1) \right]. \quad (61)$$

Thus, a straightforward "guess" for the GK relations based on results for normal fluids would miss the contributions proportional to $c^*(\alpha)$. Since this is small, for not too large inelasticity the quantitative effect would not be significant. However, such a guess might also miss the factors of $e^{\pm \frac{1}{2} s' \zeta^*}$ in (49) and (50) for similar reasons and these could have quantitative as well as conceptual consequences.

Linear response methods typically construct the response function for spatial perturbation of the homogeneous state of a specific type: those that couple only to the microscopic conserved densities. This follows from consideration of an initial local equilibrium state or maximum entropy state. Then manipulation of the response function for the conserved densities using the microscopic conservation laws leads to GK expressions in terms of the microscopic fluxes. One such quite reasonable approach has been described in ref. 10. As a specific example of those results, the shear viscosity at low density is given by (49) except with $\Phi_{2,ij}^*$ replaced by its elastic limit $\Phi_{2,ij}^* \rightarrow D_{ij}^*$. Thus the factor $e^{-\frac{1}{2}st^*}$, due to collisional cooling, is properly accounted for in the analysis, as is the stationary state dynamics of the scaled variables. Still, there is a difference due to their assumed perturbation of the HCS by linear combinations of the conserved fluxes. As this does not agree with the Chapman-Enskog result questions about their formal analysis arise. These issues and a derivation of the GK expressions from the Liouville equation will be discussed elsewhere.

In ref. 10 spatial perturbations of the HCS are introduced via linear combinations of the local densities of mass, energy, and momentum. The linear response functions (correlation functions) are therefore defined for the HCS. Since the HCS is known to be unstable to long wavelength perturbations, the long time limit cannot be performed in a simple way. In practice, as noted above, the time correlation functions are expected to decay rapidly so if the correlation time is small compared to that for the onset of the instability the GK coefficients are meaningful. They characterize transport near the HCS for intervals of its stability. This limitation does not exist for the analysis here, derived for perturbations relative to the local HCS. The latter is a specific function of the hydrodynamic variables, determined from the Boltzmann equation, but whose time dependence occurs only through those variables. Hence there can be no question of its stability. The more general Chapman-Enskog solution determines the time dependence of those hydrodynamic variables so the space and time dependence of the local HCS remains well defined as long as the nonlinear Navier-Stokes equations provide a good description on the macroscopic scale. There is growing evidence that this is the case, and that linear instability does not imply any pathology for the solution to the nonlinear equations.

The GK expressions and the Chapman-Enskog solution implicitly presume the existence of a hydrodynamic description on appropriate length and time scales. Given that existence, they provide the details of the description. To explore the approach to a hydrodynamic stage and the conditions for its validity, more detailed information about the nonhydrodynamic or microscopic modes is required. The study here does not bear on those questions.

APPENDIX A: EQUIVALENCES

The viscosity is given by (43) with (37)

$$\eta = \frac{2nm\ell v_0(t)}{d^2+d-2} \int_0^s ds' \int d\mathbf{V}^* D_{ij}^*(\mathbf{V}^*) e^{-s'(\bar{\mathcal{L}}^* + \frac{1}{2}\zeta^*)} f^{(0)*} \Phi_{2,ij}^*. \quad (\text{A1})$$

The equivalence of this GK expression with the shear viscosity obtained by the Chapman–Enskog method is shown as follows. Take $s \gg 1$ and perform the time integral in (A1) to get

$$\eta = \frac{2nm\ell v_0(t)}{d^2+d-2} \int d\mathbf{V}^* D_{ij}^*(\mathbf{V}^*) \left(\bar{\mathcal{L}}^* + \frac{1}{2}\zeta^* \right)^{-1} f^{(0)*} \Phi_{2,ij}^*. \quad (\text{A2})$$

The results (A.11) and (A.9) of refs. 4 and 7 are

$$\eta = \frac{1}{d^2+d-2} \int d\mathbf{V} D_{ij}(\mathbf{V}) \mathcal{C}_{ij}(\mathbf{V}), \quad (\text{A3})$$

where \mathcal{C}_{ij} is the solution to the integral equation

$$\left(\bar{L} - \zeta^{(0)T} \frac{\partial}{\partial T} \right) \mathcal{C}_{ij} = f^{(0)} \Phi_{2,ij}. \quad (\text{A4})$$

In the dimensionless units defined above this becomes

$$\left(\bar{\mathcal{L}}^* + \frac{1}{2}\zeta^* \right) \mathcal{C}_{ij}^*(\mathbf{V}^*) = f^{(0)*} \Phi_{2,ij}^*, \quad (\text{A5})$$

with

$$\mathcal{C}_{ij} \equiv \frac{2n\ell}{v_0^{d+1}(t)} \mathcal{C}_{ij}^*. \quad (\text{A6})$$

The change from $\bar{L} \rightarrow \bar{\mathcal{L}}^*$ is due to the change from the derivative with respect to T at constant \mathbf{V} to derivative with respect to T at constant \mathbf{V}^* , when account is taken of the different units used. Substitution of (A4)–(A6) into (A3) confirms equivalence with the GK result (A2). The analysis is similar for the other two transport coefficients.

Now consider the limit $\alpha \rightarrow 1$ in (A1),

$$\eta = \frac{2nm\ell v_0(t)}{d^2+d-2} \int_0^s ds' C^*(s), \quad (\text{A7})$$

with the correlation function

$$C^*(s) = \int d\mathbf{V}^* D_{ij}^* e^{-s\bar{L}^*} f^{(0)*} D_{ij}^*.$$

Use has been made of $\Phi_{2,ij}^* \rightarrow D_{ij}^*$, $\zeta^* \rightarrow 0$, and $\bar{\mathcal{L}}^* \rightarrow \bar{L}^*$ in this limit. Moreover, $f^{(0)*}$ becomes the Maxwellian. This is in fact the dimensionless form of the GK stress tensor autocorrelation function in the low density limit, with the time in units of the constant average collision time ℓ/v_0 .

ACKNOWLEDGMENTS

The research of J.W.D. was supported in part by the Department of Energy Grant (DE-FG03-98DP00218). The research of J.J.B. was partially supported by the Dirección General de Investigación Científica y Técnica (Spain) through Grant No. PB98-1124.

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