Transport coefficients for the hard-sphere granular fluid

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In the preceding paper, linear response methods have been applied to obtain formally exact expressions for the parameters of Navier-Stokes order hydrodynamics. The analysis there is general, applying to both normal and granular fluids with a wide range of collision rules. Those results are specialized here to the case of smooth, inelastic, hard spheres with constant coefficient of normal restitution, for further elaboration. Explicit expressions for the cooling rate, pressure, and transport coefficients are given and compared with the corresponding expressions for a system of elastic hard spheres. The scope of the results for further analytical explorations and possible numerical evaluation is discussed.

I. INTRODUCTION

Granular materials frequently exhibit flows similar to those of normal fluids, and for practical purposes these flows are often described by phenomenological hydrodynamic equations [1,2]. In the simplest cases, such equations have the form of Navier-Stokes hydrodynamics with an energy sink representing collisional "cooling." The parameters of these equations (cooling rate, pressure, and transport coefficients) are unknown in general. For normal fluids, methods of nonequilibrium statistical mechanics, e.g., linear response, have been applied to derive formally exact expressions for these parameters in a form that is suitable for introducing approximations. In the preceding paper [3], this analysis has been extended to granular fluids with similar results. The objective of the present work is to make those results more explicit by specializing to the idealized model granular fluid: a system of smooth, inelastic, hard spheres or disks. As has been shown in Ref. [3], this idealization is a limiting form for more realistic collisions, where the interaction energy scale, e.g., energy of deformation, is small compared to characteristic kinetic energies. This can be controlled by sufficient activation of the fluid, so the predictions of this model are more than academic [4]. Also, as in the case of simple atomic fluids, this idealized model of hard particles provides the most tractable setting for further theoretical analysis of the results obtained in this work.

A significant advantage of this limit is a scaling form of the reference homogeneous cooling state (HCS) to which linear response is applied. This scaling property results in several simplifications to the formalism described in [3]. For example, a stationary representation for the statistical mechanics of this granular fluid follows from the use of dimensionless phase space variables, where the particle velocities are scaled with the cooling thermal velocity in the HCS ensemble [5,6]. Furthermore, the hydrodynamic response functions for small spatial perturbations of the HCS are given in

terms of stationary time correlation functions in this representation. These time correlation functions are composed from two biorthogonal sets of observables, referred to here as the direct and conjugate functions. The direct functions are the microscopic observables whose ensemble averages are the hydrodynamic fields. The conjugate functions are generated by functional derivatives of a *local* HCS with respect to the hydrodynamic fields. For hard spheres or disks, it is possible to transform these functional derivatives into ordinary phase space derivatives. Generally, the simplifications made possible for hard spheres allow a somewhat more transparent interpretation of the dynamics and the structure involved in the formal expressions for transport coefficients. They also provide potentially better access to evaluation of these expressions using molecular dynamics (MD) simulations.

The purpose of this companion paper is twofold. The first is to specialize the results obtained in [3] to the particular system of inelastic hard particles, to give explicit expressions for the various hydrodynamic parameters, and to take advantage of this simplified setting to interpret their content [7]. The second is to record the various tools of nonequilibrium statistical mechanics of a system of inelastic hard particles, whose utility transcends the context of their application in this work. Regarding the first purpose, details of the analysis are suppressed in the main text, with the reader referred to the preceding paper or to the Appendixes here. Instead, emphasis is placed on the final results, and similarities or differences between Helfand and Green-Kubo representations for normal and granular fluid transport coefficients.

The second purpose is accomplished in most of the eight Appendixes, which summarize the statistical mechanics and dynamics for inelastic hard spheres. Although much of the formalism appears in part elsewhere, there are many new results as well. In addition to the generators for dynamics of phase space observables and the Liouville equation, the generator for time-reversed dynamics is identified. Also, the microscopic conservation laws for both the forward and time-reversed dynamics are given, and the two sets of different fluxes are identified. Although straightforward to obtain, these results do not appear in the literature even for elastic hard spheres. Similarly, although the Helfand representation for transport coefficients has been used in MD simulations of

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elastic hard spheres, the corresponding Green-Kubo expressions have not been discussed explicitly until recently [8,9]. All such elastic hard sphere coefficients are given in detail in Appendix F using the more general granular fluid formalism developed here. Dimensionless forms of the Liouville equation, including one suitable for MD simulation [10,11], the microscopic conservation laws, and a new set of balance equations for the conjugate functions noted above are derived in these Appendixes. All of these results are critical for interpreting the exact expressions given here for the transport coefficients, but are also the building blocks for more general future investigations of granular fluid properties using the nonequilibrium statistical mechanics of hard spheres.

The layout of this presentation is as follows. In the next section, the primary results of the previous paper are specialized for the case of inelastic hard particles whose collisional loss in energy is characterized by a constant coefficient of normal restitution α. Only a broad outline of the results is given in the main text, with the details of the dynamics and statistical mechanics of hard spheres recorded in the Appendixes. Then explicit expressions for the various hydrodynamic parameters are given. The cooling rate and pressure are obtained as averages over the HCS, which also can be expressed in terms of integrals over the associated reduced two-particle distribution function. The transport coefficients are given in both Helfand [12] and Green-Kubo [13] representations, in terms of the long-time limit of appropriate stationary time correlation functions for the HCS. Next, the relationship of these results to those obtained from kinetic theories is sketched briefly, as well as the possibility of numerical evaluation of the results using molecular dynamics simulation. Finally the key points in this work are summarized and some concluding remarks are made.

II. LINEAR RESPONSE

The microscopic model considered here is a system of smooth monodisperse hard spheres ($d=3$) or disks ($d=2$) of mass m and diameter σ, whose collisional loss in energy is characterized by a constant coefficient of normal restitution α. The details of the model, the statistical mechanics of this system, the generators of dynamics, and time correlation functions are given in Appendix A. In this section, the simplifications to the linear response theory developed in the previous paper, due to this choice of collision model, are identified and the results there translated to the case at hand.

A. Homogeneous cooling state

The reference state with respect to which the linear response of this system is studied, is the homogeneous hydrodynamic state whose entire time dependence arises due to the cooling temperature. This is the so-called homogeneous cooling state. First this reference state is characterized in the context of both the phenomenological macroscopic hydrodynamics, and the more fundamental statistical mechanics. At the level of hydrodynamics, this state is described by a solution with constant number density n_h and flow velocity U_h, and a homogeneous but time-dependent temperature $T_h(t)$, that obeys the hydrodynamic equation

$$\{\partial_t + \zeta_0[n_h, T_h(t)]\}T_h(t) = 0, \tag{1}$$

where $\zeta_0[n_h, T_h(t)]$ is a cooling rate that must be specified from the microscopic theory. By means of a Galilean transformation, it is always possible to consider $U_h = 0$. For the case of inelastic hard spheres or disks considered here, there is no microscopic energy scale associated with the collision model. Therefore, the temperature dependence of the cooling rate can be determined by dimensional arguments as $\zeta_0[n_h, T_h(t)] \propto T_h^{1/2}(t)$. Equation (1) then can be integrated to obtain the time dependence of the temperature,

$$T_h(t) = T_h(0)\left(1 + \frac{v_0(0)\zeta_0^* t}{2l}\right)^{-2} \tag{2}$$

with

$$\zeta_0^* \equiv \frac{l\zeta_0}{v_0(t)}, \quad v_0(t) \equiv \left(\frac{2T_h(t)}{m}\right)^{1/2} \tag{3}$$

being a dimensionless cooling rate and a "thermal velocity," respectively. Moreover, l is an appropriate length scale; for example, the mean free path. Equation (2) is the familiar Haff's cooling law [2] that is well established for inelastic hard sphere fluids as one of the signatures of the HCS.

At the level of statistical mechanics, the reference ensemble corresponding to this macrostate, the HCS ensemble, is given by a homogeneous "normal" solution to the Liouville equation, i.e., one whose entire time dependence occurs through the cooling temperature. Furthermore, the absence of any additional microscopic energy scale for hard spheres, implies that this temperature dependence can occur only through the scaling of the particle velocities v_r with the thermal velocity $v_0[T_h(t)]$,

$$\rho_h[\Gamma; T_h(t)]) = [lv_0(t)]^{-Nd}\rho_h^*\left(\left\{\frac{q_{rs}}{l}, \frac{v_r - U_h}{v_0(t)};\right.\right.$$
$$\left.\left. r, s = 1, \ldots, N\right\}\right), \tag{4}$$

where $\Gamma \equiv \{q_r, v_r; \ r = 1, \ldots, N\}$ is a point in the phase space of the system and $q_{rs} \equiv q_r - q_s$ the relative position of particle r with respect to particle s. This special form of the N-particle distribution function allows the temperature dependence of many average properties such as the cooling rate, pressure, and transport coefficients to be determined without explicit calculation. Another interesting consequence of the scaling nature of the HCS ensemble is its restriction to a constant total momentum surface in phase space,

$$\rho_h[\Gamma; n_h, T_h(t)]$$
$$= \delta\left(\frac{P - mNU_h}{mv_0(t)}\right)[\ell v_0(t)]^{-Nd}\bar{\rho}_h^*\left(\left\{\frac{q_{rs}}{l}, \frac{v_r - U_h}{v_0(t)};\right.\right.$$
$$\left.\left. r, s = 1, \ldots, N\right\}\right). \tag{5}$$

Here $\delta(x)$ is the Dirac delta function and $P = \Sigma_r m v_r$ the total momentum. The proof of this result is given in Appendix B.

It is useful to represent the dynamics more generally for other states in terms of the same dimensionless scaled vari-

ables as occur in the HCS, i.e., in terms of $\Gamma^* \equiv \{q_r^*, v_r^*; \ r = 1, \ldots, N\}$, with $q_r^* = q_r/l$ and $v_r^* = v_r/v_0(t)$, where $v_0(t)$ is defined from the temperature of a reference HCS state having the same intial total energy as the system under consideration. In this way, it is seen that the HCS is a stationary solution to the dimensionless Liouville equation, and the HCS time correlation functions also become stationary. Thus, this representation for the statistical mechanics, allows the problem of linear response about a nonequilibrium time dependent reference state to be mapped onto one where the reference is stationary, in closer correspondence to the equilibrium case for normal fluids. More details of this transformation are given in Appendix B.

B. Hydrodynamic response

In this section, the response of the fluid to small spatial perturbations about the reference state described above is considered. The macroscopic variables of interest are the dimensionless deviations δy_α^* of the hydrodynamic fields y_α from their HCS values $y_{\alpha,h}$. They are defined by

$$\{\delta y_\alpha^*\} \equiv \{\delta n^*, \delta T^*, \delta U^*\}, \tag{6}$$

$$\delta n^* \equiv \frac{\delta n}{n_h} = \frac{n - n_h}{n_h}, \quad \delta T^* \equiv \frac{\delta T}{T_h(t)} = \frac{T - T_h(t)}{T_h(t)},$$

$$\delta U^* \equiv \frac{\delta U}{v_0(t)} = \frac{U - U_h}{v_0(t)}, \tag{7}$$

where $n(r,t)$, $T(r,t)$, and $U(r,t)$ denote, respectively, the number density, temperature, and flow velocity fields. The dynamics of these hydrodynamic fields is given by a response equation of the form

$$\delta \tilde{y}_\alpha^*(k^*, s) = \sum_\beta \tilde{C}_{\alpha\beta}^*(k^*, s) \delta \tilde{y}_\beta^*(k^*, 0). \tag{8}$$

A Fourier representation in the reduced space variable has been introduced to take advantage of the homogeneity of the reference state. Also, the dimensionless time scale s defined through

$$ds = \frac{v_0(t)dt}{l} \tag{9}$$

is used. The matrix of response functions $\tilde{C}^*$ gives the effect of weak spatial perturbations of the hydrodynamic fields on the dynamics of this fluid. Such response functions can be identified in two ways [3]: either from the linearized phenomenological hydrodynamic equations or from nonequilibrium statistical mechanics. Equating the two in their common domain of validity (large space and time scales) allows identification of exact expressions for the parameters of the phenomenological hydrodynamic equations.

The solution to the dimensionless, linearized, phenomenological hydrodynamic equations gives

$$\tilde{C}^{*\text{hyd}}(k^*, s) = e^{-s\mathcal{K}^{*\text{hyd}}(k^*)}. \tag{10}$$

If the components of the flow velocity are chosen to be the longitudinal component relative to k^*, $\delta \tilde{U}_\parallel^* \equiv k^* \cdot \delta \tilde{U}^*/k^*$, and $d-1$ orthogonal transverse components, $\delta \tilde{U}_{\perp i}^*$, the dimensionless transport matrix $\mathcal{K}^{*\text{hyd}}$ is block diagonal,

$$\mathcal{K}^{*\text{hyd}} = \begin{pmatrix} \mathcal{K}_1^{*\text{hyd}} & 0 \\ 0 & \mathcal{K}_2^{*\text{hyd}} \end{pmatrix}. \tag{11}$$

Here $\mathcal{K}_1^{*\text{hyd}}$ is the "longitudinal" part, corresponding to $\{\delta \tilde{n}^*, \delta \tilde{T}^*, \delta \tilde{U}_\parallel^*\}$, and it is given by

$$\mathcal{K}_1^{*\text{hyd}}(k^*) = \begin{pmatrix} 0 & 0 & -ik^* \\ \zeta_0^* \dfrac{\partial \ln \zeta_0}{\partial \ln n_h} + \left(\dfrac{2\mu^*}{d} - \zeta^{*n} \right)k^{*2} & \dfrac{\zeta_0^*}{2} + \left(\dfrac{2\lambda^*}{d} - \zeta^{*T} \right)k^{*2} & -i\left(\dfrac{2p_h^*}{d} + \zeta^{*U} \right)k^* \\ -\dfrac{ip_h^*}{2}\dfrac{\partial \ln p_h}{\partial \ln n_h}k^* & -\dfrac{ip_h^*}{2}k^* & -\dfrac{\zeta_0^*}{2} + \left(\dfrac{2(d-1)}{d}\eta^* + \kappa^* \right)k^{*2} \end{pmatrix}, \tag{12}$$

while $\mathcal{K}_2^{*\text{hyd}}$ is associated with the "transverse" components $\delta \tilde{U}_{\perp i}$, which are decoupled from the former,

$$\mathcal{K}_2^{*\text{hyd}}(k^*) = \left(-\frac{\zeta_0^*}{2} + \eta^* k^{*2} \right) I, \tag{13}$$

where I is the unit matrix of dimension $d-1$. The dimensionless parameters and transport coefficients in the above equations are defined by

$$p_h^* = \frac{p_h}{n_h T_h}, \quad \zeta_0^* = \frac{l\zeta_0}{v_0}, \quad \lambda^* = \frac{\lambda}{ln_h v_0},$$

$$\mu^* = \frac{\mu}{lT_h v_0}, \quad \eta^* = \frac{\eta}{mn_h l v_0}, \quad \kappa^* = \frac{\kappa}{mn_h l v_0}, \tag{14}$$

$$\zeta^{*U} = \zeta^U, \quad \zeta^{*n} = \frac{n_h \zeta^n}{lv_0}, \quad \zeta^{*T} = \frac{T_h \zeta^T}{lv_0}.$$

Above, p_h is the pressure of the granular fluid, ζ_0 is the cooling rate, λ is the thermal conductivity, μ is the new transport coefficient associated with granular fluids that measures the contribution of density gradients to the heat flux, η is the shear viscosity, and κ is the bulk viscosity. Finally, ζ^U,

ζ^n, and ζ^T are transport coefficients arising from the local cooling rate. The phenomenological definition of all these quantities has been given in Ref. [3]. The associated dimensionless quantities have been introduced in Eqs. (14), and advantage has been taken of the already mentioned fact that the temperature dependence of all the parameters in the hydrodynamic equations can be determined by dimensional arguments, as a consequence of dealing with hard particles.

The dimensionless transport matrix $\mathcal{K}^{*\mathrm{hyd}}$ is a constant independent of time s and, consequently, the response function $\widetilde{C}^*$ is related to the transport matrix by the simple exponential form given in Eq. (10). This is one of the primary simplifications that occur for this hard-sphere or -disk system. Further, the eigenvalues of the $\mathcal{K}^{*\mathrm{hyd}}$ matrix give the hydrodynamic modes of the system, and its eigenfunctions identify the particular excitations of the hydrodynamic fields that give rise to these modes. These can be used to get physical insight into the hydrodynamic response of this fluid. Some of these considerations are addressed in Appendix C.

Alternatively, an exact response equation of the form of Eq. (8) can be identified by carrying out a linear response analysis at the level of statistical mechanics of the system. In this way, the response function $\widetilde{C}^*$ is found to be a matrix of time correlation functions of the form

$$\widetilde{C}^*_{\alpha\beta}(\mathbf{k}^*;s) = V^{*-1}\int d\Gamma^*\widetilde{a}^*_\alpha(\Gamma^*;\mathbf{k}^*)e^{-s\bar{\mathcal{L}}^*}\widetilde{\psi}^*_\beta(\Gamma^*,-\mathbf{k}^*). \quad (15)$$

Here, V^* is the volume of the system in reduced units and the "direct" functions $\widetilde{a}^*_\alpha$ are dimensionless Fourier transforms of linear combinations of the microscopic densities whose ensemble average gives the hydrodynamic fields,

$$\widetilde{a}^*_\alpha(\mathbf{k}^*) = l^{-d}\int d\mathbf{r}\, e^{i\mathbf{k}\cdot\mathbf{r}}a^*_\alpha(\mathbf{r}) = \int d\mathbf{r}^* e^{i\mathbf{k}^*\cdot\mathbf{r}^*}a^*_\alpha(\mathbf{r}), \quad (16)$$

$$\{a^*_\alpha\} \equiv \left\{\mathcal{N}^*, \frac{2}{d}\left(\mathcal{E}^* - \frac{d}{2}\mathcal{N}^*\right), \mathcal{G}^*\right\}, \quad (17)$$

where

$$\{\mathcal{N}^*,\mathcal{E}^*,\mathcal{G}^*\} \equiv \left\{\frac{\mathcal{N}(\Gamma;\mathbf{r})}{n_h}, \frac{\mathcal{E}(\Gamma;\mathbf{r})}{n_h T_h(t)}, \frac{\mathcal{G}(\Gamma;\mathbf{r})}{n_h m v_0(t)}\right\}. \quad (18)$$

The phase functions $\mathcal{N}$, $\mathcal{E}$, and $\mathcal{G}$ are the microscopic number density, energy density, and momentum density, respectively. Their mathematical expressions are given in Ref. [3]. The "conjugate" functions $\widetilde{\psi}^*_\beta$ in Eq. (15) are generated by functional derivatives of the local HCS ensemble $\rho_{lh}[\,\Gamma|\{y_\alpha\}]$ as also described in [3],

$$\widetilde{\psi}^*_\beta(\Gamma^*;\mathbf{k}^*) = M_\beta\int d\mathbf{r}\, e^{i\mathbf{k}\cdot\mathbf{r}}\left[\frac{\delta\rho_{lh}[\,\Gamma|\{y_\alpha\}]}{\delta y_\beta(\mathbf{r})}\right]_{\{y_\alpha\}=\{n_h,T_h(t),0\}}. \quad (19)$$

In the above expression, the M_β's are factors that render the functions ψ^*_β dimensionless, namely,

$$M_1 = [lv_0(T_h)]^{dN}n_h, \quad M_2 = [lv_0(T_h)]^{dN}T_h,$$

$$M_\parallel = M_{\perp i} = [lv_0(T_h)]^{dN}v_0(T_h). \quad (20)$$

The local HCS inherits some of the scaling nature of the true HCS ensemble, and is identified as [14]

$$\rho_{lh}[\,\Gamma|\{y_\alpha\}] = \left(\prod_{r=1}^N [lv_0(\mathbf{q}_r)]^{-d}\right)\rho^*_h\left(\left\{\frac{\mathbf{q}_{rs}}{l}, \frac{\mathbf{v}_r - U(\mathbf{q}_r)}{v_0(\mathbf{q}_r)}\right\}\Big| n\right), \quad (21)$$

where $v_0(\mathbf{q}_r) \equiv v_0[T(\mathbf{q}_r)]$. The functional dependence on the density field is obtained by considering the HCS in an external inhomogeneous field and inverting the relation giving the density profile [14]. Clearly, for uniform hydrodynamic fields this becomes the HCS of Eq. (4).

The generator of the dynamics $\bar{\mathcal{L}}^*$ in Eq. (15), is a composition of the dimensionless Liouville operator $\bar{L}^*$ that generates the trajectories in phase space plus a velocity scaling operator,

$$\bar{\mathcal{L}}^* = \bar{L}^* + \frac{\zeta^*_0}{2}\sum_{r=1}^N \frac{\partial}{\partial\mathbf{v}^*_r}\cdot\mathbf{v}^*_r, \quad (22)$$

$$\bar{L}^* = \frac{l}{v_0(t)}\bar{L} = [L]_{\{q_r=q^*_r, v_r=v^*_r\}}. \quad (23)$$

The Liouville operator $\bar{L}$ associated with this system of hard particles is identified explicitly in Appendix A. The second operator on the right-hand side of Eq. (22) rescales the velocities with an s dependence associated with the thermal velocity, and represents the effects of cooling in the reference HCS. This simplified form of the modified generator of dynamics in the time correlation functions is another special feature of the hard-sphere collision model, or, equivalently, of the absence of any other microscopic energy scale.

Using the form of the local HCS given in Eq. (21), the functional derivatives with respect to the temperature and flow velocity in Eq. (19), can be simplified to the forms

$$\widetilde{\psi}^*_2(\Gamma^*;\mathbf{k})$$

$$= M_2\int d\mathbf{r}\, e^{i\mathbf{k}\cdot\mathbf{r}}\sum_{s=1}^N\left[\frac{\partial\rho_{lh}[\,\Gamma|\{y_\alpha\}]}{\partial T(\mathbf{q}_s)}\right]_{\{y_\alpha\}=\{n,T,0\}}\delta(\mathbf{r}-\mathbf{q}_s)$$

$$= -\frac{1}{2}\sum_{s=1}^N e^{i\mathbf{k}^*\cdot\mathbf{q}^*_s}\frac{\partial}{\partial\mathbf{v}^*_s}\cdot[\mathbf{v}^*_s\rho^*_h(\Gamma^*)], \quad (24)$$

$$\widetilde{\psi}^*_{\parallel,\perp i}(\Gamma^*;\mathbf{k})$$

$$= M_\parallel\int d\mathbf{r}\, e^{i\mathbf{k}\cdot\mathbf{r}}\sum_{s=1}^N\left[\frac{\partial\rho_{lh}[\,\Gamma|\{y_\alpha\}]}{\partial U_{\parallel,\perp i}(\mathbf{q}_s)}\right]_{\{y_\alpha\}=\{n,T,0\}}\delta(\mathbf{r}-\mathbf{q}_s)$$

$$= -\sum_{s=1}^N e^{i\mathbf{k}^*\cdot\mathbf{q}^*_s}\frac{\partial}{\partial v^*_{s,\parallel,\perp i}}\rho^*_h(\Gamma^*). \quad (25)$$

If this linear response analysis were done for a normal fluid using the canonical Gibbs ensemble $\rho_c(\Gamma)$, the functions $\widetilde{\psi}^*_\alpha$

would reduce to quantities proportional to the familiar microscopic densities $\tilde{a}_\alpha$ multiplied by the Gibbs equilibrium ensemble ρ_c. Hence, the different forms of the conjugate densities appearing in Eq. (15) for the case of granular fluids, are a manifestation of the fact that the linear response is now being measured about a nonequilibrium macrostate.

Two different representations for the hydrodynamic response matrix C^* have been identified in Eqs. (10) and (15), respectively. The latter representation is exact and valid for all times and for all length scales. On the other hand, the former representation is obtained from the phenomenological hydrodynamic equations, which are the relevant description of the fluid on length scales long compared to the mean free path and time scales long compared to the mean free time. In this limit, the exact response functions (15) must go over to that given in Eq. (10), thereby providing an exact identification of all the hydrodynamic parameters in terms of time correlation functions. To facilitate this identification, the exact analog of the hydrodynamic transport matrix $\mathcal{K}^{*\mathrm{hyd}}$ defined in Eqs. (11)–(13) above is identified as

$$\mathcal{K}^*(\boldsymbol{k}^*,s) = -[\partial_s \widetilde{C}^*(\boldsymbol{k}^*;s)]\widetilde{C}^{*-1}(\boldsymbol{k}^*;s), \quad (26)$$

and the crossover to hydrodynamics stated above is

$$\mathcal{K}^{*\mathrm{hyd}}(\boldsymbol{k}^*) = \lim_{s \gg 0, k^* \ll 1} \mathcal{K}^*(\boldsymbol{k}^*,s). \quad (27)$$

This is the prescription carried out in Ref. [3] to obtain Helfand and Green-Kubo representations for the transport coefficients of a granular fluid. To lowest order, $k^*=0$, the exact expression for the cooling rate of the fluid is identified. At Euler order, linear order in k^*, the pressure and the Euler transport coefficient ζ^U are identified. Finally, to order k^{*2} the six Navier-Stokes transport coefficients are all obtained.

III. HYDRODYNAMIC PARAMETERS AND TRANSPORT COEFFICIENTS

A. Overview

In this section, the exact explicit expressions for each of the parameters occurring in the phenomenological hydrodynamic equations at Navier-Stokes order are given, and their technical and physical content is noted. Dimensionless units are used throughout, and for simplicity the length scale is now chosen by the condition $n_h l^d = 1$.

The required "equations of state" are expressions for the cooling rate and the pressure as functions of the density and temperature. These are given as averages of specific phase functions over the HCS distribution function. The phase functions are sums of functions involving the phase coordinates of pairs of particles, and so the averages can be expressed as integrals over the associated reduced two-particle distribution function defined by

$$f_h^{*(2)}(\boldsymbol{q}_{12}^*,\boldsymbol{v}_1^*,\boldsymbol{v}_2^*) = N(N-1)$$

$$\times \int d\boldsymbol{q}_3^* \int d\boldsymbol{v}_3^* \cdots \int d\boldsymbol{q}_N^* \int d\boldsymbol{v}_N^* \rho_h^*(\Gamma^*). \quad (28)$$

This function depends on the positions of particles only through $\boldsymbol{q}_{12}^* \equiv \boldsymbol{q}_1^* - \boldsymbol{q}_2^*$, as a consequence of the translational invariance of the HCS (homogeneity). The occurrence of $f_h^{*(2)}$ for the properties considered here, depends on $\boldsymbol{q}_{12}^*$ only on the sphere for the pair at contact, i.e., for $q_{12}^* = \sigma^* \equiv \sigma/l$. The velocity dependence can be represented in terms of the relative velocity $\boldsymbol{g}_{12}^* = \boldsymbol{v}_1^* - \boldsymbol{v}_2^*$, and the center of mass velocity $\boldsymbol{G}_{12}^* = (\boldsymbol{v}_1^* + \boldsymbol{v}_2^*)/2$. If the center of mass velocity can be integrated out, the result is a probability distribution for the magnitude of the relative velocity and the cosine of the impact angle, i.e., $x = |\boldsymbol{q}_{12}^* \cdot \boldsymbol{g}_{12}^*|/q_{12}^* g_{12}^*$ at contact,

$$F_h^*(g_{12}^*,x) = \int d\boldsymbol{G}_{12}^* f_h^{*(2)}(\boldsymbol{q}_{12}^*,\boldsymbol{v}_1^*,\boldsymbol{v}_2^*). \quad (29)$$

As shown below, the cooling rate, the pressure, and some parts of the transport coefficients can be expressed as low-degree moments of $F_h^*(g_{12}^*,x)$.

The dimensionless transport coefficients ϖ^* will be given in two equivalent representations. The (intermediate) Helfand expressions are long-time limits of time correlation functions, while the Green-Kubo expressions are given in terms of time integrals of related time correlation functions. These two representations are related by the simple identities

$$\varpi^* = \lim \Omega_H(s) = \Omega_0 + \lim \int_0^s ds' \Omega_G(s'), \quad (30)$$

with

$$\Omega_0 = \Omega_H(s=0), \quad \Omega_G(s) = \frac{\partial}{\partial s}\Omega_H(s). \quad (31)$$

The first equality in Eq. (30) identifies the Helfand expression, while the second one is the Green-Kubo representation. The symbol lim denotes the ordered limits of $V^* \to \infty$ followed by $s \to \infty$. Note that what is called here the Helfand representation for the sake of simplicity was termed the intermediate Helfand representation in Ref. [3]. The correlation functions $\Omega_H(s)$ appearing in the Helfand representation have the general form

$$\Omega_H(s) = V^{*-1} \int d\Gamma^* F^{*S,f}(\Gamma^*) e^{-s(\bar{\mathcal{L}}^* - \lambda)s} \mathcal{M}^*(\Gamma^*). \quad (32)$$

The phase functions $F^{*S,f}$ are defined in terms of either a volume-integrated source S or a flux f present in the microscopic conservation laws for the direct functions a_α^* defined in Eq. (17). The phase functions $\mathcal{M}^*(\Gamma^*)$ are the first space moments of the functional derivatives of the local HCS distribution function. They are obtained from Eq. (19) to first order in k, then having the general structure

$$\mathcal{M}^*(\Gamma^*) = M \int d\boldsymbol{r}\hat{\boldsymbol{k}} \cdot \boldsymbol{r} \left[\frac{\delta\rho_{lh}[\,\Gamma|\{y_\alpha\}]}{\delta y(\boldsymbol{r})}\right]_{\{y_\alpha\}=\{n_h,T_h(t),\boldsymbol{0}\}}. \quad (33)$$

Finally, the dynamics in Eq. (32) is generated by the modified operator $\bar{\mathcal{L}}^*$ of the Liouville equation, minus one of its eigenvalues λ_α, determined from

$$(\bar{\mathcal{L}}^* - \lambda_\alpha)\widetilde{\psi}_\alpha^*(\Gamma^*;\mathbf{0}) = 0. \tag{34}$$

As discussed in Refs. [3] and [14], the functions $\widetilde{\psi}_\alpha^*(\Gamma^*;\mathbf{0})$ are the exact eigenfunctions of the modified Liouville operator, representing *homogeneous* perturbations of the HCS hydrodynamics. The eigenvalues $\lambda_\alpha = 0, \zeta_0^*/2, -\zeta_0^*/2$, the last one being d-fold degenerate, are therefore the same as those of the transport matrix $\mathcal{K}^{*\mathrm{hyd}}(\mathbf{0})$. Since the transport coefficients characterize the response to *spatial* variations, it is reasonable that the dynamics in their representation as time correlation functions does not include such homogeneous excitations.

The correlation functions $\Omega_G(s)$ present in the Green-Kubo representation have the corresponding forms

$$\Omega_G(s) = V^{*-1}\int d\Gamma^* F^{*S,f}(\Gamma^*)e^{-s(\bar{\mathcal{L}}^* - \lambda)}\Upsilon^*(\Gamma^*), \tag{35}$$

with the new "fluxes" $\Upsilon^*(\Gamma^*)$ given by

$$\Upsilon^*(\Gamma^*) = -(\bar{\mathcal{L}}^* - \lambda)\mathcal{M}^*(\Gamma^*). \tag{36}$$

The terminology "flux" for these functions is justified in Appendix E, where it is shown that they are the volume integrals of fluxes occurring in the microscopic balance equations for the conjugate functions $\widetilde{\psi}_\alpha^*$. In detail, it is found that the $F^{*S,f}(\Gamma^*)$ are projected orthogonal to the set of eigenfunctions $\{\widetilde{\psi}_\alpha^*(\Gamma^*;\mathbf{0})\}$, so that the zeros of the operator $\bar{\mathcal{L}}^* - \lambda$ do not occur in the dynamics. Consequently, the limit on the time integral in Eq. (30) is expected to exist. This is the analog of the "subtracted fluxes" present for the same reason in the Green-Kubo expressions for normal fluids [13].

B. The cooling rate and the pressure

The cooling rate was identified in Ref. [3] as proportional to the average (negative) rate of change of the total energy in the HCS. Its dimensionless value is given by

$$\zeta_0^* = V^{*-1}\int d\Gamma^* W^*(\Gamma^*)\rho_h^*(\Gamma^*) \tag{37}$$

where

$$W^*(\Gamma^*) = \frac{2}{d}\int d\mathbf{r}^* w^*(\Gamma^*;\mathbf{r}^*), \tag{38}$$

w^* being the source term in the dimensionless balance equation for the energy, Eq. (D27). Then, using Eqs. (D30) and (D16), it is found that

$$W(\Gamma^*) = \frac{1-\alpha^2}{2d}\sum_{r=1}^N \sum_{s\neq r}^N \delta(q_{rs}^* - \sigma^*)\Theta(-\hat{\mathbf{q}}_{rs}^* \cdot \mathbf{g}_{rs}^*)|\hat{\mathbf{q}}_{rs}^* \cdot \mathbf{g}_{rs}^*|^3. \tag{39}$$

Here, $\hat{\mathbf{q}}_{rs}^* \equiv \mathbf{q}_{rs}^*/q_{rs}$ and $\Theta(x)$ is the Heaviside step function. Therefore, ζ_0^* is proportional to the third moment of the normal component of the relative velocities of all pairs at contact, averaged over one of the collision hemispheres, in the HCS, weighted by the fractional loss in the kinetic energy of

the two particles which is proportional to $(1-\alpha^2)$. Since the cooling rate is determined by the average of a sum of phase functions involving only phase coordinates of pairs of particles, it can be expressed in the reduced form

$$\zeta_0^* = \frac{1-\alpha^2}{2V^*d}\int d\mathbf{q}_1^*\int d\mathbf{v}_1^*\int d\mathbf{q}_2^*\int d\mathbf{v}_2^* \delta(q_{12} - \sigma^*)$$
$$\times \Theta(\hat{\mathbf{q}}_{12}^* \cdot \mathbf{g}_{12}^*)|\hat{\mathbf{q}}_{12}^* \cdot \mathbf{g}_{12}^*|^3 f_h^{*(2)}(\mathbf{q}_{12},\mathbf{v}_1,\mathbf{v}_2). \tag{40}$$

Transforming to relative and center of mass coordinates allows further simplification to

$$\zeta_0^* = \frac{(1-\alpha^2)\pi^{d/2}\sigma^{*d-1}}{\Gamma(d/2)d}\int d\mathbf{g}_{12}^*\Theta(x)g_{12}^{*3}x^3 F_h^*(g_{12}^*,x), \tag{41}$$

where $x = \cos\phi$ is now the projection of $\hat{\mathbf{g}}_{12}$ along an arbitrary direction. This rather simple result is still exact, and retains all of the two-particle (position and velocity) correlations representative of the HCS. The two forms (37) and (41) are suitable for complementary molecular dynamics simulations of the cooling rate.

Similarly, the pressure is identified as the HCS average of the trace of the microscopic momentum flux

$$p^* = \frac{2}{V^*d}\int d\Gamma^* \rho_h^*(\Gamma^*)\mathrm{tr}\,\mathbf{H}^*(\Gamma^*). \tag{42}$$

Here the phase tensor $\mathbf{H}^*$ is the volume integral of the dimensionless flux defined in Eq. (D28),

$$\mathbf{H}^*(\Gamma^*) = \int d\mathbf{r}^* \mathbf{h}^*(\Gamma^*;\mathbf{r}^*)$$
$$= \sum_{r=1}^N \mathbf{v}_r^*\mathbf{v}_r^* + \frac{(1+\alpha)\sigma^*}{4}\sum_{r=1}^N \sum_{s\neq r}^N \delta(q_{rs}^* - \sigma^*)$$
$$\times \Theta(-\hat{\mathbf{q}}_{rs}^* \cdot \mathbf{g}_{rs}^*)(\hat{\mathbf{q}}_{rs}^* \cdot \mathbf{g}_{rs}^*)^2\hat{\mathbf{q}}_{rs}^*\hat{\mathbf{q}}_{rs}^*. \tag{43}$$

The pressure can be partitioned into two terms,

$$p^* = p_K^* + p_C^*, \tag{44}$$

where

$$p_K^* = \frac{2}{d}\int d\Gamma^* \rho_h^*(\Gamma^*)v_1^{*2} = 1 \tag{45}$$

and

$$p_C^* = \frac{(1+\alpha)\sigma^*}{2V^*d}\int d\mathbf{q}_1^*\int d\mathbf{v}_1^*\int d\mathbf{q}_2^*\int d\mathbf{v}_2^* \delta(q_{12} - \sigma^*)$$
$$\times \Theta(-\hat{\mathbf{q}}_{12}^* \cdot \mathbf{g}_{12}^*)(\hat{\mathbf{q}}_{12}^* \cdot \mathbf{g}_{12}^*)^2 f_h^{*(2)}(\mathbf{q}_{12},\mathbf{v}_1,\mathbf{v}_2)$$
$$= \frac{\pi^{d/2}(1+\alpha)\sigma^{*d}}{\Gamma(d/2)d}\int d\mathbf{g}_{12}^* g_{12}^{*2}\Theta(x)x^2 F_h^*(g_{12}^*,x). \tag{46}$$

The first term on the right-hand side of Eq. (44) is the kinetic part of the pressure. It arises purely from the transport of momentum associated with the free streaming of the particles and implies that $p_K = n_h T_h(t)$. The second term, determined by the two-particle distribution function at contact, is the collisional transfer part of the pressure. Like the cooling rate, it is given by a moment of the simple distribution

$F_h^*(g_{12}^*, x)$. Again, Eqs. (42) and (44)–(46) provide different, complementary expressions for the evaluation of the pressure by means of molecular dynamics simulations.

The pressure and the cooling rate, as functions of the hydrodynamic fields n and T, are the required equations of state for the hydrodynamics equations which are determined entirely by the HCS. This is analogous to the case of normal fluids where the dependence of the pressure on n and T is given by the equilibrium Gibbs state. Note that this definition is independent of the presence or absence of other normal stresses, which appear as additional independent dissipative contributions to the hydrodynamic equations. Similarly, the cooling rate has additional independent dissipative contributions characterized by transport coefficients.

C. Euler transport coefficient ζ^U

As already indicated, a new transport coefficient ζ^U occurs at Euler order in the temperature equation of the granular fluid. It is a measure of the contribution to heat transport from divergences in the flow velocity, and does not occur in the "perfect fluid" Euler equations for a normal fluid which have no dissipation. In Appendix F, the intermediate Helfand representation for the dimensionless form of this transport coefficient is identified as

$$\zeta^{*U} = \lim \Omega_H^{\zeta^U}(s), \tag{47}$$

where the time correlation function is

$$\Omega_H^{\zeta^U}(s) = V^{*-1} \int d\Gamma^* W^S(\Gamma^*) e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} \mathcal{M}_{\zeta^U}^*(\Gamma^*). \tag{48}$$

Here $W^S(\Gamma^*)$ is the volume-integrated source term $W(\Gamma^*)$ given in Eq. (39), projected orthogonal to the set $\{\tilde{\psi}_\alpha^*(\Gamma^*; \mathbf{0})\}$, as discussed above. More precisely, it is

$$W^S(\Gamma^*) = (1 - P^{*\dagger}) W(\Gamma^*) = W(\Gamma^*) - \frac{3\zeta_0^*}{d}\left(E^* - \frac{d}{2}N\right)$$
$$- \zeta_0^*\left(\frac{\partial \ln \zeta_0}{\partial \ln n_h} + 1\right)N. \tag{49}$$

The projection gives the additional terms proportional to the total number of particles N and the total energy $E^* = \Sigma_r v_r^{*2}$. The moment $\mathcal{M}_{\zeta^U}^*$ in Eq. (48) is given by

$$\mathcal{M}_{\zeta^U}^*(\Gamma^*) = -\sum_{r=1}^{N} \mathbf{q}_r^* \cdot \frac{\partial}{\partial \mathbf{v}_r^*} \rho_h^*(\Gamma^*), \tag{50}$$

which is a space first moment of the velocity derivative of the HCS distribution. To provide some interpretation for $\mathcal{M}_{\zeta^U}^*$, note that for a normal fluid, when the canonical Gibbs ensemble $\rho_c(\Gamma)$ is considered as the reference state,

$$\mathcal{M}_{\zeta^U}^* = 2\sum_{r=1}^{N} \mathbf{q}_r^* \cdot \mathbf{v}_r^* \rho_c, \tag{51}$$

which is the space moment of the momentum density of the fluid. This is modified for granular fluids to account for the nonequilibrium nature of the HCS.

The generator of the dynamics in Eq. (48) consists of the scaled Liouville operator $\bar{\mathcal{L}}^*$ together with the factor $\zeta_0^*/2$. The latter is one of the eigenvalues $(\lambda = -\zeta_0^*/2)$ solution of Eq. (34), and occurs here because $\mathcal{M}_{\zeta^U}^*$ has a nonvanishing component along the corresponding eigenfunction in this set of zeros for $\bar{\mathcal{L}}^* - \lambda$. The projected form of $W^S(\Gamma^*)$ assures that this component does not contribute to ζ^{*U}. Further discussion of this effect for the other transport coefficients is given below.

The equivalent Green-Kubo representation is

$$\zeta^{*U} = \Omega_0^{\zeta^U} + \lim \int_0^s ds' \Omega_G^{\zeta^U}(s'), \tag{52}$$

with $\Omega_0^{\zeta^U} = \Omega_H^{\zeta^U}(0)$ and

$$\Omega_G^{\zeta^U}(s) = V^{*-1} \int d\Gamma^* W^S(\Gamma^*) e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} Y_{\zeta^U}^*(\Gamma^*), \tag{53}$$

where

$$Y_{\zeta^U}^* = -\left(\bar{\mathcal{L}}^* + \frac{\zeta_0^*}{2}\right)\mathcal{M}_{\zeta^U}^* \tag{54}$$

is a conjugate flux, associated with the new conserved quantities of the dynamics of this system [3]. The usual integrands of the time integral in Green-Kubo expressions are flux-flux correlation functions. Here, one of the fluxes has been replaced by the source in the energy equation due to collisional loss of energy. This is characteristic of the Green-Kubo expressions for transport coefficients arising from the cooling rate. For all other transport coefficients, the familiar flux-flux correlation form occurs, although involving both a direct and a conjugate flux. This difference in the two sets of fluxes is due to both the dissipation in the collision rule and the singular nature of hard spheres. The occurrence of the instantaneous part of the Green-Kubo relation, $\Omega_0^{\zeta^U}$, has similar origins and is not present for normal fluids with nonsingular forces.

The instantaneous part of the Green-Kubo representation can be simplified further to

$$\Omega_0^{\zeta^U} = (V^* d)^{-1} \int d\Gamma^* W^S(\Gamma^*) \mathcal{M}_{\zeta^U}^*(\Gamma^*) = -\frac{3}{d}(1-\alpha) p_C^*, \tag{55}$$

where p_C^* is the collisional part of the pressure given in Eq. (46). Hence, ζ^{*U} is the contribution of the source to what would physically constitute the effects of hydrostatic pressure at the Euler order, where it enters in the combination $(2p^*/d) + \zeta^{*U}$. If a small volume element of the fluid is considered, then the amount of pressure that the fluid element can exert on its boundaries is decreased by the energy lost locally due to collisions. Part of the effect of this transport coefficient is to decrease the effective pressure in the system. At the level of linear hydrodynamics, the two coefficients are indistinguishable in their physical consequences.

D. Shear viscosity

The (intermediate) Helfand and Green-Kubo expressions for the dimensionless shear viscosity η^* are also elaborated in Appendix F to the the form

$$\eta^* = \lim \Omega_H^\eta(s) = \Omega_0^\eta + \lim \int_0^s ds' \, \Omega_G^\eta(s'), \qquad (56)$$

where the correlation functions are defined by

$$\Omega_H^\eta(s) = -\frac{V^{*-1}}{d^2 + d - 2} \sum_{i=1}^d \sum_{j=1}^d \int d\Gamma^* \mathbf{H}_{ij}^*(\Gamma^*) \\ \times e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} \mathcal{M}_{\eta,ij}^*(\Gamma^*), \qquad (57)$$

$$\Omega_G^\eta(s) = -\frac{V^{*-1}}{d^2 + d - 2} \sum_{i=1}^d \sum_{j=1}^d \int d\Gamma^* \mathbf{H}_{ij}^*(\Gamma^*) e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} \Upsilon_{\eta,ij}^*(\Gamma^*), \qquad (58)$$

and $\Omega_0^\eta = \Omega_H^\eta(0)$. In the above expressions, $\mathbf{H}_{ij}^*(\Gamma^*)$ is the volume-integrated momentum flux given by Eq. (43), $\mathcal{M}_{\eta,ij}^*$ is the traceless tensor

$$\mathcal{M}_{\eta,ij}^*(\Gamma^*) = -\frac{1}{2} \sum_{r=1}^N \left(q_{r,i}^* \frac{\partial}{\partial v_{r,j}^*} + q_{r,j}^* \frac{\partial}{\partial v_{r,i}^*} - \frac{2}{d} \delta_{ij} \mathbf{q}_r^* \cdot \frac{\partial}{\partial \mathbf{v}_{r,}^*} \right) \rho_h^*(\Gamma^*). \qquad (59)$$

and the associated Green-Kubo conjugate flux $\Upsilon_{\eta,ij}^*$ is

$$\Upsilon_{\eta,ij}^* = -\left(\bar{\mathcal{L}}^* + \frac{\zeta_0^*}{2} \right) \mathcal{M}_{\eta,ij}^*(\Gamma^*). \qquad (60)$$

The generator of the dynamics is now $(\bar{\mathcal{L}}^* + \frac{\zeta_h^*}{2})$ and, therefore, has the $k=0$ mode of Eq. (34) with $\lambda = -\zeta_0^*/2$ subtracted out.

In order to better understand the differences from the corresponding expression for a normal fluid, note that for the latter with the canonical Gibbs reference state $\rho_c(\Gamma)$, the expression is

$$\mathcal{M}_{\eta,ij}^*(\Gamma^*) = \sum_{r=1}^N \left(q_{r,i}^* v_{r,j}^* + q_{r,j}^* v_{r,i}^* - \frac{2}{d} \delta_{ij} \mathbf{q}_r^* \cdot \mathbf{v}_r^* \right) \rho_c^*(\Gamma^*), \qquad (61)$$

and

$$\Upsilon_{\eta,ij}^*(\Gamma^*) = -\bar{L}^* \mathcal{M}_{\eta,ij}^*(\Gamma^*). \qquad (62)$$

Using the property (A27) and taking into account that $\bar{L}^* \rho_c^* = 0$, we obtain that, for a normal fluid,

$$\Upsilon_{\eta,ij}^*(\Gamma^*) = -2\left(\mathbf{H}_{ij}^{*-} - \frac{1}{d} \delta_{ij} \mathrm{tr} \, \mathbf{H}^{*-} \right) \rho_c^*(\Gamma^*), \qquad (63)$$

where $\mathbf{H}_{ij}^{*-}$ is the volume-integrated momentum flux for the time reversed microscopic conservation laws identified in Appendix D, namely,

$$\mathbf{H}^{*-}(\Gamma^*) = \sum_{r=1}^N \mathbf{v}_r^* \mathbf{v}_r^* + \frac{\sigma^*}{2} \sum_{r=1}^N \sum_{s \neq r}^N \delta(q_{rs}^* - \sigma^*) \\ \times \Theta(\hat{\mathbf{q}}_{rs}^* \cdot \mathbf{g}_{rs})(\hat{\mathbf{q}}_{rs}^* \cdot \mathbf{g}_{rs})^2 \hat{\mathbf{q}}_{rs} \hat{\mathbf{q}}_{rs}. \qquad (64)$$

Therefore, the normal fluid version of Eq. (56) is

$$\eta^* = \Omega_0^\eta + \lim \frac{2V^{*-1}}{d^2 + d - 2} \sum_{i=1}^d \sum_{j=1}^d \int_0^s ds' \int d\Gamma^* \mathbf{H}_{ij}^* \\ \times e^{-s\bar{L}^*} \left(\mathbf{H}_{ij}^{*-}(\Gamma^*) - \frac{1}{d} \delta_{ij} \, \mathrm{tr} \, \mathbf{H}^{*-} \right) \rho_c^*(\Gamma^*). \qquad (65)$$

The normal fluid shear viscosity is given by the long-time integral of the equilibrium time correlation functions of the forward momentum flux $\mathbf{H}^*$ with the time-reversed momentum flux $\mathbf{H}^{*-}$, together with an instantaneous part. This instantaneous term remains nonzero in the elastic limit, as an artifact of the singular nature of the hard-particle interaction. Note that, in the elastic limit, the hydrodynamic modes defined through Eq. (34) all have the same eigenvalue $\lambda = 0$, so the generator for the dynamics in both the elastic and inelastic case can be thought of as having the $k^*=0$ mode subtracted out.

The instantaneous contribution Ω_0^η for the granular fluid can be expressed in terms of the reduced pair distribution function, just as in the case of the pressure above, with the result

$$\Omega_0^\eta = -\frac{V^{*-1}}{d^2 + d - 2} \int d\Gamma^* \mathbf{H}_{ij}^*(\Gamma^*) \mathcal{M}_{\eta,ij}^*(\Gamma^*) \\ = \frac{1 + \alpha}{4(d^2 + 2d)} \sigma^{*2} \nu_{\mathrm{av}}, \qquad (66)$$

where ν_{av} is the average collision frequency as determined by the loss part of the right-hand side of the hard-sphere Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy [13] for the HCS,

$$\nu_{\mathrm{av}} = \frac{4\pi^{d/2} \sigma^{*d-1}}{\Gamma(d/2)} \int d\mathbf{g}_{12}^* \Theta(\hat{\mathbf{q}}_{12}^* \cdot \mathbf{g}_{12}^*) \hat{\mathbf{q}}_{12}^* \cdot \mathbf{g}_{12}^* F_h^*(\mathbf{g}_{12}^*, x). \qquad (67)$$

This is a purely collisional quantity, arising from the boundary condition associated with hard-sphere dynamics at the point of contact.

E. Bulk viscosity

The bulk viscosity has forms similar to those reported above for the shear viscosity, although it represents resistance to volume dilation rather than shear,

$$\kappa^* = \lim \Omega_H^\kappa(s) = \Omega_0^\kappa + \lim \int_0^s ds' \, \Omega_G^\kappa(s'). \qquad (68)$$

The correlation functions in the above expressions are shown in Appendix F to be given by

$$\Omega_H^\kappa(s) = -(V^* d^2)^{-1} \int d\Gamma^* \, \mathrm{tr} \, \mathbf{H}^{*f}(\Gamma^*) e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} \mathcal{M}_\kappa^*(\Gamma^*), \tag{69}$$

$$\Omega_G^\kappa(s) = -(V^* d^2)^{-1} \int d\Gamma^* \, \mathrm{tr} \, \mathbf{H}^{*f}(\Gamma^*) e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} \mathbf{Y}_\kappa^*(\Gamma^*), \tag{70}$$

and $\Omega_0^\kappa = \Omega_H^\kappa(0)$. Here $\mathbf{H}^{*f}$ is the projection of the integrated momentum flux, whose trace is

$$\mathrm{tr} \, \mathbf{H}^{*f}(\Gamma^*) = \mathrm{tr} \, \mathbf{H}^*(\Gamma^*) - \frac{p_h^* d}{2} \frac{\partial \ln p_h}{\partial \ln n_h} N - \left(E^* - \frac{d}{2} N \right) p_h^*, \tag{71}$$

where $\mathbf{H}^*(\Gamma^*)$ is given by Eq. (43). The additional terms on the right-hand side of the above equation, proportional to N and E^*, result from projection of $\mathrm{tr} \, \mathbf{H}^*$ orthogonal to the eigenfunctions defined in Eq. (34). Further details can be seen in Appendix F and Ref. [3]. The moment $\mathcal{M}_\kappa^*$ is the same as that for the Euler transport coefficient ζ^{*U}, i.e.,

$$\mathcal{M}_\kappa^* = \mathcal{M}_{\zeta^U}^* = -\sum_{r=1}^N \boldsymbol{q}_r^* \cdot \frac{\partial}{\partial \boldsymbol{v}_r^*} \rho_h^*(\Gamma^*). \tag{72}$$

Then also for the associated Green-Kubo conjugate flux $\mathbf{Y}_\kappa^*$,

$$\mathbf{Y}_\kappa^* = \mathbf{Y}_{\zeta^U}^* = -\left(\bar{\mathcal{L}}^* + \frac{\zeta_0^*}{2} \right) \mathcal{M}_\kappa^*. \tag{73}$$

The instantaneous part of the bulk viscosity, Ω_0^κ, is simply related to that for the shear viscosity by

$$\Omega_0^\kappa = \frac{d+2}{d} \Omega_0^\eta = \frac{(1+\alpha)\sigma^{*2}}{4d^2} \nu_{\mathrm{av}}, \tag{74}$$

with the average collision frequency ν_{av} given by Eq. (67).

F. Thermal conductivity

The expressions for the dimensionless thermal conductivity λ^* of the granular fluid of hard spheres or disks obtained in Appendix F are

$$\lambda^* = \lim \Omega_H^\lambda(s) = \Omega_0^\lambda + \lim \int_0^s ds' \, \Omega_G^\lambda(s'), \tag{75}$$

where

$$\Omega_H^\lambda(s) = -(V^* d)^{-1} \int d\Gamma^* \boldsymbol{S}^{*f}(\Gamma^*) \cdot e^{-s(\bar{\mathcal{L}}^* - \zeta_0^*/2)} \mathcal{M}_\lambda^*(\Gamma^*), \tag{76}$$

$$\Omega_G^\lambda(s) = -(V^* d)^{-1} \int d\Gamma^* \boldsymbol{S}^{*f}(\Gamma^*) \cdot e^{-s(\bar{\mathcal{L}}^* - \zeta_0^*/2)s} \mathbf{Y}_\lambda^*(\Gamma^*), \tag{77}$$

and $\Omega_0^\lambda = \Omega_H^\lambda(0)$. In the above expressions, the projected energy flux $\boldsymbol{S}^{*f}$ is

$$\boldsymbol{S}^{*f}(\Gamma^*) = \boldsymbol{S}^*(\Gamma^*) - \left(\frac{d}{2} + p_h^* \right) \boldsymbol{P}^*, \tag{78}$$

with $\boldsymbol{S}^*(\Gamma^*) \equiv \boldsymbol{s}^*(\Gamma^*; \mathbf{0})$ being the volume-integrated heat flux obtained from Eqs. (D15) and (D29),

$$\boldsymbol{S}^*(\Gamma^*) = \sum_{r=1}^N v_r^{*2} \boldsymbol{v}_r^* + \frac{(1+\alpha)\sigma^*}{2} \sum_{r=1}^N \sum_{s \neq r}^N \delta(q_{rs}^* - \sigma^*)$$
$$\times \Theta(-\hat{\boldsymbol{q}}_{rs}^* \cdot \boldsymbol{g}_{rs}^*)(\hat{\boldsymbol{q}}_{rs}^* \cdot \boldsymbol{g}_{rs}^*)^2 (\hat{\boldsymbol{q}}_{rs}^* \cdot \boldsymbol{G}_{rs}^*)\hat{\boldsymbol{q}}_{rs}^*. \tag{79}$$

As with the previous transport coefficients, the additional term proportional to the total momentum $\boldsymbol{P}^*$ in Eq. (78) results from projection of $\boldsymbol{S}^*$ orthogonal to the eigenfunctions defined by Eq. (34). The moment $\mathcal{M}_\lambda^*$ is

$$\mathcal{M}_\lambda^*(\Gamma^*) = -\frac{1}{2} \sum_{r=1}^N \boldsymbol{q}_r^* \frac{\partial}{\partial \boldsymbol{v}_r^*} \cdot [\boldsymbol{v}_r^* \rho_h^*(\Gamma^*)] \tag{80}$$

and the expression of the associated Green-Kubo conjugate flux $\mathbf{Y}_\lambda^*$ is

$$\mathbf{Y}_\lambda^*(\Gamma^*) = -\left(\bar{\mathcal{L}}^* - \frac{\zeta_0^*}{2} \right) \mathcal{M}_\lambda^*. \tag{81}$$

The relevant hydrodynamic excitation that is subtracted from the generator of the dynamics is now that for $\lambda = \zeta_0^*/2$.

The instantaneous part of the thermal conductivity in the Green-Kubo representation can be simplified to

$$\Omega_0^\lambda = \frac{(1+\alpha)\sigma^{*d+1}}{16d} \int d\hat{\boldsymbol{\sigma}}^* \int d\boldsymbol{g}_{12}^* \int d\boldsymbol{G}_{12}^* \Theta(\hat{\boldsymbol{\sigma}}^* \cdot \boldsymbol{g}_{12}^*)(\hat{\boldsymbol{\sigma}}^* \cdot \boldsymbol{g}_{12}^*)$$
$$\times [8(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{G}_{12}^*)^2 + (\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{g}_{12}^*)^2] f_h^{*(2)}(\boldsymbol{\sigma}^*, \boldsymbol{v}_1^*, \boldsymbol{v}_2^*), \tag{82}$$

with $\boldsymbol{\sigma}^* = \sigma^* \hat{\boldsymbol{\sigma}}^*$. Again, the instantaneous contribution to the transport coefficient is purely collisional, reflecting its origin as the discontinuity in time for colliding configurations at contact. Also note that this is the first transport coefficient where the center of mass momentum of the pair, in addition to the relative velocity, occurs in the final average.

The corresponding normal fluid expression for this transport coefficient can be analyzed along the lines done for the viscosities above. The Green-Kubo integrand for the time integral is a flux-flux correlation function as in Eq. (65), with both the direct flux $\boldsymbol{S}^*$ and a conjugate flux, the volume-integrated time-reversed energy flux $\boldsymbol{S}^{*-}$. This and the nonvanishing instantaneous part are peculiarities of the singular hard-sphere interactions and neither effect occurs for nonsingular forces in the elastic limit. For the granular fluid, the conjugate flux is further modified by its generation from the HCS.

G. The μ coefficient

The μ coefficient is a measure of the contribution to heat transport in the fluid due to spatial gradients in the density field. It is directly related to the inelasticity of the collisions and it is unique to granular fluids with no analog for normal fluids. The simplest form for this transport coefficient is obtained when considering the linear combination

$$\bar{\mu}^* = \mu^* - 2 \frac{\partial \ln \zeta_0}{\partial \ln n_h} \lambda^*, \tag{83}$$

where λ^* is the dimensionless thermal conductivity discussed in the previous subsection. The intermediate Helfand and Green-Kubo representations for $\bar{\mu}^*$ are identified in Appendix F as

$$\bar{\mu}^* = \lim \Omega_H^{\bar{\mu}}(s) = \Omega_0^{\bar{\mu}} + \lim \int_0^s ds' \Omega_G^{\bar{\mu}}(s'). \tag{84}$$

The expression of the Helfand correlation function is

$$\Omega_H^{\bar{\mu}}(s) = -(V^*d)^{-1} \int d\Gamma^* \mathbf{S}^{*f}(\Gamma^*) \cdot e^{-s\bar{\mathcal{L}}^*} \mathcal{M}_{\bar{\mu}}^*(\Gamma^*), \tag{85}$$

where $\mathbf{S}^{*f}$ is the subtracted heat flux given in Eq. (78). The moment $\mathcal{M}_{\bar{\mu}}^*$ is

$$
\begin{aligned}
\mathcal{M}_{\bar{\mu}}^* &= [\ell v_0(T)]^{Nd} \int d\mathbf{r}\, \mathbf{r} \left[n \frac{\delta \rho_{lh}}{\delta n(\mathbf{r})} \right. \\
&\quad \left. -2 \frac{\partial \ln \zeta_0}{\partial \ln n} T \frac{\delta \rho_{lh}}{\delta T(\mathbf{r})} \right]_{\{y_\alpha\}=\{n,T,\mathbf{0}\}} \\
&= [\ell v_0(T)]^{Nd} n \int d\mathbf{r}\, \mathbf{r} \left[\left(\frac{\delta \rho_{lh}[\Gamma|\{y_\alpha\}]}{\delta n(\mathbf{r})} \right)_{\zeta_0} \right]_{\{y_\alpha\}=\{n,T,\mathbf{0}\}}.
\end{aligned}
\tag{86}
$$

As indicated, in the last expression the functional derivative with respect to the density field is to be carried out at constant cooling rate. This suggests that $\bar{\mu}^*$ is characterizing density gradients under conditions of constant cooling rate.

The Green-Kubo correlation functions are

$$\Omega_0^{\bar{\mu}} = \Omega_H^{\bar{\mu}}(0), \tag{87}$$

$$\Omega_G^{\bar{\mu}}(s) = -(V^*d)^{-1} \int d\Gamma^* \mathbf{S}^{*f}(\Gamma^*) \cdot e^{-s\bar{\mathcal{L}}} \mathbf{Y}_{\bar{\mu}}^*(\Gamma^*), \tag{88}$$

with the associated flux $\mathbf{Y}_{\bar{\mu}^*}$ having the expression

$$\mathbf{Y}_{\bar{\mu}}^* = -\bar{\mathcal{L}}^* \mathcal{M}_{\bar{\mu}}^*. \tag{89}$$

The hydrodynamic mode subtracted from the generator $\bar{\mathcal{L}}^*$ in this case has the eigenvalue $\lambda = 0$. Unlike the previous transport coefficients discussed so far, the moment $\mathcal{M}_{\bar{\mu}}^*$ and the flux $\mathbf{Y}_{\bar{\mu}}^*$ are still given implicitly in terms of the *local* HCS state. Further analysis requires determination of the density dependence of the *inhomogeneous* HCS, i.e., that in an external conservative field. This is beyond the discussion here and remains an open problem for applications of these representations for the μ^* coefficient.

It is shown in Appendix G that this transport coefficient vanishes in the elastic limit, as expected. However, that result is specific to the choice of an equilibrium Gibbs state for the reference ensemble. More generally, for nonequilibrium reference states, it is $\mu^* \neq 0$. As noted above, the linear combination $\bar{\mu}^* = \mu^* - 2 \frac{\partial \ln \zeta_0}{\partial \ln n_h} \lambda^*$ is the transport coefficient mea-

suring the effects of density gradients on the heat flux when the cooling rate instead of the temperature is held fixed. The Helfand moment $\mathcal{M}_{\bar{\mu}}^*$ is the space moment associated with $\tilde{\psi}_1^*(\Gamma^*; \mathbf{0}) - 2 \frac{\partial \ln \zeta_0}{\partial \ln n_h} \tilde{\psi}_2^*(\Gamma^*; \mathbf{0})$. It is shown in Appendix C that this same combination determines the eigenfunction of the specific hydrodynamic mode solution of Eq. (34) with eigenvalue $\lambda = 0$. Hence, it appears that in some respects the pair $\delta \zeta_0, \delta n$ are more natural independent variables than $\delta T, \delta n$.

IV. EVALUATION OF TRANSPORT COEFFICIENTS

The (intermediate) Helfand and Green-Kubo expressions for the various transport coefficients obtained above are formal results since the full N-particle problem has not been solved yet. Instead, the linear response method gives a valuable exact and direct relationship of the macroscopic properties to the microscopic statistics and dynamics. Their utility is determined by the fact that they are the ideal setting to explore controlled analytic approximations and exact numerical evaluations. The transport coefficients have been obtained in the form of stationary time correlation functions. This suggests the possible generalization to granular fluids of the extensively developed many-body tools for the analysis of time correlation functions of a normal fluid, such as short-time expansions, mode-coupling theories, and formal kinetic theories. Also, for normal fluids such expressions have proved particularly suitable for evaluation by MD simulation to extend the studies of hydrodynamic descriptions to otherwise inaccessible domains in the density of the fluid. In this section, this potential for future studies is illustrated in two directions. First, the applicability of a kinetic theory of time correlation functions is outlined and discussed. Then, a scheme for implementing the stationary representation of the dynamics considered in this work in an MD simulation is discussed.

A. Kinetic theory

The results for the various transport coefficients obtained in the present work are expressed in terms of time correlation functions over an N-particle distribution. However, an equivalent expression involving two-particle time-dependent reduced functions is possible as well. This reduced representation serves as the appropriate starting point for construction of a kinetic theory for the correlation functions, and application of formal cluster expansion techniques. Consider the Helfand representation for a generic transport coefficient ϖ^* as given by Eqs. (30) and (32),

$$\varpi^* = \lim V^{*-1} \int d\Gamma^* F^{*S,f}(\Gamma^*) e^{-s(\bar{\mathcal{L}}^* - \lambda)} \mathcal{M}^*(\Gamma^*). \tag{90}$$

The projected source or flux, $F^{*S,f}(\Gamma^*)$, is the sum of single-particle or pair functions in all cases, so it has the form

$$F^{*S,f}(\Gamma^*) = \sum_{r=1}^N F_1(x_r^*) + \sum_{r=1}^N \sum_{s \neq r}^N F_2(x_r^*, x_s^*), \tag{91}$$

with $x_r^* \equiv \{\mathbf{q}_r^*, \mathbf{v}_r^*\}$ denoting the one-particle phase point for particle r, and F_1 and F_2 being one- and two-particle func-

tions of the phase point, respectively. Define a set of "reduced correlation functions" $\mathcal{M}^{*(m)}(x_1^*, \dots, x_m^*, s)$ by

$$
\mathcal{M}^{*(m)}(x_1^*, \dots, x_m^*, s) \equiv \frac{N!}{(N-m)!} \int dx_{m+1}^* \cdots
$$

$$
\times \int dx_N^* e^{-s(\bar{\mathcal{L}}^* - \lambda)} \mathcal{M}^*(\Gamma^*). \quad (92)
$$

Then the generic expression for the transport coefficient (90) becomes

$$
\varpi^* = \lim V^{*-1} \Big[\int dx_1^* F_1(x_1^*) \mathcal{M}^{*(1)}(x_1^*, s)
$$

$$
+ \int dx_1^* \int dx_2^* F_2(x_1^*, x_2^*) \mathcal{M}^{*(2)}(x_1^*, x_2^*, s) \Big]. \quad (93)
$$

In this way, the full N-body correlation function is mapped onto one that involves only the one- and two-particle reduced correlation functions.

It follows by direct differentiation with respect to s of Eq. (92) that the functions $\mathcal{M}^{*(m)}$ obey a hierarchy of equations,

$$
\left(\frac{\partial}{\partial s} - \lambda + \bar{\mathcal{L}}^{*(m)} \right) \mathcal{M}^{*(m)}(x_1^*, \dots, x_m^*, s)
$$

$$
= \sum_{r=1}^{m} \int dx_{m+1}^* \bar{T}^*(r, m+1) \mathcal{M}^{*(m+1)}(x_1^*, \dots, x_{m+1}^*, s),
$$

$$
(94)
$$

where $\bar{\mathcal{L}}^{*(m)}$ is the same operator as $\bar{\mathcal{L}}^*$ but now defined for only m particles, and the $\bar{T}^*(r, s)$ operator is the dimensionless form of the operator defined in Eq. (A24). This hierarchy is formally the same as the dimensionless BBGKY hierarchy of the reduced distribution functions representing the nonequilibrium state of the fluid [13,15]. Only the initial conditions needed to solve the equations are different.

Formally, a kinetic theory represents a closure of the hierarchy at the level of the first equation, through the identification of a representation for the two-body function $\mathcal{M}^{*(2)}(x_1^*, x_2^*, s)$ as a functional of the one-body function $\mathcal{M}^{*(1)}(x_1^*, s)$. With such a functional relationship, the first hierarchy equation becomes a closed, autonomous equation for $\mathcal{M}^{*(1)}(x_1^*, s)$. This equation is called a kinetic equation, and the functional relationship defines the kinetic theory. It is important to recognize that this concept of a kinetic theory does not imply any *a priori* restrictions to low density, weak inelasticity, or absence of correlations. Such restrictions occur only in the justification of specific choices for approximate closure functionals.

To obtain a functional relationship for $\mathcal{M}^{*(2)}(x_1^*, x_2^*, s)$, it is postulated that there exists a functional expressing the two-body reduced distribution function associated with the local HCS in terms of the one-body distribution function,

$$
f_{lh}^{(2)}(x_1, x_2, t) = f_{lh}^{(2)}[\, x_1, x_2, t | f_{lh}^{(1)}], \quad (95)
$$

where the reduced local HCS distributions are defined by

$$
f_{lh}^{(m)}(x_1 \dots, x_m, t) \equiv \frac{N!}{(n-m)!} \int dx_{m+1} \cdots \int dx_N e^{-t\bar{L}} \rho_{lh}(\Gamma).
$$

$$
(96)
$$

The formal construction of a functional as in Eq. (95) for normal fluids, where ρ_{lh} is replaced by the local equilibrium ensemble, is a well-studied problem, e.g., inversion of formal cluster expansions for the reduced distribution functions. This is the first point at which extensions of kinetic theory to granular fluids can be explored. From the definition of $\mathcal{M}^*$ in Eq. (33), it follows that Eq. (95) implies a similar but linear functional relationship for $\mathcal{M}^{*(2)}$,

$$
\mathcal{M}^{*(2)}(x_1^*, x_2^*, s) = \int dx^{*\prime} K(x_1^*, x_2^*, x^{*\prime}, s) \mathcal{M}^{*(1)}(x^{*\prime}, s),
$$

$$
(97)
$$

with

$$
K(x_1^*, x_2^*, x^{*\prime}, s) = [l v_0(T_h)]^d \left[\frac{\delta f_{lh}^{(2)}[\, x_1, x_2, t | f_{lh}^{(1)}]}{\delta f_{lh}^{(1)}(x', t)} \right]_{\{y_\alpha\} = \{n_h, T_h, \mathbf{0}\}}.
$$

$$
(98)
$$

The linear kernel K is a functional derivative of the two-body distribution function with respect to the one-body distribution, evaluated in the homogeneous limit. This latter evaluation leads to the linearity of this functional. The prefactor in the above expression just transforms to dimensionless variables as in Eq. (19). Substitution of this form for the two body correlation function in the first equation of the hierarchy leads to the kinetic equation

$$
(\partial_s - \lambda + \bar{\mathcal{L}}^{*(1)} - \mathcal{I}(s)) \mathcal{M}^{(1)}(x_1^*, s) = 0, \quad (99)
$$

with the formal linear "collision operator"

$$
\mathcal{I}(s) \mathcal{M}^{*(1)}(x_1^*, s) \equiv \int dx_2^* \bar{T}^*(1, 2) \int dx^{*\prime} K(x_1^*, x_2^*, x^{*\prime}, s)
$$

$$
\times \mathcal{M}^{*(1)}(x^{*\prime}, s). \quad (100)
$$

This is the kinetic equation governing the dynamics of $\mathcal{M}^{*(1)}$. Since this quantity also determines $\mathcal{M}^{*(2)}$ through the functional relationship given by Eq. (97), the transport coefficient can be calculated from Eq. (93).

The above is exact but formal, and the aim here is only to provide a flavor of the potential for developing a practical kinetic theory for time correlation functions. Details of this method and the explicit evaluation of the various transport coefficients an Enskog-like approximation will be given elsewhere [16]. The latter is obtained by estimating $f^{(2)}[\, x_1, x_2, t | f^{(1)}] \approx f^{(2)}[\, x_1, x_2, 0 | f^{(1)}]$, which is exact at $t=0$, and furthermore neglecting velocity correlations. The resulting kinetic theory for the correlation functions leads to cooling rate, pressure, and transport coefficients identical to those from the Chapman-Enskog solution to the Enskog kinetic theory [17,18]. At low density, these results agree with those from the Boltzmann equation [19].

B. Molecular dynamics simulation

The formal expressions for the various transport coefficients derived in this work, are given in the dimensionless representation for the phase space dynamics that leave the HCS ensemble stationary and defined by the thermal velocity associated with the HCS. But for practical purposes this is a complicated representation as it must be solved self-consistently with the cooling equation. It is then convenient to consider a different scaling, in which the function $v_0(t)$ is replaced by a known function chosen in an appropriate way. A useful choice is defined by

$$q_r^{**} = q_r^* = \frac{q_r^*}{l}, \quad v_r^{**} = \frac{\xi_0 t}{2l} v_r \quad (101)$$

where ξ_0 is an arbitrary time-independent dimensionless frequency. The rationale for his choice and some more details are given in Appendix H. The particle dynamics in the new variables consists of an acceleration streaming between collisions,

$$\frac{\partial q^{**}(\tau)}{\partial \tau} = v^{**}(\tau), \quad (102)$$

$$\frac{\partial v^{**}(\tau)}{\partial \tau} = \frac{\xi_0}{2} v^{**}(\tau), \quad (103)$$

while the effect of a collision between two particles r and s is to instantaneously alter their relative velocity according to the same rule as in the original scale. This invariance of the interation law is another consequence of the singular character of hard-particle collisions.

The quantity ξ_0 and the dimensionless cooling rate ζ_0^* are related through the steady state temperature obtained in the simulations in the scaled variables [20,27]. The relationship is given in Eq. (G15). This method has already been implemented in event-driven molecular dynamics simulation to measure the self-diffusion transport coefficient of a granular fluid [20]. That is a simpler case than those considered here, since the correlation functions appearing in its Helfand and Green-Kubo expressions are not moments of the conjugate densities, but simply the velocities of the particles.

The low-density limits of the Green-Kubo expressions for a granular gas have been evaluated by means of the direct simulation Monte Carlo method in Refs. [21] and [22], also by using the steady representation introduced above. The conjugate fluxes were determined from the simulation themselves. Although the technical problems are much harder beyond the low-density limit, this shows the way to evaluate the general expression derived here at arbitrary densities.

V. DISCUSSION

The parameters of Navier-Stokes hydrodynamics for a system of smooth, inelastic hard spheres with constant restitution coefficient have been given formally exact representations starting from the underlying nonequilibrium statistical mechanics. General linear response functions for small initial spatial perturbations of the HCS are given by Eq. (15). These

are stationary time correlation functions, composed of densities of the hydrodynamic fields and corresponding conjugate densities defined by functional derivatives of the local HCS with respect to these fields. They are similar to the response functions for a normal fluid, where the local HCS is replaced by a local equilibrium ensemble. Such response functions provide the basis for exploration of a wide range of phenomena in granular gases at the fundamental level of statistical mechanics, beyond the specific case of transport coefficients considered here [23].

In the long-wavelength, long-time limit these response functions exhibit the hydrodynamic behavior of the system. This is the analog of the Onsager regression property for normal fluids [24,25]. This limit has been extracted by defining a general transport matrix for the response functions, and expanding it to order k^2 to identify the Navier-Stokes parameters in terms of corresponding HCS averages or stationary time correlation functions. The cooling rate is given as the HCS average rate of change of the global energy, and the pressure is expressed as the average fluctuation in the global momentum flux. Such averages can be studied directly by MD simulation. Furthermore, they have been expressed in terms of the reduced two-particle distribution function for pairs of particles at contact. This representation is suitable for inquiry about new features of granular fluids, such as two-particle velocity correlations.

The transport coefficients obtained in this way have been considered in two representations, the (intermediate) Helfand and Green-Kubo forms. The former is the long-time limit of a correlation function constructed from a global flux associated with the energy or momentum densities, and a space moment of one of the conjugate densities. This is quite similar to the corresponding Helfand results for a normal fluid, if the HCS ensemble is replaced by the equilibrium Gibbs ensemble. There is an important additional difference, however, in the generator for the time dependence. The dimensionless generator for hard-sphere trajectories $\bar{L}^*$ is replaced by $\bar{\mathcal{L}}^*$ of Eq. (22), which contains an additional velocity scaling operator. The latter represents the cooling of the reference HCS and it is essential for the stationary representation given here. In addition, the time correlation functions for transport coefficients have the further modification $\bar{\mathcal{L}}^* \to \bar{\mathcal{L}}^* - \lambda$, where λ is one of the eigenvalues of the hydrodynamic transport matrix $\mathcal{K}^{*\text{hyd}}(\mathbf{0})$. These eigenvalues describe the dynamics of homogeneous perturbations to the HCS. Since the transport coefficients measure only spatial correlations, it is perhaps not surprising that this homogeneous dynamics does not occur in their representation. These same eigenvalues occur in the exact spectrum of $\bar{\mathcal{L}}^*$, so this generator $\bar{\mathcal{L}}^* - \mathcal{K}^{*\text{hyd}}(\mathbf{0})$ has invariants (zeros of the spectrum). In the elastic limit, these invariants are proportional to the usual global conserved total number, energy, and momentum.

The equivalent Green-Kubo expressions have a time-independent part plus the familiar time integral of a flux-flux correlation function. The time-independent part is absent for normal fluids with conservative, nonsingular forces. More generally, for either singular forces (e.g., hard spheres) and/or nonconservative forces, this contribution is nonzero.

For normal fluids, it can be evaluated exactly and represents the high-density contribution to the transport coefficients in the Enskog kinetic theory. Here, it can be reduced to an average over the two-particle distribution function, just as described for the cooling rate and pressure. The flux-flux time correlation functions in the Green-Kubo integrands are constructed from a global flux of the energy or momentum densities and a global flux associated with the conjugate densities. The dynamics is generated by $\bar{\mathcal{L}}^* - \mathcal{K}^{*\mathrm{hyd}}(\mathbf{0})$ as described above, so the associated invariants must not occur in order for the time integral to exist in the long-time limit. In fact, the expressions obtained have the fluxes orthogonal to these invariants. This is the analog of subtracted fluxes for a normal fluid [13].

There are additional transport coefficients associated with spatial gradients of the hydrodynamic fields contribution to the cooling rate. These also have Helfand and Green-Kubo forms as described above, but with the global flux of energy replaced by the volume-integrated source in the microscopic balance equation for energy. One of these transport coefficients, ζ^U, appears at the Euler level hydrodynamics and gives a correction to the pressure in the coefficient of $\nabla \cdot \mathbf{U}$. The other two give corrections to the macroscopic heat flux proportional to ∇T and ∇n. These vanish for a normal fluid.

As with normal fluids, the value of such formal expressions is direct access to the transport coefficients before approximations are introduced. Often this avoids (or postpones) conceptual difficulties associated with the particular many-body method used for evaluation. Here, the two most common approaches for normal fluids have been briefly discussed for extension to granular fluids. The first is a kinetic theory for time correlation functions. It is inherently simpler than constructing a corresponding kinetic theory for the reduced distribution functions, since the latter are nonlinear while that for the correlation functions is linear. Furthermore, the special solution required for hydrodynamics (normal solution and Chapman-Enskog construction) has already been incorporated implicitly in the linear response analysis here. The necessary functional assumption for a kinetic theory of granular time correlation functions has been identified as a property of the local HCS. In this restricted context, it should be possible to explore the validity or failure of such an assumption, although the detailed investigations for normal fluids need to be reconsidered. It is shown elsewhere [16] that an *ad hoc* neglect of velocity correlations, something that is justified in the case of normal fluids, leads to transport coefficients identical to those from the Enskog kinetic theory. The formalism developed in this paper and the preceding one, provides the basis for critiquing that theory and correcting it for granular fluids.

The second approach for evaluating the formal expressions given here is MD simulation. In this case, the extension of approach from normal fluids is not direct either. The conjugate moments (Helfand representation) or the conjugate fluxes (Green-Kubo representation) are not known explicitly, but rather given by derivatives of the HCS ensemble. Thus the simulation of these expressions requires new method for developing properties of the HCS from the simulation itself.

APPENDIX A: HARD-SPHERE DYNAMICS

In this appendix, the details of the dynamics and statistical mechanics of a system of hard particles are given. Consider a system of N monodisperse smooth hard spheres ($d=3$) or disks ($d=2$) of mass m and diameter σ. A complete specification of the initial state of the system involves knowing a point in the $2Nd$-dimensional phase space $\Gamma \equiv \{\mathbf{q}_r, \mathbf{v}_r;\ r=1,\ldots,N\}$, which gives the position $\mathbf{q}_r$ and velocity $\mathbf{v}_r$ of each particle r of the system. At a later time t, the state will be characterized by another point in phase space, $\Gamma \equiv \{\mathbf{q}_r(t), \mathbf{v}_r(t);\ r=1,\ldots,N\}$. The dynamics of the particles consists of free streaming (straight line motion along the direction of the velocity), until a pair of particles, r and s, are at contact, at which time their velocities $\mathbf{v}_r, \mathbf{v}_s$ change instantaneously to $\mathbf{v}'_r, \mathbf{v}'_s$ according to the collision rule

$$\mathbf{v}'_r = \mathbf{v}_r - \frac{1+\alpha}{2}(\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})\hat{\mathbf{q}}_{rs},$$

$$\mathbf{v}'_s = \mathbf{v}_s + \frac{1+\alpha}{2}(\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})\hat{\mathbf{q}}_{rs}, \tag{A1}$$

where $\hat{\mathbf{q}}_{rs}$ is a unit vector along the relative position $\mathbf{q}_{rs} = \mathbf{q}_r - \mathbf{q}_s$ at contact and α is the coefficient of normal restitution, defined in the interval $0 < \alpha \leq 1$, and which will be taken here as constant, i.e., velocity independent. In terms of the relative velocity $\mathbf{g}_{rs} = \mathbf{v}_r - \mathbf{v}_s$ and the center of mass velocity $\mathbf{G}_{rs} = (\mathbf{v}_r + \mathbf{v}_s)/2$, the above collision rule reads

$$\mathbf{G}'_{rs} = \mathbf{G}_{rs}, \quad \mathbf{g}'_{rs} = \mathbf{g}_{rs} - (1+\alpha)(\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})\hat{\mathbf{q}}_{rs}. \tag{A2}$$

The energy loss on collision is

$$\Delta E = \frac{m}{4}(g'^2_{rs} - g^2_{rs}) = -\frac{m}{4}(1-\alpha^2)(\hat{\mathbf{q}}_{rs} \cdot \mathbf{g}_{rs})^2. \tag{A3}$$

It is seen that $\alpha=1$ corresponds to elastic collisions. Subsequent to the change in relative velocity for the pair $\{r,s\}$, the free streaming of all particles continues until another pair is at contact, and the corresponding instantaneous change in their relative velocities is performed. The sequence of free streaming and binary collisions determines a unique trajectory in phase space, Γ_t, for given initial conditions. The collision rule is invertible so the trajectory can be reversed, although with the inverted collision rule ("restituting" collisions).

The statistical mechanics for this system [26] is comprised of the dynamics just described, an initial macrostate

specified in terms of a probability density $\rho(\Gamma)$, and a set of microscopic observables (measurables). The macroscopic variables of interest are the expectation value for the observables at time $t > 0$ for an initial state $\rho(\Gamma)$. Given an observable $A(\Gamma)$, its expectation value is defined by the two equivalent forms

$$\langle A(t);0 \rangle \equiv \int d\Gamma \, \rho(\Gamma) e^{Lt} A(\Gamma) = \int d\Gamma \, A(\Gamma) e^{-\bar{L}t} \rho(\Gamma).$$
(A4)

In the above expression, L is the generator of the dynamics of phase functions and $\bar{L}$ is the generator of dynamics for distribution functions. The explicit forms of these generators will be derived in the following.

1. Generator of trajectories

The hard-sphere dynamics described above is characterized by piecewise constant velocities that change instantaneously (and discontinuously) at the time of collision. This allows the generator of trajectories to be derived using geometric arguments [10]. Consider first a system of two inelastic hard spheres or disks. The particles move freely until they eventually contact, at which time their velocities change instantaneously according to Eq. (A1) above. Suppose that the two particles, named 1 and 2, respectively, collide at time τ. This time is determined as a function of the initial separation $\boldsymbol{q}_{12}$ and relative velocity $\boldsymbol{g}_{12}$ from

$$\boldsymbol{q}_{12} + \boldsymbol{g}_{12} \tau = \boldsymbol{\sigma},$$
(A5)

with $\boldsymbol{\sigma}$ being an arbitrary vector of modulus σ. Of course, if this equation does not have a real and positive solution for τ, the particles do not collide. Then, for $0 < t \leq \tau$ the trajectory is given by free streaming with the initial velocities, i.e., $\Gamma(t) = \Gamma_0(t) \equiv \{\boldsymbol{q}_t + \boldsymbol{v}_r t, \boldsymbol{v}_r; \; r = 1, 2\}$. For $t > \tau$, it is $\Gamma(t) = \Gamma'(t) = \{\boldsymbol{q}_r + \boldsymbol{v}_r \tau + \boldsymbol{v}'_r(t-\tau), \boldsymbol{v}'_r; \; r = 1, 2\}$, where the velocities $\boldsymbol{v}'_r$ are determined by the collision rule (A1). Therefore, the value of any phase function $A(\Gamma)$ at time t can be given compactly expressed as

$$A[\Gamma(t)] = \{1 - \Theta[t - \tau(\Gamma)]\} A[\Gamma_0(t)] + \Theta[t - \tau(\Gamma)] A[\Gamma'(t)],$$
(A6)

where $\Theta(x)$ is the Heaviside step function, defined by $\Theta(x) = 0$ for $x \leq 0$ and $\Theta(x) = 1$ for $x > 0$. Differentiation with respect to time of the above equation leads to

$$\frac{\partial A[\Gamma(t)]}{\partial t}$$

$$= \sum_{r=1}^{2} \boldsymbol{v}_r(t) \cdot \frac{\partial A[\Gamma(t)]}{\partial \boldsymbol{q}_r(t)} + \delta[t - \tau(\Gamma)]\{A[\Gamma'(t)] - A[\Gamma_0(t)]\}$$

$$= \sum_{r=1}^{2} \boldsymbol{v}_r(t) \cdot \frac{\partial A[\Gamma(t)]}{\partial \boldsymbol{q}_r(t)} + \delta[t - \tau(\Gamma)](b_{12} - 1) A[\Gamma(t)]. \quad \text{(A7)}$$

Here, b_{12} is a substitution operator that changes the velocities into their postcollisional values as given by Eq. (A1),

$$b_{12} X(\boldsymbol{v}_1, \boldsymbol{v}_2) = X(b_{12}\boldsymbol{v}_1, b_{12}\boldsymbol{v}_2) = X(\boldsymbol{v}'_1, \boldsymbol{v}'_2). \quad \text{(A8)}$$

Of course, the vector $\hat{\boldsymbol{q}}_{12}$ to be used in the collision rule is $\boldsymbol{q}_{12}(\tau)/q_{12}(\tau)$.

It is convenient to substitute the δ function involving the time t in Eq. (A7) by a more geometrical quantity. To begin with, notice that not every solution of Eq. (A5) corresponds to a physical collision. In fact, it is easily realized that, for every contact representing a physical collision, there is another solution to Eq. (A5) corresponding to the time at which the two particles would separate if they were allowed to stream through each other. The physical value of τ can be identified as that for which $\hat{\boldsymbol{q}}_{12}(\tau) \cdot \boldsymbol{g}_{12} < 0$, while for the unphysical solution of Eq. (A5) it is $\hat{\boldsymbol{q}}_{12}(\tau) \cdot \boldsymbol{g}_{12} > 0$. Next, take into account that the solutions of Eq. (A5) are the same as those of $q_{12}(\tau) - \sigma = 0$. Hence

$$\delta[t - \tau(\Gamma)] = \Theta[-\hat{\boldsymbol{q}}_{12}(t) \cdot \boldsymbol{g}_{12}(t)] \delta[q_{12}(t) - \sigma] \left| \frac{\partial q_{12}(t)}{\partial t} \right|$$

$$= \Theta[-\hat{\boldsymbol{q}}_{12}(t) \cdot \boldsymbol{g}_{12}(t)] \delta[q_{12}(t) - \sigma] |\hat{\boldsymbol{q}}_{12}(t) \cdot \boldsymbol{g}_{12}(t)|. \quad \text{(A9)}$$

Use of this in Eq. (A7) yields

$$\frac{\partial A[\Gamma(t)]}{\partial t} = \sum_{r=1}^{2} \boldsymbol{v}_r(t) \cdot \frac{\partial A[\Gamma(t)]}{\partial \boldsymbol{q}_r(t)} + \delta[q_{12}(t) - \sigma]$$

$$\times \Theta[-\hat{\boldsymbol{q}}_{12}(t) \cdot \boldsymbol{g}_{12}(t)] |\hat{\boldsymbol{q}}_{12}(t) \cdot \boldsymbol{g}_{12}(t)|$$

$$\times (b_{12} - 1) A[\Gamma(t)]. \quad \text{(A10)}$$

The generator of trajectories is defined by

$$A[\Gamma(t)] = e^{Lt} A(\Gamma), \quad \text{(A11)}$$

so L is identified as

$$L = \sum_{r=1}^{2} \boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} + T(1,2), \quad \text{(A12)}$$

with the binary collision operator $T(1,2)$ given by

$$T(1,2) = \delta(q_{12} - \sigma) \Theta(-\hat{\boldsymbol{q}}_{12} \cdot \boldsymbol{g}_{12}) |\hat{\boldsymbol{q}}_{12} \cdot \boldsymbol{g}_{12}| (b_{12} - 1). \quad \text{(A13)}$$

This expression can be rewritten in a form that is often more suitable for explicit calculations, by employing the relation

$$\int d\hat{\boldsymbol{\sigma}} \, \delta(\boldsymbol{q}_{12} - \boldsymbol{\sigma}) = \sigma^{-(d-1)} \delta(q_{12} - \sigma), \quad \text{(A14)}$$

where $d\hat{\boldsymbol{\sigma}}$ is the solid angle element associated with $\boldsymbol{\sigma}$. In this way, we obtain

$$T(1,2) = \sigma^{d-1} \int d\hat{\boldsymbol{\sigma}} \, \delta(\boldsymbol{q}_{12} - \boldsymbol{\sigma}) \Theta(-\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{g}_{12}) |\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{g}_{12}| (b_{12} - 1). \quad \text{(A15)}$$

The generator of trajectories for the system of N particles considered here entails the additional *assumption* that only binary collisions occur between particles, i.e., there are no collisions involving three or more particles simultaneously at contact. Then, for a system of N particles,

$$L = \sum_{r=1}^{N} \boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} + \frac{1}{2} \sum_{r}^{N} \sum_{s \neq r}^{N} T(r,s). \qquad \text{(A16)}$$

2. Adjoint dynamics

Next, consider the generator $\bar{L}$ defined by the second equality in Eq. (A4). It can be identified from

$$\int d\Gamma \, A(\Gamma) \bar{L} \rho[\Gamma] \equiv -\int d\Gamma [LA(\Gamma)] \rho(\Gamma)$$

$$= -\sum_{r=1}^{N} \int d\Gamma \, \rho(\Gamma) \boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} A(\Gamma)$$

$$- \frac{1}{2} \int \sum_{r}^{N} \sum_{s \neq r}^{N} \int d\Gamma \, \rho(\Gamma) \delta(q_{rs} - \sigma)$$

$$\times \Theta(-\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}) |\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}| (b_{rs} - 1) A(\Gamma). \tag{A17}$$

Define the inverse, b_{rs}^{-1}, of b_{rs} by $b_{rs}^{-1} b_{rs} = b_{rs} b_{rs}^{-1} = 1$. Equation (A2) gives directly

$$b_{rs}^{-1} \boldsymbol{g}_{rs} \equiv \boldsymbol{g}_{rs}'' = \boldsymbol{g}_{rs} - \frac{1 + \alpha}{\alpha} (\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}) \hat{\boldsymbol{q}}_{rs}. \qquad \text{(A18)}$$

A useful identity is given by

$$\int d\Gamma \, X(\Gamma) b_{rs} Y(\Gamma) = \int d(b_{rs}^{-1} \Gamma) X(b_{rs}^{-1} \Gamma) Y(\Gamma)$$

$$= \alpha^{-1} \int d\Gamma \, X(b_{rs}^{-1} \Gamma) Y(\Gamma) \qquad \text{(A19)}$$

for arbitrary functions $X(\Gamma)$ and $Y(\Gamma)$. The first equality is obtained by changing integration variables from $(\boldsymbol{v}_r, \boldsymbol{v}_s)$ to $(b_{rs} \boldsymbol{v}_r, b_{rs} \boldsymbol{v}_s)$. The factor α^{-1} is the Jacobian for this change of variables. Also,

$$b_{rs}^{-1}(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}) = -\alpha^{-1} \hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}. \qquad \text{(A20)}$$

Equation (A17) therefore can be rewritten as

$$\int d\Gamma \, A(\Gamma) \bar{L} \rho(\Gamma) = \sum_{r=1}^{N} \int d\Gamma \, A(\Gamma) \boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} \rho(\Gamma)$$

$$- \sum_{r=1}^{N} \int_S d\boldsymbol{S}_r \cdot \int d\boldsymbol{v}_r \int d\Gamma^{(r)} \boldsymbol{v}_r \rho(\Gamma) A(\Gamma)$$

$$- \frac{1}{2} \sum_{r=1}^{N} \sum_{s \neq r}^{N} \int d\Gamma \, A(\Gamma) \delta(q_{rs} - \sigma) |\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}|$$

$$\times [\Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}) \alpha^{-2} b_{rs}^{-1} - \Theta(-\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})] \rho(\Gamma). \tag{A21}$$

An integration by parts has been performed in the first term, leaving a surface integral for which boundary conditions must be specified. Then $d\boldsymbol{S}_r$ is the surface element vector

associated with $\boldsymbol{q}_r$ and $d\Gamma^{(r)}$ is the element of volume of the $2(N-1)d$ phase space obtained by eliminating $\boldsymbol{q}_r$ and $\boldsymbol{v}_r$ in the original one. This surface term identically vanishes when, for instance, periodic boundary conditions are considered for the system and $A(\Gamma)$ is a compact function of the positions. In the following it will always be considered that this is the case. The adjoint Liouville operator is formally identified from the other nonsurface terms as

$$\bar{L} = \sum_{r=1}^{N} \boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} - \frac{1}{2} \sum_{r}^{N} \sum_{s \neq r}^{N} \bar{T}(r,s), \qquad \text{(A22)}$$

where the new binary collision operator is

$$\bar{T}(r,s) = \delta(q_{rs} - \sigma) |\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}| [\Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}) \alpha^{-2} b_{rs}^{-1} - \Theta(-\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})]. \tag{A23}$$

The integral representation of this operator, similar to Eq. (A15), is

$$\bar{T}(r,s) = \sigma^{d-1} \int d\hat{\boldsymbol{\sigma}} \Theta(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{g}_{rs}) |\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{g}_{rs}|$$

$$\times [\alpha^{-2} \delta(\boldsymbol{q}_{rs} - \boldsymbol{\sigma}) b_{rs}^{-1} - \delta(\boldsymbol{q}_{rs} + \boldsymbol{\sigma})]. \tag{A24}$$

3. Time correlation functions and time-reversed generator

The response functions in statistical mechanics take the form of time correlation functions over the macrostate under consideration, and can be written in two equivalent ways, corresponding to each of the two representations in Eq. (A4),

$$C_{AB}(t) = \int d\Gamma [e^{tL} A(\Gamma)] B(\Gamma) \rho(\Gamma)$$

$$= \int d\Gamma \, A(\Gamma) e^{-t\bar{L}} [\rho(\Gamma) B(\Gamma)], \qquad \text{(A25)}$$

where $A(\Gamma)$ and $B(\Gamma)$ are two phase functions. A third representation can be identified in the form

$$C_{AB}(t) = \int d\Gamma \, A(\Gamma) [e^{-tL_-} B(\Gamma)] e^{-t\bar{L}} \rho(\Gamma). \qquad \text{(A26)}$$

Comparison of Eqs. (A25) and (A26) shows that the operator L_- must satisfy the relation

$$\bar{L}(\rho B) = (\bar{L} \rho) B + \rho L_- B. \qquad \text{(A27)}$$

It follows that

$$\rho L_- B = \rho \sum_{r=1}^{N} \boldsymbol{v}_r \cdot \frac{\partial B}{\partial \boldsymbol{q}_r} - \frac{1}{2} \sum_{r=1}^{N} \sum_{s \neq r}^{N} [\bar{T}(r,s)(\rho B) - B\bar{T}(r,s)\rho]. \tag{A28}$$

Next, consider the action of $\bar{T}(r,s)$ on ρB in detail using the definition (A23),

$$\bar{T}(r,s)(\rho B) = \delta(q_{rs} - \sigma)|\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}|[\Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})\alpha^{-2}(b_{rs}^{-1}\rho)(b_{rs}^{-1}B)$$
$$- \Theta(-\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})\rho B]$$
$$= B\bar{T}(r,s)\rho + \delta(q_{rs} - \sigma)|\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}|$$
$$\times \Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})(\alpha^{-2}b_{rs}^{-1}\rho)(b_{rs}^{-1} - 1)B$$
$$= B\bar{T}(r,s)\rho + \rho\delta(q_{rs} - \sigma)|\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}|$$
$$\times \Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})(b_{rs}^{-1} - 1)B. \tag{A29}$$

In the last equality, use has been made of the identity

$$\delta(q_{rs} - \sigma)|\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}|\Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})\alpha^{-2}b_{rs}^{-1}\rho$$
$$= \delta(q_{rs} - \sigma)|\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}|\Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})\rho, \tag{A30}$$

valid for hard-sphere or -disk distribution functions [27]. This identity follows from the requirement that the flux for a pair of particles at contact with relative velocity $\boldsymbol{g}_{rs}$ on the precollision hemisphere, should be the same as that for $\boldsymbol{g}_{rs}''$ on the postcollision hemisphere. See Ref. [27] for further details and applications.

Use of Eq. (A29) in Eq. (A28) gives

$$\rho L_- B = \rho \sum_r \boldsymbol{v}_r \cdot \frac{\partial B}{\partial \boldsymbol{q}_r} - \frac{\rho}{2}\sum_{r=1}^{N}\sum_{s \neq r}^{N} \delta(q_{rs} - \sigma)|\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs}|\Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{g}_{rs})$$
$$\times (b_{rs}^{-1} - 1). \tag{A31}$$

This in turn gives the identification

$$L_- = \sum_{r=1}^{N} \boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} - \frac{1}{2}\sum_{r=1}^{N}\sum_{s \neq r}^{N} T_-(r,s), \tag{A32}$$

with a third binary collision operator $T_-(r,s)$ defined as

$$T_-(r,s) = \delta(q_{rs} - \sigma)\Theta(\hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{q}_{rs})|\ \hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{q}_{rs}|(b_{rs}^{-1} - 1)$$
$$= \sigma^{d-1}\int d\hat{\boldsymbol{\sigma}}\Theta(\hat{\boldsymbol{\sigma}} \cdot \boldsymbol{g}_{rs})|\ \hat{\boldsymbol{q}}_{rs} \cdot \boldsymbol{q}_{rs}|\delta(q_{rs} - \boldsymbol{\sigma})(b_{rs}^{-1} - 1). \tag{A33}$$

It is a simple task using standard techniques to verify that Eq. (A27) implies

$$e^{-t\bar{L}}(\rho B) = (e^{-t\bar{L}}\rho)e^{-tL_-}B, \tag{A34}$$

and Eq. (A26) follows. For the particular case $\rho = \rho_h$, the HCS ensemble, we have

$$e^{-t\bar{L}}\rho_h[\Gamma; T(0)] = \rho_h[\Gamma; T(t)] \tag{A35}$$

and, therefore, the correlation functions defined in Eq. (A26) can be expressed in the form

$$C_{AB}(t) = \int d\Gamma\, A(\Gamma)[e^{-tL_-}B(\Gamma)]\rho_h[\Gamma; T(t)]. \tag{A36}$$

It is seen that L_- is the same as the trajectory generator identified in Eq. (A16), but with the restituting collision rule in place of the direct collision rule. Therefore, L_- is the generator of time-reversed trajectories in phase space.

APPENDIX B: DIMENSIONLESS REPRESENTATION

The time dependence of the reference HCS ensemble has the scaling form indicated in Eq. (4). This means that the time dependence can be removed entirely by a change of variables, leaving a universal dimensionless function of the scaled velocities. It is useful to introduce these same variables more generally for other states as well, to partially account for collisional cooling. The advantages will be apparent in the final results. The set of dimensionless variables are chosen to be

$$\boldsymbol{q}_r^* = \frac{\boldsymbol{q}_r}{l}, \quad \boldsymbol{v}_r^* = \frac{\boldsymbol{v}_r}{v_0(t)}, \quad ds = \frac{v_0(t)}{l}dt, \tag{B1}$$

where $v_0(t) \equiv v_0[T_h(t)]$ is defined in terms of the temperature of a HCS reference state having the same initial total energy as the actual system under consideration. The Liouville equation then becomes

$$\left(\frac{\partial}{\partial s} + \bar{\mathcal{L}}^*\right)\rho^*(\Gamma^*, s) = 0, \tag{B2}$$

with the reduced distribution function $\rho^*(\Gamma^*, s)$ defined by

$$\rho^*(\Gamma^*, s) = [\ell v_0(t)]^{Nd}\rho(\Gamma, t), \tag{B3}$$

where $\Gamma^* \equiv \{\boldsymbol{q}_r^*, \boldsymbol{v}_r^*;\ r = 1, \dots, N\}$ and the operator $\bar{\mathcal{L}}^*$ is given by

$$\bar{\mathcal{L}}^*\rho^* = \bar{L}^*\rho^* + \frac{\zeta_0^*}{2}\sum_{r=1}^{N} \frac{\partial}{\partial \boldsymbol{v}_r^*} \cdot (\boldsymbol{v}_r^*\rho^*). \tag{B4}$$

Here,

$$\bar{L}^* = \frac{l}{v_0(t)}\bar{L} = [\bar{L}]_{\Gamma = \Gamma^*} \tag{B5}$$

and ζ_0^* is the dimensionless cooling rate

$$\zeta_0^* = \frac{l\zeta_0(T)}{v_0(T)}. \tag{B6}$$

The first term $\bar{L}^*$ of the generator $\bar{\mathcal{L}}^*$ for dynamics in this dimensionless Liouville equation generates the usual hard-sphere trajectories in scaled variables. The second term rescales the velocities along the trajectories, to represent their change due to the average cooling associated with the HCS. A first advantage of this representation is the fact that the HCS ensemble is a stationary solution of the Liouville equation,

$$\bar{\mathcal{L}}^*\rho_h^* = 0. \tag{B7}$$

Consider a phase function $A(\Gamma)$ whose dimensions scale out as a factor with the above change of variables, i.e.,

$$A(\Gamma) = c_A[v_0(t)]A^*(\Gamma^*), \tag{B8}$$

where $c_A[v_0(t)]$ contains the dimensions of $A(\Gamma)$ so that $A^*(\Gamma^*)$ is dimensionless. The ensemble average of $A(\Gamma)$ at time t is

$$\langle A(t) \rangle \equiv \int d\Gamma\, \rho(\Gamma,t)A(\Gamma) = c_A[v_0(t)]\langle A^*(s)\rangle^*. \quad \text{(B9)}$$

The dimensionless average is then given by

$$\langle A^*(s)\rangle^* \equiv \frac{\langle A(t)\rangle}{c_A[v_0(t)]} = \int d\Gamma^*[e^{-s\bar{\mathcal{L}}^*}\rho^*(\Gamma^*,0)]A^*(\Gamma^*). \quad \text{(B10)}$$

Adjoint operators can be introduced just as in Appendix A for equivalent representations. For example,

$$\langle A^*(s)\rangle^* = \int d\Gamma^*\rho^*(\Gamma^*,0)e^{s\mathcal{L}^*}A^*(\Gamma^*) \quad \text{(B11)}$$

with

$$\mathcal{L}^* = L^* + \frac{\zeta_0^*}{2}\sum_{r=1}^{N} \boldsymbol{v}_r^* \cdot \frac{\partial}{\partial \boldsymbol{v}_r}; \quad \text{(B12)}$$

$$L^* = \frac{l}{v_0(t)}L = [L]_{\Gamma=\Gamma^*}. \quad \text{(B13)}$$

To illustrate the utility of this formulation, consider an average over the HCS. Then Eq. (B10) gives $\langle A^*(s)\rangle^* = \langle A^*(0)\rangle^*$, since ρ_h^* is stationary. Using Eq. (B11), the time derivative at $s=0$ is seen to be given by

$$\int d\Gamma^*\rho_h^*(\Gamma^*)\mathcal{L}^*A^*(\Gamma^*) = 0. \quad \text{(B14)}$$

Suppose now that A^* is an arbitrary differentiable function of the scaled total momentum of the system $\boldsymbol{P}^* = \Sigma_r \boldsymbol{v}_r^*$, i.e., $A^* = A^*(\boldsymbol{P}^*)$. By momentum conservation, $L^*A^*(\boldsymbol{P}^*)=0$ and Eq. (B14) becomes

$$\frac{\zeta_0^*}{2}\int d\Gamma^*\rho_0^*(\Gamma^*)\sum_{r=1}^{N} \boldsymbol{v}_r^* \cdot \frac{\partial}{\partial \boldsymbol{v}_r}A^*(\boldsymbol{P}^*)$$

$$= \frac{\zeta_0^*}{2}\int d\Gamma^*\rho_0^*(\Gamma^*)\boldsymbol{P}^* \cdot \frac{\partial}{\partial \boldsymbol{P}^*}A^*(\boldsymbol{P}^*) = 0. \quad \text{(B15)}$$

Since this holds for any function $A^*(\boldsymbol{P}^*)$, it follows that $\rho_h^*(\Gamma^*)$ must be proportional to a δ function in the total momentum,

$$\rho_h^*(\Gamma^*) = \delta(\boldsymbol{P}^*)\bar{\rho}_h^*(\Gamma^*). \quad \text{(B16)}$$

This is the result quoted in Eq. (5) in the text.

The dimensionless forms for correlation functions defined in Eq. (A25) are obtained by using the representation in Eq. (B11),

$$C_{AB}^*(s) = \frac{C_{AB}(t)}{c_A[v_0(t)]c_B[v_0(0)]}$$

$$= \int d\Gamma^*[e^{s\mathcal{L}^*}A^*(\Gamma^*)]B^*(\Gamma^*)\rho^*(\Gamma^*,0). \quad \text{(B17)}$$

The adjoint representation follows directly as well,

$$C_{AB}^*(s) = \int d\Gamma^*A^*(\Gamma^*)e^{-s\bar{\mathcal{L}}^*}[\rho^*(\Gamma^*,0)B^*(\Gamma^*)]. \quad \text{(B18)}$$

Finally, the representation in Eq. (A26) gives the third equivalent form:

$$C_{AB}^*(s) = \int d\Gamma^*A^*(\Gamma^*)[e^{-s\mathcal{L}^*}\rho^*(\Gamma^*,0)]e^{-s\mathcal{L}_-^*}B^*(\Gamma^*), \quad \text{(B19)}$$

with

$$\mathcal{L}_-^* = L_-^* + \frac{\zeta_0^*}{2}\sum_{r=1}^{N} \boldsymbol{v}_r^* \cdot \frac{\partial}{\partial \boldsymbol{v}_r^*} \quad \text{(B20)}$$

and

$$L_-^* = \frac{l}{v_0(t)}L_- = [L_-]_{\Gamma=\Gamma^*}. \quad \text{(B21)}$$

For the particular case of the HCS, in Eqs. (B17)–(B19) we have

$$e^{-s\bar{\mathcal{L}}^*}\rho_h^*(\Gamma^*,0) = \rho_h^*(\Gamma^*,0) = \rho_h^*(\Gamma^*), \quad \text{(B22)}$$

due to the stationarity of the distribution of the HCS in the reduced scales.

The results of this appendix, starting from hard-sphere dynamics, agree with those obtained in Ref. [3], starting from more general interaction potentials and taking the scaling limit (see Sec. VIII in Ref. [3]).

APPENDIX C: HYDRODYNAMIC MODES

In this appendix, the eigenvalues of the hydrodynamic transport matrix $\mathcal{K}^{*\text{hyd}}(\boldsymbol{k}^*)$, whose expression is given by Eqs. (11)–(13), are presented and some comments made on their implication for transport in a granular fluid. Similar results, but restricted to the low-density limit, have been reported in [28]. The eigenvalues of the matrix $\mathcal{K}^{*\text{hyd}}$ are the solutions γ_α to the cubic equation

$$\gamma^3 - \left[\frac{2(d-1)\eta^*}{d} + \kappa^* + \frac{2\lambda^*}{d} - \zeta^{*T}\right]k^{*2}\gamma^2 - \left\{\frac{\zeta_0^{*2}}{4}\right.$$

$$- \left[\frac{\zeta_0^*}{2}\left(\frac{2(d-1)\eta^*}{d} + \kappa^* - \frac{2\lambda^*}{d} + \zeta^{*T}\right) - \frac{p_h^*}{2}\left(\frac{2p_h^*}{d} + \zeta^{*U}\right)\right.$$

$$\left.- \frac{p_h^*}{2}\frac{\partial\ln p_h}{\partial\ln n_h}\right]k^{*2}\left.\right\}\gamma + \frac{\zeta_0^*p_h^*}{4}\left(\frac{\partial}{\partial\ln n_h}\ln\frac{\zeta_0^2}{p_h}\right)k^{*2} = 0, \quad \text{(C1)}$$

plus the $(d-1)$-fold-degenerate shear modes

$$\gamma_\perp = -\frac{\zeta_0^*}{2} + \eta^*k^{*2}. \quad \text{(C2)}$$

If the limit $\alpha \to 1$ is taken for this equation, $\zeta_0^* \to 0$, and the solutions to order k^{*2} give the familiar hydrodynamic modes associated with normal fluids: the two propagating sound modes, the heat mode, and the $d-1$ transverse shear modes [13]. But, when the solution to the above equation is considered at finite α, the modes to order k^{*2} are quite different,

$$\gamma_1(k^*) = \frac{p_h^*}{\zeta_0^*}\left(\frac{\partial}{\partial \ln n_h}\ln\frac{\zeta_0^2}{p_h}\right)k^{*2}, \tag{C3}$$

$$\gamma_2(k^*) = \frac{\zeta_0^*}{2} - \left[\frac{p_h^*}{2\zeta_0^*}\left(\frac{2p_h^*}{d} + 2\frac{\partial \ln \zeta_0}{\partial \ln n_h} + \zeta^{*U}\right) - \frac{2\lambda^*}{d} + \zeta^{*T}\right]k^{*2}, \tag{C4}$$

$$\gamma_3(k^*) \equiv \gamma_\parallel(k^*) = -\frac{\zeta_0^*}{2} + \left[\frac{p_h^*}{2\zeta_0^*}\left(\frac{2p_h^*}{d} - 2\frac{\partial \ln \zeta_0}{\partial \ln n_h} + \zeta^{*U}\right.\right.$$
$$\left.\left. + 2\frac{\partial \ln p_h}{\partial \ln n_h}\right) + \frac{2(d-1)\eta^*}{d} + \kappa^*\right]k^{*2}. \tag{C5}$$

All eigenvalues are real and hence there are no propagating modes. Also, the limit $\alpha \to 1$ is singular so these modes in this limit do not represent the familiar hydrodynamic excitations of a normal fluid. The drastic difference in the nature of the hydrodynamic modes obtained as the elastic limit of the above eigenvalues is due to the nonanalyticity of the eigenvalues and eigenvectors about the point $\alpha = 1$ and $k = 0$. Close to the elastic limit, both $\zeta_0^* \propto (1-\alpha^2)$ and k are small parameters, and the type of modes obtained depends on how these parameters approach zero [28]. This is an indication of the fact that the inelasticity, even when small, gives rise to drastically different transport in the fluid. For the purposes at hand, attention is restricted here to the $\alpha \neq 1$ forms of these modes.

There exists a critical wavelength $k_\perp^{*c}$ defined by

$$k_\perp^{*c} = \frac{\zeta_0^*}{2\eta^*}, \tag{C6}$$

such that for $k^* < k_\perp^{*c}$ the shear modes become unstable. Similarly, there exists a threshold wavelength for the $\gamma_\parallel$ mode such that it becomes unstable as well. This means that the homogeneous state characterized by these hydrodynamic equations is unstable to sufficiently long-wavelength perturbations that excite these modes. This instability of the HCS has been well established in the literature [29,30]. This implies physically that the response due to the unstable modes grows until such time as the linear theory breaks down, and further analysis of the dynamics has to be carried out using the full nonlinear hydrodynamic equations. It is still an open question as to the nature of the final state [31].

Further insight into the nature of the hydrodynamic response of this fluid can be obtained by looking at the corresponding eigenvectors. To lowest order in k these are found to be

$$\varphi_1(k^*) = \begin{pmatrix} 1 \\ -2\dfrac{\partial \ln \zeta_0}{\partial \ln n_h} \\ 0 \\ \mathbf{0} \end{pmatrix}, \quad \varphi_2(k^*) = \begin{pmatrix} 0 \\ 1 \\ 0 \\ \mathbf{0} \end{pmatrix},$$

$$\varphi_\parallel(k^*) = \begin{pmatrix} 0 \\ 0 \\ 1 \\ \mathbf{0} \end{pmatrix}, \quad \varphi_{\perp,i}(k^*) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \hat{\boldsymbol{i}} \end{pmatrix}. \tag{C7}$$

Here, $\mathbf{0}=0$ and $\hat{\boldsymbol{i}}=\hat{\mathbf{1}}=1$, for $d=2$, while $\mathbf{0}=\binom{0}{0}$ and $i=1,2$, with $\hat{\mathbf{1}}=\binom{1}{0}$ and $\hat{\mathbf{2}}=\binom{0}{1}$, for $d=3$.

The first of these modes is excited by the condition

$$\delta T^* = -2\frac{\partial \ln \zeta_0}{\partial \ln n_h}\delta n^* \tag{C8}$$

and zero flow velocity. This can be interpreted as follows. The cooling rate has the form $\zeta_0(n_h,T_h)=T_h^{1/2}\overline{\zeta}_0(n_h)$. It then follows that this condition for exciting the first mode corresponds to variations in the temperature and density that leave the cooling rate constant. The second mode in Eq. (C7) is due to a temperature perturbation at constant density and also zero velocity, while the third one is due to a longitudinal velocity perturbation at constant temperature and density. The last $d-1$ modes are the response to a transverse velocity perturbation, again at constant temperature and density.

APPENDIX D: MICROSCOPIC CONSERVATION LAWS

The aim here is to derive the conservation laws (more precisely, balance equations) for the microscopic observables of interest, namely, the number density $\mathcal{N}(\Gamma;\boldsymbol{r})$, energy density $\mathcal{E}(\Gamma;\boldsymbol{r})$, and momentum density $\mathcal{G}(\Gamma;\boldsymbol{r})$. Their ensemble averages give the hydrodynamic fields. One set of balance equations is associated with the dynamics for $t>0$, whose generator is the L operator given by Eq. (A16). Another set of balance equations describes the dynamics for $t<0$, as generated by L_- defined in Eq. (A32). Both dynamics lead to forms of fluxes that appear in the Green-Kubo expressions for both elastic and inelastic hard sphere transport coefficients (see Appendix H).

Let $\{\mathcal{A}_\alpha(\Gamma;\boldsymbol{r},t)\}$ denote the set of phase functions $\{\mathcal{N},\mathcal{E},\mathcal{G}\}$. Consider first $t>0$. The phase functions obey the equation

$$\frac{\partial \mathcal{A}_\alpha(\Gamma;\boldsymbol{r},t)}{\partial t} - L(\Gamma)\mathcal{A}_\alpha(\Gamma;\boldsymbol{r},t) = 0, \tag{D1}$$

where $L(\Gamma)$ is given in Eq. (A16). The aim here is to evaluate the action of the L operator on the density $\mathcal{A}_\alpha$ to identify a balance equation of the form

$$\frac{\partial \mathcal{A}(\Gamma;\boldsymbol{r},t)}{\partial t} + \boldsymbol{\nabla} \cdot \boldsymbol{j}_\alpha(\Gamma;\boldsymbol{r},t) = -w_\alpha(\Gamma;\boldsymbol{r},t). \tag{D2}$$

Here, $\boldsymbol{j}_\alpha$ is the flux associated with the density $\mathcal{A}_\alpha$, and w_α is a source that signifies a local loss contribution in this density that cannot be expressed as a divergence. It is nonzero only in the equation for the energy density.

The number density is defined as

$$\mathcal{N}(\Gamma;\boldsymbol{r}) \equiv \sum_{r=1}^{N} \delta(\boldsymbol{r}-\boldsymbol{q}_r), \tag{D3}$$

so

$$L\mathcal{N}(\Gamma;\mathbf{r}) = \sum_{r=1}^{N} \boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} \delta(\boldsymbol{r}-\boldsymbol{q}_r) = -\boldsymbol{\nabla} \cdot \sum_{r=1}^{N} \boldsymbol{v}_r \delta(\boldsymbol{r}-\boldsymbol{q}_r). \tag{D4}$$

This gives the microscopic continuity equation,

$$\frac{\partial \mathcal{N}(\Gamma;\boldsymbol{r},t)}{\partial t} + \boldsymbol{\nabla} \cdot \frac{\mathcal{G}(\Gamma;\boldsymbol{r},t)}{m} = 0, \tag{D5}$$

where the number flux density is seen to be proportional to the momentum density,

$$\mathcal{G}(\Gamma;\boldsymbol{r}) \equiv \sum_{r=1}^{N} m\boldsymbol{v}_r \delta(\boldsymbol{r}-\boldsymbol{q}_r). \tag{D6}$$

Consider now the equation for this density. It is

$$L\mathcal{G}(\Gamma;\boldsymbol{r}) = \sum_{r=1}^{N} m\boldsymbol{v}_r\boldsymbol{v}_r \cdot \frac{\partial}{\partial \boldsymbol{q}_r} \delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{m}{2}\sum_{r=1}^{N}\sum_{s\neq r}^{N} T(r,s)[\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \boldsymbol{v}_s\delta(\boldsymbol{r}-\boldsymbol{q}_s)]$$

$$= -\boldsymbol{\nabla} \cdot \left[\sum_{r=1}^{N} m\boldsymbol{v}_r\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{(1+\alpha)m\sigma}{4}\sum_{r=1}^{N}\sum_{s\neq r}^{N} \delta(q_{rs}-\sigma)\Theta(-\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs}) \times |\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs}|^2\hat{\boldsymbol{q}}_{rs}\hat{\boldsymbol{q}}_{rs}\int_0^1 d\gamma\, \delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs}) \right]. \tag{D7}$$

In the second equality, use has been made of the relation

$$(b_{rs}-1)\boldsymbol{v}_r = -(b_{rs}-1)\boldsymbol{v}_s = -\frac{1+\alpha}{2}(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})\hat{\boldsymbol{q}}_{rs} \tag{D8}$$

and the identity

$$\delta(\boldsymbol{r}-\boldsymbol{q}_r) - \delta(\boldsymbol{r}-\boldsymbol{q}_s) = -\int_0^1 d\gamma \frac{\partial}{\partial \gamma} \delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs})$$

$$= -\boldsymbol{q}_{rs} \cdot \boldsymbol{\nabla} \int_0^1 d\gamma\, \delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs}). \tag{D9}$$

Equation (D7) gives the conservation law for the momentum,

$$\frac{\partial}{\partial t}\mathcal{G}(\Gamma;\boldsymbol{r},t) + \boldsymbol{\nabla} \cdot \mathbf{h}(\Gamma;\boldsymbol{r},t) = 0, \tag{D10}$$

with the tensor momentum flux density $\mathbf{h}$ identified as

$$\mathbf{h}(\Gamma;\boldsymbol{r}) = \sum_{r=1}^{N} m\boldsymbol{v}_r\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{m(1+\alpha)\sigma}{4}\sum_{r=1}^{N}\sum_{s\neq r}^{N} \delta(q_{rs}-\sigma)$$

$$\times \Theta(-\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})^2\hat{\boldsymbol{q}}_{rs}\hat{\boldsymbol{q}}_{rs}\int_0^1 d\gamma$$

$$\times \delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs}). \tag{D11}$$

The first term on the right-hand side is called the kinetic part of the momentum flux, while the second term is the collisional transfer part.

Finally, the energy density is given by

$$\mathcal{E}(\Gamma;\boldsymbol{r}) = \sum_{r=1}^{N} \frac{mv_r^2}{2}\delta(\boldsymbol{r}-\boldsymbol{q}_r). \tag{D12}$$

Proceeding in a similar way as for the momentum density,

$$L\mathcal{E}(\Gamma;\boldsymbol{r}) = -\boldsymbol{\nabla} \cdot \sum_{r=1}^{N} \frac{mv_r^2}{2}\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{m}{4}\sum_{r=1}^{N}\sum_{s\neq r}^{N} T(r,s)[v_r^2\delta(\boldsymbol{r}-\boldsymbol{q}_r) + v_s^2\delta(\boldsymbol{r}-\boldsymbol{q}_s)]$$

$$= -\boldsymbol{\nabla} \cdot \left(\sum_{r=1}^{N} \frac{mv_r^2}{2}\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{m(1+\alpha)\sigma}{4}\sum_{r=1}^{N}\sum_{s\neq r}^{N} \delta(q_{rs}-\sigma)\Theta(-\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs}) \times (\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})^2\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{G}_{rs}\hat{\boldsymbol{q}}_{rs} \right.$$

$$\left. \times \int_0^1 d\gamma\delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs}) \right) \frac{m(1-\alpha^2)}{8}\sum_{r=1}^{N}\sum_{s\neq r}^{N} \delta(q_{rs}-\sigma)\Theta(-\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})|\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs}|^3\delta(\boldsymbol{r}-\boldsymbol{q}_r). \tag{D13}$$

This consists of two parts, one that can be expressed as a gradient and a second one that is inherently local, characterizing the loss in energy due to the inelastic character of collisions. The energy balance equation becomes

$$\frac{\partial}{\partial t}\mathcal{E}(\Gamma;\boldsymbol{r},t) + \boldsymbol{\nabla} \cdot \boldsymbol{s}(\Gamma;\boldsymbol{r},t) = -w(\Gamma;\boldsymbol{r},t), \qquad \text{(D14)}$$

with the energy flux density

$$\boldsymbol{s}(\Gamma;\boldsymbol{r}) = \sum_{r=1}^{N} \frac{mv_r^2}{2}\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{m(1+\alpha)\sigma}{4}\sum_{r=1}^{N}\sum_{s\neq r}^{N}\delta(q_{rs}-\sigma)$$

$$\times\Theta(-\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{ij})(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})^2(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{G}_{rs})\hat{\boldsymbol{q}}_{rs}$$

$$\times\int_0^1 d\gamma\,\delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs}), \qquad \text{(D15)}$$

and the energy source

$$w(\Gamma;\boldsymbol{r}) = \frac{m(1-\alpha^2)}{8}\sum_{r=1}^{N}\sum_{s\neq r}^{N}\delta(q_{rs}-\sigma)\Theta(-\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})$$

$$\times|\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs}|^3\delta(\boldsymbol{r}-\boldsymbol{q}_r). \qquad \text{(D16)}$$

This completes the identification of the flux and source terms in the microscopic balance equations for the forward dynamics.

A similar analysis can be done for the balance equations associated with the backward dynamics of the phase functions, described by the equations

$$\frac{\partial\mathcal{A}_\alpha(\Gamma;\boldsymbol{r},-t)}{\partial(-t)} - L_-\mathcal{A}_\alpha(\Gamma;\boldsymbol{r},-t) = 0, \qquad \text{(D17)}$$

where $t>0$. The form of the conservation laws now is

$$\frac{\partial\mathcal{A}_\alpha(\Gamma;\boldsymbol{r},-t)}{\partial(-t)} + \boldsymbol{\nabla}\cdot\boldsymbol{j}_\alpha^-(\Gamma;\boldsymbol{r},-t) = w_\alpha^-(\Gamma;\boldsymbol{r},-t). \qquad \text{(D18)}$$

If the generators L and L_- were the same, then this would just be the time reversal of Eq. (D2). However, the contributions for positive times from the binary collision operators $T(i,j)$ are replaced by those from $T_-(i,j)$ when considering negative times. Repeating the above analysis for this case gives the time-reversed fluxes as

$$\boldsymbol{h}^-(\Gamma;\boldsymbol{r}) = m\sum_{r=1}^{N}\boldsymbol{v}_r\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{m(1+\alpha)\sigma}{4\alpha}\sum_{r=1}^{N}\sum_{s\neq r}^{N}\delta(q_{rs}-\sigma)$$

$$\times\Theta(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})^2\hat{\boldsymbol{q}}_{rs}\hat{\boldsymbol{q}}_{rs}$$

$$\times\int_0^1 d\gamma\,\delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs}), \qquad \text{(D19)}$$

$$\boldsymbol{s}^-(\Gamma;\boldsymbol{r}) = \frac{m}{2}\sum_{r=1}^{N}v_r^2\boldsymbol{v}_r\delta(\boldsymbol{r}-\boldsymbol{q}_r) + \frac{m(1+\alpha)\sigma}{4\alpha}\sum_{r=1}^{N}\sum_{s\neq r}^{N}\delta(q_{rs}-\sigma)$$

$$\times\Theta(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})^2(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{G}_{rs})\hat{\boldsymbol{q}}_{rs}$$

$$\times\int_0^1 d\gamma\,\delta(\boldsymbol{r}-\boldsymbol{q}_r+\gamma\boldsymbol{q}_{rs}), \qquad \text{(D20)}$$

while the expression for the reverse energy source is

$$w^-(\Gamma;\boldsymbol{r}) = \frac{m(1-\alpha^2)}{8\alpha^2}\sum_{r=1}^{N}\sum_{s\neq r}^{N}\delta(q_{rs}-\sigma)\Theta(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})$$

$$\times(\hat{\boldsymbol{q}}_{rs}\cdot\boldsymbol{g}_{rs})^3\delta(\boldsymbol{r}-\boldsymbol{q}_r). \qquad \text{(D21)}$$

The superscript $-$ is used here to indicate that the quantities are associated with the time-reversed equations. The source term w^- in the balance equation for the energy is now positive, accounting for collisional increase in energy on moving backward along a trajectory originally generated forward in time. In the elastic limit, this latter effect vanishes. However, the fluxes still differ from those for $t>0$, with the collisional transfer contributions being defined on different precollision hemispheres.

1. Dimensionless balance equations

The purpose of this section is twofold. First, the dimensionless forms of the various fluxes that determine the hydrodynamic parameters are identified. Second, a special property of the source term in the equation for the energy noted in Ref. [3], namely, that it is orthogonal to the set of conjugate densities $\{\widetilde{\psi}_\alpha^*\}$ in the homogeneous limit, is briefly reviewed here.

Dimensionless forms for the microscopic densities $\mathcal{N}$, $\mathcal{G}$, and $\mathcal{E}$ are defined by (recall the choice $l=n_h^{-1/d}$ made for the length scale)

$$\mathcal{N}^*(\Gamma^*;\boldsymbol{r}^*) \equiv \frac{\mathcal{N}(\Gamma;\boldsymbol{r})}{n_h} = \sum_{r=1}^{N}\delta(\boldsymbol{r}^*-\boldsymbol{q}_r^*), \qquad \text{(D22)}$$

$$\mathcal{E}^*(\Gamma^*;\boldsymbol{r}^*) \equiv \frac{\mathcal{E}(\Gamma;\boldsymbol{r})}{n_hT_h} = \sum_{r=1}^{N}v_r^{*2}\delta(\boldsymbol{r}^*-\boldsymbol{q}_r^*), \qquad \text{(D23)}$$

$$\mathcal{G}^*(\Gamma^*;\boldsymbol{r}^*) \equiv \frac{\mathcal{G}(\Gamma;\boldsymbol{r})}{mn_hv_0(T_h)} = \sum_{r=1}^{N}\boldsymbol{v}_r^*\delta(\boldsymbol{r}^*-\boldsymbol{q}_r^*). \qquad \text{(D24)}$$

With this choice, the balance equations in the dimensionless form become

$$\frac{\partial\mathcal{N}^*}{\partial s} + \frac{\partial}{\partial\boldsymbol{r}^*}\cdot\boldsymbol{\mathcal{G}}^* = 0, \qquad \text{(D25)}$$

$$\left(\frac{\partial}{\partial s} - \frac{\xi_0^*}{2}\right)\boldsymbol{\mathcal{G}}^* + \frac{\partial}{\partial\boldsymbol{q}_r^*}\cdot\boldsymbol{h}^* = 0, \qquad \text{(D26)}$$

$$\left(\frac{\partial}{\partial s} - \zeta_0^*\right)\mathcal{E}^* + \frac{\partial}{\partial\boldsymbol{r}^*}\cdot\boldsymbol{s}^* = -w^*. \qquad \text{(D27)}$$

The functional forms of the fluxes and source terms are related to those given above by

$$\boldsymbol{h}^*(\Gamma^*;\boldsymbol{r}^*) = \frac{\boldsymbol{h}(\Gamma;\boldsymbol{r})}{mn_hv_0^2(T_h)} = [\boldsymbol{h}(\Gamma;\boldsymbol{r})]_{\Gamma=\Gamma^*,\boldsymbol{r}=\boldsymbol{r}^*}, \qquad \text{(D28)}$$

$$\boldsymbol{s}^*(\Gamma^*;\boldsymbol{r}^*) = \frac{\boldsymbol{s}(\Gamma;\boldsymbol{r})}{n_hT_hv_0(T_h)} = 2[\boldsymbol{s}(\Gamma;\boldsymbol{r})]_{\Gamma=\Gamma^*,\boldsymbol{r}=\boldsymbol{r}^*}, \qquad \text{(D29)}$$

$$w^*(\Gamma^*;\boldsymbol{r}^*) = \frac{lw(\Gamma;\boldsymbol{r})}{n_h T_h v_0(T_h)} = 2[w(\Gamma;\boldsymbol{r})]_{\Gamma=\Gamma^*,\boldsymbol{r}=\boldsymbol{r}^*}. \quad \text{(D30)}$$

It is understood that, in addition to the indicated substitutions, the changes $\sigma \to \sigma^* = \sigma/l$ and $m \to 1$, are made. The direct density functions $a_\alpha^*(\Gamma^*;\boldsymbol{r}^*)$ appearing in the response functions are defined by Eq. (17). In the case of a_2^*, the balance equations give

$$\frac{\partial a_2^*}{\partial s} - \frac{2\zeta_0^*}{d}\mathcal{E}^* + \frac{\partial}{\partial \boldsymbol{r}^*} \cdot \left(\frac{2\boldsymbol{s}^*}{d} - \boldsymbol{\mathcal{G}}^*\right) = -\frac{2w^*}{d}. \quad \text{(D31)}$$

For reasons that become apparent below, add a term $\Sigma_\alpha \mathcal{K}_{2\alpha}^{*\text{hyd}}(\boldsymbol{0})a_\alpha^*$ on both sides of the above equation to write

$$\frac{\partial a_2^*}{\partial s} + \sum_\alpha \mathcal{K}_{2\alpha}^{*hyd}(\boldsymbol{0})a_\alpha^* + \frac{\partial}{\partial \boldsymbol{r}^*} \cdot \left(\frac{2\boldsymbol{s}^*}{d} - \boldsymbol{\mathcal{G}}^*\right) = -\ell^*, \quad \text{(D32)}$$

where the new source ℓ^* is

$$\ell^*(\Gamma^*;\boldsymbol{r}^*,s) \equiv \frac{2w^*}{d} - \zeta_0^*\left[\frac{3}{2}a_2^* + \left(\frac{\partial \ln \zeta_0}{\partial \ln n_h} + 1\right)a_1^*\right]. \quad \text{(D33)}$$

Evidently, the Fourier representation of Eq. (D32) is

$$\frac{\partial \widetilde{a}_2^*}{\partial s} + \sum_\alpha \mathcal{K}_{2\alpha}^{*\text{hyd}}(\boldsymbol{0})\widetilde{a}_\alpha - i\boldsymbol{k}^* \cdot \left(\frac{2\widetilde{\boldsymbol{s}}^*}{d} - \widetilde{\boldsymbol{\mathcal{G}}}^*\right) = \widetilde{\ell}^*(\boldsymbol{k}^*,s). \quad \text{(D34)}$$

The homogeneous limit of the source term, $\widetilde{\ell}^*(\boldsymbol{0},s)$, has an important orthogonality property, which is the reason for adding the contribution $\Sigma_\alpha \mathcal{K}_{2\alpha}^{*\text{hyd}}(\boldsymbol{0})a_\alpha^*$ above. To see this, the Fourier transform for $\boldsymbol{k}^*=\boldsymbol{0}$ of the second term on the right-hand side of Eq. (D33) is written in the equivalent form

$$\zeta_0^*\left[\frac{3}{2}\widetilde{a}_2^*(\boldsymbol{0},s) + \left(\frac{\partial \ln \zeta_0}{\partial \ln n_h} + 1\right)\widetilde{a}_1^*(\boldsymbol{0},s)\right]$$

$$= e^{s\mathcal{L}}\left[\frac{3}{2}\zeta_0^*\widetilde{a}_2^*(\boldsymbol{0}) + \zeta_0^*\left(\frac{\partial \ln \zeta_0}{\partial \ln n_h} + 1\right)\widetilde{a}_1^*(\boldsymbol{0})\right]$$

$$= e^{s\mathcal{L}}\left(\sum_\gamma \widetilde{a}_\gamma^*(\boldsymbol{0})\frac{2}{V^*d}\int d\Gamma^* \widetilde{w}^*(\boldsymbol{0})\widetilde{\psi}_\gamma^*(\boldsymbol{0})\right). \quad \text{(D35)}$$

The last equality is obtained as follows. From the definition of $\widetilde{\psi}_\alpha^*$ in Eq. (19) we have

$$\frac{2}{V^*d}\int d\Gamma^* \widetilde{w}^*(\boldsymbol{0})\widetilde{\psi}_\alpha^*(\boldsymbol{0}) = \frac{2}{d}[lv_0(T_h)]^{-Nd}\frac{N_\alpha l}{n_h T_h v_0(T_h)V}\int d\Gamma \widetilde{w}(\Gamma;\boldsymbol{0})\left(\frac{\partial \rho_h(\Gamma;n_h,T_h)}{\partial n_h}\delta_{\alpha 1} + \frac{\partial \rho(\Gamma;n_h,T_h)}{\partial T_h}\delta_{\alpha 2}\right)$$

$$= \frac{2l}{n_h T_h v_0(T_h)Vd}\left(\delta_{\alpha 1}n_h\frac{\partial}{\partial n_h} - \delta_{\alpha 2}T_h\frac{\partial}{\partial T_h}\right)\int d\Gamma \widetilde{w}(\Gamma;\boldsymbol{0})\rho_h(\Gamma;n_h,T_h). \quad \text{(D36)}$$

Moreover, from Eq. (D14),

$$\int d\Gamma \widetilde{w}(\Gamma;\boldsymbol{0})\rho_h(\Gamma;n_h,T_h) = \frac{d}{2}n_h V\zeta_0(n_h,T_h)T_h, \quad \text{(D37)}$$

so that Eq. (D36) can be rewritten as

$$\frac{2}{V^*d}\int d\Gamma^* \widetilde{w}^*(\boldsymbol{0})\widetilde{\psi}_\alpha^*(\boldsymbol{0})$$

$$= \zeta_0^*\left[\delta_{\alpha 1}\left(1 + \frac{\partial \ln \zeta_0(n_h,T_h)}{\partial \ln n_h}\right) + \delta_{\alpha 2}\frac{3}{2}\right]. \quad \text{(D38)}$$

This proves Eq. (D35). Use of it in the Fourier transform of Eq. (D33) particularized for $\boldsymbol{k}^*=\boldsymbol{0}$ yields

$$\widetilde{\ell}^*(\Gamma^*;\boldsymbol{0},s) = e^{s\mathcal{L}^*}(1 - P^\dagger)\frac{2}{d}\widetilde{w}^*(\boldsymbol{0}) \quad \text{(D39)}$$

with the operator $P^\dagger$ given by

$$P^\dagger X(\Gamma^*) = V^{*-1}\sum_\alpha \widetilde{a}_\alpha^*(\Gamma^*;\boldsymbol{0})\int d\Gamma^* \widetilde{\psi}_\alpha^*(\Gamma^*;\boldsymbol{0})X(\Gamma^*). \quad \text{(D40)}$$

This is a projection operator since the quantities $\{\widetilde{a}_\alpha^*(\Gamma^*;\boldsymbol{0})\}$ and $\{\widetilde{\psi}_\beta^*(\Gamma^*;\boldsymbol{0})\}$ form a biorthogonal set, in the sense that

$$V^{*-1}\int d\Gamma^* \widetilde{a}_\alpha^*(\Gamma^*;\boldsymbol{0})\widetilde{\psi}_\beta^*(\Gamma^*;\boldsymbol{0}) = \delta_{\alpha\beta}, \quad \text{(D41)}$$

as shown in Ref. [3]. The utility of this result is that $\widetilde{\ell}^*(\boldsymbol{0},s)$ is the source phase function for the transport coefficient ζ^U, as shown in Eq. (F2). Then, the presence of this orthogonal projection is essential for the existence of the large-s limit in the Green-Kubo representation for ζ^U, as discussed in Ref. [3]. A similar orthogonal projection occurs for all of the direct fluxes $F^{S,f}$ occurring in the representation (32) for transport coefficients.

In summary, the conservation laws associated with the chosen phase functions $\{a_\alpha\}$ in dimensionless variables take the form

$$\frac{\partial \widetilde{a}_\alpha^*(\Gamma^*;\boldsymbol{k}^*,s)}{\partial s} + \sum_\beta \mathcal{K}_{\alpha\beta}^{*hyd}(\Gamma^*;\boldsymbol{0})\widetilde{a}_\beta^*(\Gamma^*;\boldsymbol{k}^*,s)$$
$$- i\boldsymbol{k}^* \cdot \widehat{\boldsymbol{f}}_\alpha^*(\Gamma^*;\boldsymbol{k}^*,s) = \delta_{\alpha 2}\widetilde{\ell}^*(\Gamma^*;\boldsymbol{k}^*,s), \quad \text{(D42)}$$

where $\mathcal{K}_{\alpha\beta}^{*hyd}(\Gamma^*;\boldsymbol{0})$ is the $\boldsymbol{k}^*=\boldsymbol{0}$ limit of the matrix given in Eqs. (11)–(13) and

$$\boldsymbol{f}_1^*(\Gamma^*;\boldsymbol{r}^*) = \boldsymbol{\mathcal{G}}^*(\Gamma^*;\boldsymbol{r}^*), \quad \text{(D43)}$$

$$\boldsymbol{f}_2^*(\Gamma^*;\boldsymbol{r}^*) = \frac{2}{d}\boldsymbol{s}^*(\Gamma^*;\boldsymbol{r}^*) - \boldsymbol{\mathcal{G}}^*(\Gamma^*;\boldsymbol{r}^*), \quad \text{(D44)}$$

$$\boldsymbol{f}_{3,ij}^*(\Gamma^*;\boldsymbol{r}^*) = \boldsymbol{h}_{ij}^*(\Gamma^*;\boldsymbol{r}^*). \quad \text{(D45)}$$

The last equation above gives the tensor flux appearing in the equation for the dimensionless momentum $\boldsymbol{\mathcal{G}}^*(\Gamma^*;\boldsymbol{r}^*)$ $\equiv \boldsymbol{a}_3^*(\Gamma^*;\boldsymbol{r}^*)$.

APPENDIX E: CONJUGATE FUNCTIONS AND CONSERVATION LAWS

Consider the conjugate functions $\widetilde{\psi}_\alpha^*(\boldsymbol{k}^*)$ that occur in the response function (15), obtained from the linear response analysis, and are defined by Eq. (19). The dimensionless dynamical equation obeyed by these functions is

$$(\partial_s + \bar{\mathcal{L}}^*)\widetilde{\psi}_\alpha^*(\boldsymbol{k}^*,s) = 0. \quad \text{(E1)}$$

In the homogeneous limit $\boldsymbol{k}^*=\boldsymbol{0}$, these functions satisfy [3]

$$\bar{\mathcal{L}}^*\widetilde{\psi}_\alpha^*(\boldsymbol{0}) = \sum_\beta \mathcal{K}_{\beta\alpha}^{*hyd}(\boldsymbol{0})\widetilde{\psi}_\beta^*(\boldsymbol{0}), \quad \text{(E2)}$$

where $\mathcal{K}^{*hyd}(\boldsymbol{0})$ is the hydrodynamic transport matrix given by Eqs. (11) and (13) in the main text. This property allows the construction of a new set of "conservation laws"

$$\frac{\partial}{\partial s}\widetilde{\psi}_\alpha^*(\boldsymbol{k}^*,s) + \sum_\beta \mathcal{K}_{\beta\alpha}^{*hyd}(\boldsymbol{0})\widetilde{\psi}_\beta^*(\boldsymbol{k}^*,s) - i\boldsymbol{k}^* \cdot \widetilde{\boldsymbol{\gamma}}_\alpha^*(\boldsymbol{k}^*,s) = 0, \quad \text{(E3)}$$

with the conjugate fluxes $\widetilde{\boldsymbol{\gamma}}_\alpha^*(\boldsymbol{k},s)$ defined by

$$i\boldsymbol{k}^* \cdot \widetilde{\boldsymbol{\gamma}}_\alpha^*(\boldsymbol{k}^*,s) \equiv -(\bar{\mathcal{L}}^* - \sum_\beta \mathcal{K}_{\beta\alpha}^{*hyd}(\boldsymbol{0}))\widetilde{\psi}_\beta^*(\boldsymbol{k}^*,s). \quad \text{(E4)}$$

The property (E2) assures that $i\boldsymbol{k}^* \cdot \widetilde{\boldsymbol{\gamma}}_\alpha^*$ vanishes at $\boldsymbol{k}^*=\boldsymbol{0}$, justifying the introduction of $\widetilde{\boldsymbol{\gamma}}_\alpha^*$ as a flux. It is the conjugate quantity occurring in the Green-Kubo expressions of the transport coefficients, Eq. (35). More precisely, Υ^* in that expression is defined by

$$\Upsilon_\alpha^* \equiv \widetilde{\boldsymbol{k}}^* \cdot \widetilde{\boldsymbol{\gamma}}_\alpha^*(\boldsymbol{0}). \quad \text{(E5)}$$

APPENDIX F: TRANSPORT COEFFICIENTS: SOME DETAILS

The linear response analysis of Ref. [3] identified the transport coefficients in the intermediate Helfand representa-

tion by Eqs. (117)–(119). The transformation of those results to the dimensionless, hard-sphere form is outlined in Sec. VIII of that reference. Some further details for the expressions of the dimensionless transport coefficients are described briefly here.

The dimensionless response functions have a dynamics generated by $\bar{\mathcal{L}}^*$, as in Eq. (B18). However, the transport coefficients are given in terms of correlation functions whose dynamics is generated by $\bar{\mathcal{L}}^* - [\mathcal{K}^{*hyd}(\boldsymbol{0})]^T$, where the superscript T indicates transposed. As discussed in Ref. [3] and also in the main text here, this generator compensates for both the cooling of the reference state (through the change of $\bar{L}^*$ by $\bar{\mathcal{L}}^*$) and the dynamics of homogeneous perturbations of that state (through the subtraction of $\mathcal{K}^{*hyd}(\boldsymbol{0})$).

Consider first the Euler transport coefficient ζ^U given in the intermediate Helfand representation by Eq. (117) of Ref. [3], whose dimensionless form is

$$\zeta^{*U} = -\lim \widetilde{\boldsymbol{k}}^* \cdot \bar{\boldsymbol{S}}_{23}^{*(1)}(s), \quad \text{(F1)}$$

where $\bar{\boldsymbol{S}}_{23}^{*(1)}(s)$ is obtained from

$$\bar{\boldsymbol{S}}_{23}^*(\boldsymbol{k}^*,s) = \frac{v_0[T_h(t)]}{v_0[T_h(0)]}V^{*-1}\int d\Gamma^* \widetilde{\ell}^*(\Gamma^*,\boldsymbol{k}^*)e^{-s\bar{\mathcal{L}}^*}\widetilde{\psi}_\parallel^*(\Gamma^*;-\boldsymbol{k}^*)$$
$$= V^{*-1}\int d\Gamma^* \widetilde{\ell}^*(\Gamma^*;\boldsymbol{k}^*)e^{-s(\bar{\mathcal{L}}^*+\zeta_0^*/2)}\widetilde{\psi}_\parallel^*(\Gamma^*;-\boldsymbol{k}^*), \quad \text{(F2)}$$

as explained below. In this expression, $\widetilde{\ell}^*(\Gamma^*;\boldsymbol{k}^*)$ is the source term in the balance equation for the energy given in Eq. (D33) and $\widetilde{\psi}_\parallel^*(\Gamma^*;\boldsymbol{k}^*)$ is the conjugate density associated with the longitudinal component of the flow velocity. Equation (F2) is easily derived by using Eq. (167) in Ref. [3]. It can also be expressed as

$$\bar{\boldsymbol{S}}_{23}^*(\boldsymbol{k}^*,s) = V^{*-1}\int d\Gamma^* \widetilde{\ell}^*(\Gamma^*,\boldsymbol{k}^*)\widetilde{\psi}_\parallel^*(\Gamma^*;-\boldsymbol{k}^*,s), \quad \text{(F3)}$$

with

$$\widetilde{\psi}_\parallel^*(\Gamma^*;\boldsymbol{k}^*,s) \equiv \sum_\alpha \mathcal{U}_{\parallel\alpha}^*(s)\widetilde{\psi}_\alpha^*(\Gamma^*;\boldsymbol{k}^*), \quad \text{(F4)}$$

the matrix evolution operator $\mathcal{U}^*(s)$ being given by

$$\mathcal{U}_{\alpha\beta}^*(s) \equiv \widetilde{C}_{\beta\alpha}^{*hyd-1}e^{-s\bar{\mathcal{L}}^*} = [e^{s\mathcal{K}^{*hyd}(\boldsymbol{0})}]_{\beta\alpha}e^{-s\bar{\mathcal{L}}^*}. \quad \text{(F5)}$$

Here, $\mathcal{K}^{*hyd}(\boldsymbol{k}^*)$ is as always the matrix given in Eqs. (11)–(13). It will be seen in the following that, consistently with the description given at the beginning of this section, going to the dimensionless expressions of the transport coefficients implies replacing the matrix evolution $\mathcal{U}(t,T)$ used in Ref. [3] by $\mathcal{U}^*(s)$ defined above.

The quantity $\bar{\boldsymbol{S}}_{23}^{*(1)}(s)$ in Eq. (F1) is generated from $\bar{\boldsymbol{S}}_{23}^*(\boldsymbol{k}^*,s)$ by means of the Taylor series expansion around $\boldsymbol{k}^*=\boldsymbol{0}$, which for any function $X(\boldsymbol{k}^*)$ is defined as

$$X(\boldsymbol{k}^*) = X(\boldsymbol{0}) + i\boldsymbol{k}^* \cdot \boldsymbol{X}^{(1)} - \boldsymbol{k}^*\boldsymbol{k}^*:\boldsymbol{X}^{(2)} + \cdots. \quad \text{(F6)}$$

Then we have

$$S_{23}^{*(1)}(s) = - V^{*-1} \int d\Gamma^* \widetilde{\ell}^*(\Gamma^*; \mathbf{0}) e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} \widetilde{\boldsymbol{\psi}}^{*(1)}(\Gamma^*),$$

$$\text{(F7)}$$

with

$$\widetilde{\boldsymbol{\psi}}^{*(1)}(\Gamma^*) = - \sum_{r=1}^{N} \mathbf{q}_r^* \frac{\partial}{\partial v_{s,\parallel}^*} \rho_h^*(\Gamma^*). \qquad \text{(F8)}$$

In writing Eq. (F7), a contribution involving $\widetilde{\ell}^{*(1)}(\Gamma^*)$ has been omitted since it vanishes due to the symmetry of $\widetilde{\psi}_\parallel^*(\Gamma^*; \mathbf{0})$. Taking now into account Eq. (D39) and the definitions given in (D30) and (38), it is easily verified that

$$\widetilde{\ell}^*(\Gamma^*; \mathbf{0}) = (1 - P^\dagger) W^*(\Gamma^*). \qquad \text{(F9)}$$

Use of this in Eq. (F7) and later substitution of the result into Eq. (F1) leads to Eqs. (47)–(50), after using the symmetry of the integrand.

The Navier-Stokes transport coefficients at order k^2 associated with the heat and momentum flux are given by Eq. (119) of Ref. [3] and, more explicitly, they are identified in Appendix F of that reference. In dimensionless form, they are the elements of the matrix

$$\Lambda^* = \lim \widetilde{k}^* \widetilde{k}^* : [\mathbf{D}^{*(1)}(s) - \bar{\mathbf{D}}^*(\mathbf{0}, 0) \bar{\mathbf{C}}^{(1)*}(s)], \qquad \text{(F10)}$$

where the correlation functions $\bar{C}^*(\mathbf{k}^*, s)$ and $\bar{D}^*(\mathbf{k}^*, s)$ are defined by

$$\bar{C}_{\alpha\beta}^*(\mathbf{k}^*, s) = V^{*-1} \int d\Gamma^* \widetilde{a}_\alpha^*(\Gamma^*; \mathbf{k}^*) \widetilde{\psi}_\beta^*(\Gamma^*; -\mathbf{k}^*, s).$$

$$\text{(F11)}$$

$$\bar{D}_{\alpha\beta}^*(\mathbf{k}^*, s) = V^{*-1} \int d\Gamma^* \widetilde{f}_\alpha^*(\Gamma^*; \mathbf{k}^*) \widetilde{\psi}_\beta^*(\Gamma^*; -\mathbf{k}^*, s),$$

$$\text{(F12)}$$

with the direct densities $\widetilde{a}_\alpha^*$ given in Eq. (17) and the associated fluxes $\widetilde{f}_\alpha^*$ given in Eqs. (D43)–(D45).

The explicit form of the first-order-in-k^* expanded correlation matrix $\bar{\mathbf{C}}^{*(1)}(s)$ above is

$$\bar{C}_{\alpha\beta}^{*(1)}(s) = V^{*-1} \int d\Gamma^* \widetilde{\mathbf{a}}_\alpha^{*(1)}(\Gamma^*) \widetilde{\psi}_\beta^*(\Gamma^*; \mathbf{0}, s)$$

$$- V^{*-1} \int d\Gamma^* \widetilde{a}_\alpha^*(\Gamma^*; \mathbf{0}) \widetilde{\boldsymbol{\psi}}_\beta^{*(1)}(\Gamma^*; s)$$

$$= - V^{*-1} \int d\Gamma^* \widetilde{a}_\alpha^*(\Gamma^*; \mathbf{0}) \widetilde{\boldsymbol{\psi}}_\beta^{*(1)}(\Gamma^*; s). \qquad \text{(F13)}$$

The contribution involving $\widetilde{\mathbf{a}}_\alpha^{*(1)}(\Gamma^*)$ is proportional to the center of mass coordinates and vanishes from symmetry. A similar analysis of $\mathbf{D}^{*(1)}(s)$ gives

$$\mathbf{D}_{\alpha\eta}^{*(1)}(s) = - V^{*-1} \int d\Gamma^* \widetilde{f}_\alpha^*(\Gamma^*; \mathbf{0}) \widetilde{\boldsymbol{\psi}}_\beta^{*(1)}(\Gamma^*; s). \qquad \text{(F14)}$$

The two terms on the right side of Eq. (F10) now combine, and the transport matrix Λ^* takes the simple form

$$\Lambda_{\alpha\beta}^* = - \lim \hat{k}^* \hat{k}^* : V^{*-1} \int d\Gamma^* \widetilde{f}^*(\Gamma^*; \mathbf{0})(1 - P) \widetilde{\boldsymbol{\psi}}_\beta^{*(1)}(\Gamma^*; s),$$

$$\text{(F15)}$$

where P is the projection operator

$$PX(\Gamma^*) \equiv \sum_\alpha \psi_\alpha^*(\Gamma^*; \mathbf{0}) V^{*-1} \int d\Gamma^* \widetilde{a}_\alpha^*(\Gamma^*; 0) X(\Gamma^*).$$

$$\text{(F16)}$$

Since the operator $1 - P$ is orthogonal to the invariants of $\mathcal{U}^*(s)$, as shown in Ref. [3], Eq. (F15) is equivalent to

$$\Lambda_{\alpha\beta}^* = - \lim V^{*-1} \int d\Gamma^* F_\alpha^{*f}(\Gamma^*) \hat{k}^* \cdot \widetilde{\boldsymbol{\psi}}_\beta^{*(1)}(\Gamma^*; s), \quad \text{(F17)}$$

where F_α^{*f} is the projected flux

$$F_\alpha^{*f}(\Gamma^*) = (1 - P^\dagger) \hat{k}^* \cdot \widetilde{\mathbf{f}}_\alpha^*(\Gamma^*; \mathbf{0}). \qquad \text{(F18)}$$

The projection operator $P^\dagger$ is the adjoint of P, and it is the same as that given by Eq. (D40).

1. Shear viscosity

The dimensionless shear viscosity is determined from Λ_{44}^* through

$$\eta^* = \Lambda_{44}^* = - \lim V^{*-1} \hat{k}^* \hat{k}^* : \int d\Gamma^* F_4^{*f}(\Gamma^*) [\mathcal{U}^*(s) \widetilde{\boldsymbol{\psi}}^{*(1)}(\Gamma^*)]_4$$

$$= - \lim V^{*-1} \hat{k}^* \hat{k}^* : \int d\Gamma^* \widetilde{\mathbf{f}}_4^*(\Gamma^*; \mathbf{0}) e^{-s(\bar{\mathcal{L}}^* + \zeta_0^*/2)} \widetilde{\boldsymbol{\psi}}_4^{*(1)}(\Gamma^*).$$

$$\text{(F19)}$$

The projection operator in the definition of the projected fluxes, Eq. (F18), does not contribute in this case due to the symmetry of the integrand. The conjugate moment $\widetilde{\boldsymbol{\psi}}_4^{*(1)}(\Gamma^*)$ is easily obtained from the definition in Eqs. (F6) and (25),

$$\hat{k}^* \cdot \widetilde{\boldsymbol{\psi}}_4^{*(1)}(\Gamma^*) = - \sum_{r=1}^N (\hat{k}^* \cdot \mathbf{q}_r^*) \frac{\partial}{\partial v_{r,\perp 1}^*} \rho_h^*(\Gamma^*), \qquad \text{(F20)}$$

where $v_{r,\perp 1}^*$ is the first of the transversal components of $\mathbf{v}_r$. Moreover, using Eq. (D45),

$$\hat{k} \cdot \widetilde{\mathbf{f}}_4^*(\Gamma^*; \mathbf{0}) = \mathbf{H}_{\parallel \perp 1}^*(\Gamma^*), \qquad \text{(F21)}$$

so Eq. (F19) becomes

$$\eta^* = - \lim V^{*-1} \int d\Gamma^* \mathbf{H}_{xy}^*(\Gamma^*) e^{-s(\mathcal{L}^* + \zeta_0^*/2)} \mathcal{M}_\eta^*(\Gamma^*),$$

$$\text{(F22)}$$

with

$$\mathcal{M}_{\eta}^*(\Gamma^*) = -\sum_{r=1}^{N} q_{r,x}^* \frac{\partial}{\partial v_{r,y}^*} \rho_h^*(\Gamma^*). \quad (F23)$$

The x and y components in the above expression are due to the arbitrary choice of the x axis along $\hat{\boldsymbol{k}}$ and the y axis along the first tranverse direction.

An alternative expression for the shear viscosity can be derived as follows. Define

$$\mathcal{M}_{\eta,ij}^*(\Gamma^*) = -\frac{1}{2}\sum_{r=1}^{N}\left(q_{r,i}^*\frac{\partial}{\partial v_{r,j}^*} + q_{r,j}^*\frac{\partial}{\partial v_{r,i}^*} -\frac{2}{d}\delta_{ij}\boldsymbol{q}_r^*\cdot\frac{\partial}{\partial \boldsymbol{v}_r^*}\right)\rho_h^*(\Gamma^*), \quad (F24)$$

where i and j are spatial coordinates. The symmetry of Eq. (F22) implies that it is equivalent to

$$\eta^* = -\frac{1}{d^2+d+2}\lim V^{*-1}\sum_{i=1}^{d}\sum_{j=1}^{d}\int d\Gamma^* \mathbf{H}_{ij}^*(\Gamma^*) \times e^{-s(\bar{\mathcal{L}}^*+\zeta_0^*/2)}\mathcal{M}_{\eta,ij}^*(\Gamma^*). \quad (F25)$$

This is the expression presented in Eqs. (56) and (57) in the main text.

2. Bulk viscosity

The bulk viscosity κ^* occurs in the 33 matrix element of the hydrodynamic transport matrix, namely, it is

$$\kappa^* + \frac{2(d-1)\eta^*}{d} = \Lambda_{33}^*$$

$$= -\lim V^{*-1}\int d\Gamma^* F_3^{*f} e^{-s(\bar{\mathcal{L}}^*+\zeta_0^*/2)}\mathcal{M}_3^*(\Gamma^*). \quad (F26)$$

The projected flux is found to be

$$F_3^f(\Gamma^*) = \hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{f}}_3^*(\Gamma^*;\mathbf{0}) - \frac{p_h^*}{2}\frac{\partial\ln p_h}{\partial\ln n_h}\tilde{a}_1(\Gamma^*;\mathbf{0}) - \frac{p_h^*}{2}\tilde{a}_2(\Gamma^*;\mathbf{0}) \quad (F27)$$

and the conjugate moment is

$$\mathcal{M}_3^*(\Gamma^*) = \hat{\boldsymbol{k}}^*\cdot\boldsymbol{\psi}_3^{*(1)}(\Gamma^*) = -\sum_{r=1}^{N}(\hat{\boldsymbol{k}}^*\cdot\boldsymbol{q}_r^*)\hat{\boldsymbol{k}}^*\cdot\frac{\partial}{\partial\boldsymbol{v}_r^*}\rho_h^*(\Gamma^*). \quad (F28)$$

Taking into account that $\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{f}}_3^*(\Gamma^*;\mathbf{0}) = \mathbf{H}_{33}^*(\Gamma^*)$ and the symmetry of the tensor $\mathbf{H}^*$, the expressions used in Sec. III, Eqs. (68) and (69), follow directly.

3. Thermal conductivity

The dimensionless thermal conductivity λ^* is given by

$$\lambda^* = \frac{d}{2}\Lambda_{22}^*$$

$$= -\frac{d}{2}\lim V^{*-1}\int d\Gamma^* F_2^{*f}[\mathcal{U}(s)\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{\psi}}^{*(1)}(\Gamma^*)]_2$$

$$= -\frac{d}{2}\lim V^{*-1}\int d\Gamma^* F_2^{*f} e^{-s(\bar{\mathcal{L}}^*-\zeta_0^*/2)}\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{\psi}}_2^{*(1)}(\Gamma^*). \quad (F29)$$

The projected flux is

$$F_2^{*f} = \hat{\boldsymbol{k}}^*\cdot\left(\tilde{\boldsymbol{f}}_2^*(\Gamma^*;\mathbf{0}) - \frac{2p_h^*}{d}\boldsymbol{P}^*\right)$$

$$= \frac{2}{d}\hat{\boldsymbol{k}}^*\cdot\left[\tilde{\boldsymbol{s}}^*(\Gamma^*;\mathbf{0}) - \left(p_h^* + \frac{d}{2}\right)\boldsymbol{P}^*\right], \quad (F30)$$

with

$$\boldsymbol{P}^* = \sum_{r=1}^{N}\boldsymbol{v}_r^*, \quad (F31)$$

and the conjugate moment is

$$\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{\psi}}_2^{*(1)}(\Gamma^*) = -\frac{1}{2}\sum_{r=1}^{N}(\hat{\boldsymbol{k}}^*\cdot\boldsymbol{q}_r^*)\frac{\partial}{\partial\boldsymbol{v}_r^*}\cdot[\boldsymbol{v}_r^*\rho_h^*(\Gamma^*)]. \quad (F32)$$

The above expressions are equivalent to Eqs. (75) and (76).

4. The μ coefficient

The expression for the coefficient μ^* from linear response reads

$$\mu^* = \frac{d}{2}\Lambda_{21}^* = -\frac{d}{2}\lim V^{*-1}\int d\Gamma^* F_2^{*f}[\mathcal{U}^*(s)\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{\psi}}^{*(1)}(\Gamma^*)]_1$$

$$= -\frac{d}{2}\lim V^{*-1}\int d\Gamma^* F_2^{*f}$$

$$\times e^{-s\mathcal{L}^*}\left(\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{\psi}}_1^{*(1)}(\Gamma^*) - 2\frac{\partial\ln\zeta_0}{\partial\ln n_h}\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{\psi}}_2^{*(1)}(\Gamma^*)\right)$$

$$-d\frac{\partial\ln\zeta_0}{\partial\ln n_h}\lim V^{*-1}\int d\Gamma^* F_2^{*f} e^{-s(\bar{\mathcal{L}}^*-\zeta_0^*/2)}\hat{\boldsymbol{k}}^*\cdot\tilde{\boldsymbol{\psi}}_2^{*(1)}(\Gamma^*). \quad (F33)$$

Since the projected flux is the same as in Eq. (F29), the second term on the right-hand side of Eq. (F33) is proportional to λ^*, and the expression can be written

$$\bar{\mu}^* \equiv \mu^* - 2\frac{\partial \ln \zeta_0}{\partial \ln n_h}\lambda^* = -\frac{d}{2}\lim V^{*-1}\int d\Gamma^* F_2^{*f}$$

$$\times e^{-s\bar{\mathcal{L}}^*}\hat{\boldsymbol{k}}^* \cdot \left(\tilde{\boldsymbol{\psi}}_1^{*(1)}(\Gamma^*) - 2\frac{\partial \ln \zeta_0}{\partial \ln n_h}\hat{\boldsymbol{k}}^* \cdot \tilde{\boldsymbol{\psi}}_2^{*(1)}(\Gamma^*)\right).$$

$$(F34)$$

Therefore, the involved conjugate moments are

$$\hat{\boldsymbol{k}}^* \cdot \hat{\boldsymbol{\psi}}_1^{*(1)}(\Gamma^*) = [lv_0(T)]^{Nd}n\int d\boldsymbol{r}\hat{\boldsymbol{k}}^* \cdot \boldsymbol{r}^*$$

$$\times \left[\frac{\delta\rho_{lh}(\Gamma|\{y_\alpha\})}{\delta n(\boldsymbol{r})}\right]_{\{y_\alpha\}=\{n,T,\mathbf{0}\}}, \quad (F35)$$

$$\hat{\boldsymbol{k}}^* \cdot \tilde{\boldsymbol{\psi}}_2^{*(1)}(\Gamma^*) = [lv_0(T)]^{Nd}T\int d\boldsymbol{r}\hat{\boldsymbol{k}}^* \cdot \boldsymbol{r}^*$$

$$\times \left[\frac{\delta\rho_{lh}(\Gamma|\{y_\alpha\})}{\delta T(\mathbf{r})}\right]_{\{y_\alpha\}=\{n,T,\mathbf{0}\}}. \quad (F36)$$

Substitution of Eqs. (F35) and (F36) into Eq. (F34) and use of the symmetry of the integrand leads to Eqs. (84)–(86).

APPENDIX G: ELASTIC HARD SPHERES

The aim of this appendix is to give the Green-Kubo expressions for the transport coefficients in the case of elastic hard spheres or disks. The linear response method used in Ref. [3] was specifically applied to initial perturbations of a local HCS. The results apply as well in the elastic case for perturbations of a local equilibrium distribution, with only the replacement of the local HCS ensemble by a local equilibrium Gibbs ensemble. Here, for simplicity and to compare with standard results in the literature, a local grand canonical ensemble will be used. Strictly speaking, this is not the $\alpha \rightarrow 1$ limit of the results derived in this paper for a granular fluid, since the HCS ensemble in the elastic limit goes over to a microcanonical ensemble with constant total energy and momentum, i.e., the so-called MD ensemble. The results obtained by using different ensembles are known to be equivalent up to fluctuations that do not contribute in the thermodynamic limit, but the ensemble used affects the forms of the projected fluxes appearing in the Green-Kubo expressions.

The form of the representations for all transport coefficients is, of course, the same as in the inelastic case, but with some simplifications. The most obvious ones are the absence of cooling, implying that $\bar{\mathcal{L}}^*$ reduces to $\bar{L}^*$, and the absence of any dynamics for homogeneous perturbations, which reflects itself in that $\mathcal{K}^{*hyd}(\mathbf{0})=0$. Of course, both simplifications are closely related. Moreover, the dimensionless time s is now simply proportional to t. The direct fluxes F^{*S} in Eq. (35) vanish since all the source terms are zero and, consequently, also all the transport coefficients related to the cooling rate. On the other hand, the direct fluxes F^{*f} are unchanged. The generic transport coefficient in Eq. (90) then becomes

$$\omega_{el} = \lim V^{*-1}\int d\Gamma^* F^f(\Gamma^*)e^{-s\bar{L}^*}\mathcal{M}^*(\Gamma^*). \quad (G1)$$

It remains only to determine the moments $\mathcal{M}^*(\Gamma^*)$, and afterward the Green-Kubo representation can be constructed directly as is done in the main text for the general inelastic case.

The distribution of the local grand canonical ensemble is [13]

$$\rho_{\mathrm{LGC}}(\Gamma) = \Xi(\Gamma)\exp\left[-Q_L + \int d\boldsymbol{r}\left(\varrho(\boldsymbol{r})\mathcal{N}(\Gamma;\boldsymbol{r}) - \frac{\mathcal{E}(\Gamma;\boldsymbol{r})}{T(\boldsymbol{r})}\right.\right.$$

$$\left.\left. + \boldsymbol{Y}(\boldsymbol{r}) \cdot \boldsymbol{\mathcal{G}}(\Gamma;\boldsymbol{r})\right)\right], \quad (G2)$$

where the parameters of the ensemble are defined as

$$\varrho(\boldsymbol{r}) \equiv \frac{1}{T(\boldsymbol{r})}\left(\mathsf{s}(\boldsymbol{r}) - \frac{mU^2(\boldsymbol{r})}{2T(\boldsymbol{r})}\right), \quad (G3)$$

$$\boldsymbol{Y}(\boldsymbol{r}) \equiv \frac{n(\boldsymbol{r})m\boldsymbol{U}(\boldsymbol{r})}{T(\boldsymbol{r})}, \quad (G4)$$

s being the chemical potential, $\boldsymbol{U}$ the flow velocity, T the temperature in units where the Boltzmann constant is unity, and Q_L the normalization constant. Moreover, $\Xi(\Gamma)$ is the overlap function, which is zero for any configuration of overlapping pairs and unity otherwise.

Consider first the conjugate fluxes defined in Eq. (19) with the substitution of ρ_{lh} by ρ_{lGC}, i. e.,

$$\tilde{\psi}_\alpha^*(\Gamma^*;\boldsymbol{k}^*) = M_\alpha\int d\boldsymbol{r}\,e^{i\boldsymbol{k}\cdot\boldsymbol{r}}\left[\frac{\delta\rho_{\mathrm{LGC}}[\Gamma|\{y_\beta\}]}{\delta y_\alpha(\boldsymbol{r})}\right]_{\{y_\beta\}=\{n,T,\mathbf{0}\}}.$$

$$(G5)$$

The functional differentiations can be performed explicitly in this case, with the results

$$\tilde{\psi}_1^*(\Gamma^*;\boldsymbol{k}^*) = [1 + n_h\tilde{h}_e(\boldsymbol{k})]^{-1}\tilde{\mathcal{N}}^*(\Gamma^*;\boldsymbol{k}^*)\rho_{\mathrm{GC}}^*(\Gamma^*), \quad (G6)$$

$$\tilde{\psi}_2^*(\Gamma^*;\boldsymbol{k}^*) = \left[\tilde{\mathcal{E}}^*(\Gamma^*;\boldsymbol{k}^*) - \frac{d}{2}\tilde{\mathcal{N}}^*(\Gamma^*;\boldsymbol{k}^*)\right]\rho_{\mathrm{GC}}^*(\Gamma^*), \quad (G7)$$

$$\tilde{\boldsymbol{\psi}}_3^*(\Gamma^*;\boldsymbol{k}^*) = 2\hat{\boldsymbol{\mathcal{G}}}^*(\Gamma^*;\boldsymbol{k}^*)\rho_{\mathrm{GC}}^*(\Gamma^*). \quad (G8)$$

Here $\tilde{h}_e(\boldsymbol{k})$ is the Fourier transform of $g_e(\boldsymbol{r})-1$, where $g_e(\boldsymbol{r})$ is the equilibrium radial distribution function. The notation $\tilde{\boldsymbol{\psi}}_3^* \equiv \{\tilde{\psi}_\parallel^*, \tilde{\psi}_\perp^*\}$ has been used. It is seen that the $\tilde{\psi}_\alpha^*(\Gamma^*;\boldsymbol{k})$'s are linear combinations of the direct fluxes $\tilde{a}_\alpha(\Gamma^*;\boldsymbol{k})$ multiplied by the grand canonical ensemble dimensionless distribution $\rho_{\mathrm{GC}}^*(\Gamma^*)$.

The moments $\mathcal{M}^*(\Gamma^*)$ appearing in the Helfand expressions, are the coefficients of ik^* in the expansions of the $\tilde{\psi}_\alpha(\boldsymbol{k}^*)$'s, as indicated in Eq. (33),

$$\mathcal{M}^*(\Gamma^*) = \hat{\boldsymbol{k}}^* \cdot \tilde{\boldsymbol{\psi}}^{*(1)}(\Gamma^*). \quad (G9)$$

In detail, they are found to be

$$\hat{\boldsymbol{k}}^* \cdot \tilde{\boldsymbol{\psi}}_1^{*(1)}(\Gamma^*) = [1 + n_h \tilde{h}_e(\mathbf{0})]^{-1} \sum_{r=1}^{N} \hat{\boldsymbol{k}}^* \cdot \boldsymbol{q}_r^* \rho_{\text{GC}}^*(\Gamma^*),$$

(G10)

$$\hat{\boldsymbol{k}}^* \cdot \tilde{\boldsymbol{\psi}}_2^{*(1)}(\Gamma^*) = \sum_{r=1}^{N} \hat{\boldsymbol{k}}^* \cdot \boldsymbol{q}_r^* \left(v_r^{*2} - \frac{d}{2} \right) \rho_{\text{GC}}^*(\Gamma^*), \quad \text{(G11)}$$

$$\hat{\boldsymbol{k}}^* \cdot \tilde{\boldsymbol{\psi}}_\|^{*(1)}(\Gamma^*) = 2 \sum_{r=1}^{N} (\boldsymbol{k}^* \cdot \boldsymbol{q}_r^*)(\hat{\boldsymbol{k}}^* \cdot \boldsymbol{v}_r^*) \rho_{\text{GC}}^*(\Gamma^*), \quad \text{(G12)}$$

$$\hat{\boldsymbol{k}}^* \cdot \tilde{\boldsymbol{\psi}}_{\perp i}^{*(1)}(\Gamma^*) = 2 \sum_{r=1}^{N} (\hat{\boldsymbol{k}}^* \cdot \boldsymbol{q}_r^*) v_{r, \perp i}^* \rho_{\text{GC}}^*(\Gamma^*). \quad \text{(G13)}$$

Once these moments have been identified, the various transport coefficients for a system of elastic hard spheres or disks can be directly written.

1. Shear and bulk viscosities

The Helfand forms in Sec. III for the shear and bulk viscosities of the granular model in the elastic limit become

$$\eta^* = \lim \Omega_H^\eta(s), \quad \kappa^* = \lim \Omega_H^\kappa(s), \quad \text{(G14)}$$

respectively, where $\Omega_H^\eta(s)$ and $\Omega_H^\kappa(s)$ are now equilibrium time correlation functions,

$$\Omega_H^\eta(s) = -\frac{V^{*-1}}{d^2 + d - 2} \sum_{i=1}^{d} \sum_{j=1}^{d} \int d\Gamma^* \mathbf{H}_{ij}^*(\Gamma^*) e^{-s\bar{L}^*}(M_{\eta,ij}^* \rho_{\text{GC}}^*),$$

(G15)

$$\Omega_H^\kappa(s) = -2(V^* d^2)^{-1} \int d\Gamma^* \operatorname{tr} \mathbf{H}^{*f} e^{-s\bar{L}^*}(M_\kappa^* \rho_{\text{GC}}^*),$$

(G16)

with $\mathbf{H}_{ij}^*$ given by Eq. (43) and $\mathbf{H}_{ij}^*$ by Eq. (71). Moreover,

$$M_{\eta,ij}^* = \sum_{r=1}^{N} \left(q_{r,i}^* v_{r,j}^* + q_{r,j}^* v_{r,i}^* - \frac{2}{d} \delta_{ij} \boldsymbol{q}_r^* \cdot \boldsymbol{v}_r^* \right), \quad \text{(G17)}$$

$$M_\kappa^* = \sum_{r=1}^{N} \boldsymbol{q}_r^* \cdot \boldsymbol{v}_r^*. \quad \text{(G18)}$$

These are the usual well-known results for systems of elastic hard spheres or disks, in dimensionless form. The corresponding Green-Kubo expressions are

$$\eta^* = \Omega_0^\eta + \lim \int_0^s ds' \Omega_G^\eta(s'), \quad \text{(G19)}$$

$$\kappa^* = \Omega_0^\kappa + \lim \int_0^s ds' \Omega_G^\kappa(s'). \quad \text{(G20)}$$

The instantaneous parts, $\Omega_0^\eta = \Omega_H^\eta(0)$ and $\Omega_0^\kappa = \Omega_H^\kappa(0)$, now can be evaluated exactly, with the result

$$\Omega_0^\kappa = \frac{d+2}{d} \Omega_0^\eta = \frac{\sqrt{2}\pi^{(d-1)/2}\sigma^{*d+1}}{\Gamma(d/2)d^2} g_e(\sigma). \quad \text{(G21)}$$

The calculation of the conjugate fluxes in the expressions for $\Omega_G^\eta(s)$ and $\Omega_G^\kappa(s)$ requires some care. The calculation of $Y_{\eta,ij}^*$ has been discussed in detail in Sec. III, and the result is given by Eq. (63). The subsequent expression for the elastic shear viscosity is presented in Eq. (65). In a completely similar way, it is obtained that the integrand in the Green-Kubo expression for the bulk viscosity is

$$\Omega_G^\kappa(s) = (V^* d^2)^{-1} \int d\Gamma^* \operatorname{tr} \mathbf{H}^{*f}(\Gamma^*) e^{-s\bar{L}^*} [\operatorname{tr} \mathbf{H}^{*-}(\Gamma^*) \rho_{\text{GC}}^*(\Gamma^*)].$$

(G22)

2. Thermal conductivity

The expression of the thermal conductivity in the Helfand representation reads

$$\lambda^* = \lim \Omega_H^\lambda(s), \quad \text{(G23)}$$

where, for a system of elastic hard spheres or disks, Ω_H^λ is the time equilibrium correlation function

$$\Omega_H^\lambda(s) = -(V^* d)^{-1} \int d\Gamma^* \boldsymbol{S}^{*f} \cdot e^{-s\bar{L}^*}(\boldsymbol{M}_\lambda^* \rho_{GC}^*). \quad \text{(G24)}$$

The moment $\boldsymbol{M}_\lambda^*$ is identified from Eq. (G11) as

$$\boldsymbol{M}_\lambda^* = \sum_{r=1}^{N} \boldsymbol{q}_r^* \left(v_r^{*2} - \frac{d}{2} \right). \quad \text{(G25)}$$

The corresponding Green-Kubo representation is

$$\lambda^* = \Omega_0^\lambda + \lim \int_0^s ds' \Omega_G^\lambda(s'). \quad \text{(G26)}$$

Again, the instantaneous contribution $\Omega_0^\lambda = \Omega_H^\lambda(0)$ can be calculated exactly,

$$\Omega_0^\lambda = \frac{\pi^{(d-1)/2}\sigma^{*d+1}}{\sqrt{2}\Gamma(d/2)d} g_e(\sigma).$$

The analysis of the Green-Kubo flux $\boldsymbol{Y}_\lambda$ is similar to that for the viscosities, leading to the result

$$\Omega_G^\lambda(s) = (V^* d)^{-1} \int d\Gamma^* \boldsymbol{S}^{*f} \cdot e^{-s\bar{L}^*}(\boldsymbol{S}^{*-} \rho_{\text{GC}}^*), \quad \text{(G27)}$$

where $\boldsymbol{S}^{*-}(\Gamma^*)$ is the volume-integrated energy flux for the time-reversed microscopic laws identified in Appendix D as

$$\boldsymbol{S}^{*-}(\Gamma^*) = \sum_{r=1}^{N} v_r^{*2} \boldsymbol{v}_r^* + \sigma^* \sum_{r=1}^{N} \sum_{s \neq r}^{N} \delta(q_{rs}^* - \sigma^*) \Theta(\hat{\boldsymbol{q}}_{rs}^* \cdot \boldsymbol{g}_{rs}^*)$$
$$\times (\hat{\boldsymbol{q}}_{rs}^* \cdot \boldsymbol{g}_{rs}^*)^2 (\hat{\boldsymbol{q}}_{rs}^* \cdot \boldsymbol{G}_{rs}^*) \hat{\boldsymbol{q}}_{rs}^*. \quad \text{(G28)}$$

3. μ coefficient

It has been mentioned several time that the transport co-efficient μ vanishes in the elastic case, and it is instructive to see this at the formally exact level of linear response theory. The elastic limit of the Helfand form for μ^* in Eq. (F33) is

$$\mu^* = -\frac{d}{2}\lim V^{*-1}\int d\Gamma^* \boldsymbol{S}^{*f} \cdot e^{-s\bar{L}^*}(\boldsymbol{M}_\mu^*\rho_{GC}^*), \quad \text{(G29)}$$

where

$$\boldsymbol{M}_\mu^* \equiv \tilde{\boldsymbol{\psi}}_1^{*(1)} = [1 + n_h\tilde{h}(\boldsymbol{0})]^{-1}\sum_{r=1}^{N}\boldsymbol{q}_r^*. \quad \text{(G30)}$$

This is proportional to the center of mass position of the system. Its time evolution is, therefore, proportional to the total momentum $\boldsymbol{P}^*$. But, by definition, $\boldsymbol{S}^{*f}$ is projected orthogonal to $\boldsymbol{P}^*$. As, moreover, it is easily seen that the average on the right-hand side of Eq. (G29) vanishes for $s=0$, it is concluded that it vanishes for all times.

APPENDIX H: STATIONARY REPRESENTATION FOR MD SIMULATIONS

The transformation to dimensionless velocities defined in the text is based on scaling relative to $v_0(t) \equiv [2T_h(t)/m]^{1/2}$. This was done so as to be able to pose theoretical questions of interest in an elegant self-consistent form. However, this is inconvenient in practice since the cooling rate is given implicitly in terms of the stationary HCS. Instead, the same analysis can be performed by scaling with a known function $\xi(t)$ instead of $v_0(t)$ [5], to get a Liouville equation in the form

$$\frac{\partial}{\partial t}\rho^{**}(\Gamma^{**},t) - \frac{\partial \ln \xi(t)}{\partial t}\sum_{r=1}^{N}\frac{\partial}{\partial \boldsymbol{v}^{**}} \cdot [\boldsymbol{v}^{**}\rho^{**}(\Gamma^{**},t)]$$

$$+ \frac{\xi(t)}{l}\bar{L}^{**}(\Gamma^{**})\rho^{**}(\Gamma^{**},t) = 0, \quad \text{(H1)}$$

where $\Gamma^{**} \equiv \{\boldsymbol{q}^{**}, \boldsymbol{v}_r^{**}\} \equiv \{\boldsymbol{q}_r/l; \boldsymbol{v}_r/\xi(t)\}$. Here, as earlier, l is a constant characteristic length in the system,

$$\rho^{**}(\Gamma^{**},t) \equiv [\ell\chi(t)]^{Nd}\rho(\Gamma,t), \quad \text{(H2)}$$

and

$$\bar{L}^{**}(\Gamma^{**}) \equiv \frac{l}{\xi(t)}\bar{L}(\Gamma) = [\bar{L}(\Gamma)]_{\Gamma=\Gamma^{**}}. \quad \text{(H3)}$$

Next define a new time variable τ by

$$d\tau = \frac{\xi(t)dt}{l} \quad \text{(H4)}$$

and choose $\xi(t)$ to make the coefficients of the Liouville equation (H1) independent of τ, namely, verifying

$$\frac{d\xi^{-1}(t)}{dt} = \frac{\xi_0}{2l}, \quad \text{(H5)}$$

where ξ_0 is an arbitrary dimensionless constant that can be chosen for convenience. Then the choice $\xi(t) = 2l/\xi_0 t$ is made, and Eq. (H4) becomes

$$d\tau = \frac{2dt}{\xi_0 t}. \quad \text{(H6)}$$

The scaled Liouville equation (H(H1)) takes the form

$$\frac{\partial}{\partial \tau}\rho^{**} + \frac{\xi_0}{2}\sum_{r=1}^{N}\frac{\partial}{\partial \boldsymbol{v}_r^{**}} \cdot (\boldsymbol{v}_r^{**}\rho^{**}) + \bar{L}^{**}\rho^{**} = 0. \quad \text{(H7)}$$

This is formally the same as Eq. (B2), except that here the cooling rate has been replaced by the arbitrary constant ξ_0.

There is a stationary solution ρ_{st}^{**} to Eq. (H7) determined by

$$\bar{\mathcal{L}}^{**}(\Gamma^{**};\xi_0)\rho_{st}^{**}(\Gamma^{**};\xi_0) = 0, \quad \text{(H8)}$$

$$\bar{\mathcal{L}}^{**}(\Gamma^{**};\xi_0) = \frac{\xi_0}{2}\sum_{r=1}^{N}\frac{\partial}{\partial \boldsymbol{v}_r^*} \cdot \boldsymbol{v}_r^* + \bar{L}^{**}. \quad \text{(H9)}$$

Clearly $\rho^{**}(\Gamma^{**};\xi_0)$ is the same function as $\rho_h^*(\Gamma^*)$ with only the unknown value ζ_0^* replaced by the constant ξ_0. Interestingly, it is possible to determine ζ_0^* from the chosen value of ξ_0 and the measured value of the temperature T_{st}^{**} of the steady state, defined by

$$T_{st}^{**} = \frac{1}{d}\int d\Gamma^{**}v_1^{**2}\rho_{st}^{**}(\Gamma^{**};\xi_0). \quad \text{(H10)}$$

The three mentioned quantities are related by

$$\zeta_0^* = \frac{\xi_0}{\sqrt{2\tilde{T}_{st}^{**}}}. \quad \text{(H11)}$$

This relationship may be derived as follows. Define for homogeneous systems in general the temperature

$$T^{**}(\tau) = \frac{1}{d}\int d\Gamma^{**}v_1^{**2}\rho^{**}(\Gamma^{**},\tau;\xi_0) = \frac{T(t)}{m\chi^2(t)}, \quad \text{(H12)}$$

i.e., the temperature T^{**} is the actual temperature but expressed in the arbitrary scaling variables. Now consider the dynamical equation associated with this scaled temperature, which follows directly from Eq. (H10),

$$\left(\frac{\partial}{\partial \tau} - \xi_0\right)T^{**}(\tau) = -\frac{l\zeta_0(t)T^{**}(\tau)}{\xi(t)}. \quad \text{(H13)}$$

Using now the scaling property of the distribution function of the HCS and, therefore, of $\rho^{**}(\Gamma^{**};\xi_0)$, this becomes

$$\left(\frac{\partial}{\partial \tau} - \xi_0\right)T^{**}(\tau) = -\sqrt{2}\zeta_0^*T^{**3/2}(\tau), \quad \text{(H14)}$$

whose solution is

$$T^{**}(\tau) = \frac{\xi_0^2}{2\zeta_0^{*2}} \left[1 + \left(\frac{\xi_0}{\zeta_0^* \sqrt{2T^{**}(0)} - 1} \right) e^{-\tau \xi_0/2} \right]^{-2}, \quad (H15)$$

which in the long-time limit goes to Eq. (H11) above. Therefore, in practice, one imagines measuring T_{st}^{**} rather than

solving for ζ_0^* self-consistently in the HCS state. Also, the different generators defined earlier and the stationary representation of two-time correlation functions over the HCS ensemble can be translated into this language of arbitrary scaling [5,6].

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