

## Dynamics of a Hard Sphere Granular Impurity

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An impurity particle coupling to its host fluid via inelastic hard sphere collisions is considered. It is shown that the exact equation for its distribution function can be mapped onto that for an impurity with elastic collisions and an effective mass. The application of this result to the Enskog-Lorentz kinetic equation leads to several conclusions: (1) every solution in the elastic case is equivalent to a class of solutions in the granular case; (2) for an equilibrium host fluid the granular impurity approaches equilibrium at a different temperature, with a dominant diffusive mode at long times; (3) for a granular host fluid in its scaling state, the granular impurity approaches the corresponding scaling solution.

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Granular fluids are the subject of growing attention using a variety of experimental, numerical, and theoretical tools [1,2]. Among the many objectives is a theoretical characterization of important mechanisms based in the fundamentals of nonequilibrium statistical mechanics and kinetic theory [2]. In this context, an idealized model that captures the single feature of collisional energy loss has been considered extensively. This is the system of  $N$  smooth, hard spheres with pairwise inelastic collisions. It has a remarkably rich number of properties that correlate with those of real granular fluids. Of central interest are properties that differ from those of normal fluids, and the reasons behind these differences.

Perhaps the simplest test bed for such questions is a study of the dynamics of a single impurity particle of mass  $m_0$  in a one-component granular fluid. The impurity-fluid particle interactions have a “restitution coefficient”  $\alpha_0$  measuring the degree of inelasticity ( $0 < \alpha_0 \leq 1$ , with  $\alpha_0 = 1$  corresponding to elastic collisions). A complete description of impurity properties is given by the probability density for its position and velocity at each time,  $F(\mathbf{q}_0, \mathbf{v}_0, t)$ . Its time dependence is coupled to the joint distribution for the impurity and a fluid particle,  $f^{(2)}(x_0, x_1, t)$ , where  $x_i \equiv (\mathbf{q}_i, \mathbf{v}_i)$ , through collisions between the impurity and fluid particles. This coupling occurs through an exact equation

$$(\partial_t + \mathbf{v}_0 \cdot \nabla_0)F(x_0, t) = L[x_0; \alpha_0, m_0]f^{(2)}(t), \quad (1)$$

where  $L[x_0; \alpha_0, m_0|\cdot]$  is a linear functional depending on the impurity position and velocity, and its restitution coefficient and mass. Equation (1) is the exact first Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy equation [3], with its detailed form given below. A primary result being reported here is the identity

$$L[x_0; \alpha_0, m_0]f^{(2)}(t) = L[x_0; \alpha_0 = 1, m_0^*]f^{(2)}(t), \quad (2)$$

where the effective mass is

$$m_0^* = m_0 + (m_0 + m)(1 - \alpha_0)/(1 + \alpha_0), \quad (3)$$

$m$  being the mass of a fluid particle. This identity establishes an exact relationship of the coupling of the impurity to its host fluid by inelastic and elastic collisions. Therefore, it has the potential to reveal details about the differences and similarities of granular and normal fluids.

The main utility of (1) is its basis for constructing a closed kinetic equation for  $F(x_0, t)$ . In detail, the above functional  $L$  depends on  $f^{(2)}$  only for the colliding pair at contact, and on the precollision hemisphere. For this configuration, a kinetic theory results by expressing  $f^{(2)}(x_0, x_1, t)$  as a linear functional of  $F(x_0, t)$ . A simple and accurate choice is the Enskog-Lorentz approximation [4]

$$f^{(2)}(x_0, x_1, t) \rightarrow F(x_0, t)f(x_1, t)g(\mathbf{q}_0, \mathbf{q}_1|n(t)), \quad (4)$$

where  $f(x_1, t)$  is the fluid probability density and  $g(\mathbf{q}_0, \mathbf{q}_1|n)$  is the local equilibrium pair correlation function as a known functional of the nonequilibrium fluid density  $n(\mathbf{q}, t)$ . The correlation factor  $g$  accounts for the influence of the impurity particle on the joint impurity-fluid particle distribution. However, the one-particle fluid distribution  $f$  is not affected by the impurity in the thermodynamic limit ( $N \rightarrow \infty$ ).

Use of the approximation (4) in the exact result (1) gives the granular Enskog-Lorentz kinetic equation for  $F(x_0, t)$ . The utility of this equation is limited to low or moderate fluid density and impurity size small compared to the mean free path. However, within this context, its scope is quite broad, encompassing homogeneous and inhomogeneous states of the impurity and arbitrary host fluid states. The identity (2) implies that this kinetic equation is the same as that for an impurity with elastic collisions but with an effective mass. Several strong conclusions follow immedi-

ately: (1) Since the effective mass is a function of both the impurity mass and restitution coefficient, every solution in the elastic case corresponds to a continuous family of granular solutions with different  $\alpha_0$ ,  $m_0$ . Equivalently, there is a scaling for the granular solutions such that the dependence on  $\alpha_0$ ,  $m_0$  occurs only through the single combination  $m_0^*$ . (2) For the case of a host fluid at equilibrium, the granular particle approaches equilibrium as well, but at a different temperature. In addition, the long time dynamics is hydrodynamic (diffusion) at long wavelengths. (3) For the case of a host granular fluid in its homogeneous cooling state (HCS), it is shown below that the impurity particle also approaches a HCS with a different temperature, but the same cooling rate. These conclusions hold for the complete range of inelasticity,  $0 < \alpha_0 \leq 1$ .

There are some limiting cases where some of the implications discussed here have been noted before. For a massive impurity particle, the Enskog-Lorentz kinetic equation simplifies to a Fokker-Planck equation and its exact mapping to the corresponding elastic case has been given [5]. The equilibrium state of an impurity particle in an equilibrium host fluid has been discussed in [6]. It has been noted recently [7] that the impurity mass can be taken as equal to the fluid particle mass by introducing an effective restitution coefficient, while Piasecki *et al.* [8] found (considering one-dimensional systems only) that the special case  $m_0/m = \alpha_0$  is equivalent to  $\alpha_0 = 1$  with  $m_0^*/m = 1$ . All of these special cases are subsumed by the general results discussed here.

The system considered is a fluid of  $N$  hard spheres of mass  $m$  and diameter  $\sigma$ , and an impurity particle of mass  $m_0$  and diameter  $\sigma_0$ . The impurity interacts with the fluid particles by inelastic hard sphere collisions; the nature of collisions between a pair of fluid particles is left unspecified at this point. The reduced distribution function for the impurity obeys the exact Eq. (1) with the definition

$$L[x_0; \alpha_0, m_0 | f^{(2)}(t)] \equiv \bar{\sigma}^{d-1} \int d\mathbf{v}_1 d\hat{\sigma} \Theta(\mathbf{v}_{01} \cdot \hat{\sigma}) |\mathbf{v}_{01} \cdot \hat{\sigma}| \times [\alpha_0^{-2} f^{(2)}(\mathbf{q}_0, \mathbf{v}_0', \mathbf{q}_0 - \bar{\sigma}, \mathbf{v}_1', t) - f^{(2)}(\mathbf{q}_0, \mathbf{v}_0, \mathbf{q}_0 + \bar{\sigma}, \mathbf{v}_1, t)]. \quad (5)$$

Here,  $\bar{\sigma} = (\sigma_0 + \sigma)/2$  is an effective hard sphere diameter for an impurity-fluid pair,  $\bar{\sigma} \equiv \bar{\sigma} \hat{\sigma}$ ,  $d$  is the dimensionality of the system,  $\Theta$  is the Heaviside step function,  $\mathbf{v}_{01} = \mathbf{v}_0 - \mathbf{v}_1$  is the relative velocity, and

$$\begin{aligned} \mathbf{v}_0'' &= \mathbf{v}_0 - \frac{m}{m_0 + m} \frac{1 + \alpha_0}{\alpha_0} (\mathbf{v}_{01} \cdot \hat{\sigma}) \hat{\sigma}, \\ \mathbf{v}_1'' &= \mathbf{v}_1 + \frac{m_0}{m_0 + m} \frac{1 + \alpha_0}{\alpha_0} (\mathbf{v}_{01} \cdot \hat{\sigma}) \hat{\sigma} \end{aligned} \quad (6)$$

are the restituting collision values that lead to  $\{\mathbf{v}_0, \mathbf{v}_1\}$  following a binary collision. It is easily verified that the total momentum of the colliding pair is conserved. Now

make the change of variables  $\mathbf{w}_1 = \mathbf{v}_1 - (\alpha_0^{-1} - 1)(\mathbf{v}_{01} \cdot \hat{\sigma}) \hat{\sigma}$  in the first term of the integrand in (5), using  $d\mathbf{v}_1 = \alpha_0 d\mathbf{w}_1$ ,  $\mathbf{v}_{01} \cdot \hat{\sigma} = \alpha_0 \mathbf{w}_{01} \cdot \hat{\sigma}$ , and  $\mathbf{w}_{01} \equiv \mathbf{v}_0 - \mathbf{w}_1$ . After some straightforward algebra, the above scattering law becomes that for an *elastic* relationship between the pair  $(\mathbf{v}_0, \mathbf{w}_1)$  and  $(\mathbf{v}_0'', \mathbf{w}_1'')$ ,

$$\begin{aligned} \mathbf{v}_0'' &= \mathbf{v}_0 - \frac{2m}{m_0^* + m} (\mathbf{w}_{01} \cdot \hat{\sigma}) \hat{\sigma}, \\ \mathbf{w}_1'' &= \mathbf{w}_1 + \frac{2m_0^*}{m_0^* + m} (\mathbf{w}_{01} \cdot \hat{\sigma}) \hat{\sigma}, \end{aligned} \quad (7)$$

where  $m_0^*(\alpha_0, m_0)$  is defined by (3). Note that this does not imply equivalence between inelastic and elastic scattering laws. However, only the integration over  $\mathbf{v}_1$  is required in (5) and this is equivalent to an integration over the new variable  $\mathbf{w}_1$ . Finally, by renaming the dummy integration variable  $\mathbf{w}_1 \rightarrow \mathbf{v}_1$  the desired result, Eq. (2) above, is obtained.

There are some caveats to note at this formally exact level. The joint distribution  $f^{(2)}$  cannot be chosen arbitrarily. In fact, it obeys an independent second hierarchy equation for which the dependence on  $\alpha_0$  cannot be removed by this transformation. Consequently, while the functional on the right side of (2) is that for an elastic impurity, in general its argument is not. Hence there is not a complete mapping of the granular impurity problem to one with elastic collisions. However, in the approximation to be considered next this mapping is complete.

Use of the approximate functional (4) in the first hierarchy equation gives the revised Enskog-Lorentz kinetic equation [4,9]

$$(\partial_t + \mathbf{v}_0 \cdot \nabla_0) F(x_0, t) = I_E[x_0; \alpha_0, m_0 | F(t), f(t)]. \quad (8)$$

The collision operator,  $I_E$ , is a functional of both the impurity and fluid particle distribution functions,  $F(x_0, t)$  and  $f(x_1, t)$ , with the notation  $I_E[x_0; \alpha_0, m_0 | F(t), f(t)] \equiv L[x_0; \alpha_0, m_0 | F(t)f(t)g]$ . At low density  $g \rightarrow 1$  and this becomes the Boltzmann-Lorentz-Bogoliubov equation. The identity (2) gives directly the corresponding property of the collision operator  $I_E[x_0; \alpha_0, m_0 | F(t), f(t)] = I_E[x_0; \alpha_0 = 1, m_0^* | F(t), f(t)]$ . Consequently, this implies the equality of solutions, for any given fluid state,  $F(x_0, t; \alpha_0, m_0) = F(x_0, t; \alpha_0 = 1, m_0^*)$ . Thus, for any chosen positive value of  $m_0^*(\alpha_0, m_0)$  there is an equivalence class of solutions for different pairs  $(\alpha_0, m_0)$ . Furthermore, the solution for each different class is that for an impurity with elastic collisions. These are the main observations of the present work for kinetic theory. It is emphasized that they apply for all solutions, including time dependent and spatially inhomogeneous states, and for arbitrary nonequilibrium fluid states as well [10]. In the following, some of the consequences are noted for illustration.

For simplicity, the rest of the discussion is limited to cases for which the host fluid is in a spatially homogeneous

state,  $f(\mathbf{q}_1, \mathbf{v}_1, t) \rightarrow f(\mathbf{v}_1, t)$ . Then, evaluated at contact,  $g(\mathbf{q}_0, \mathbf{q}_1 | n(t))$  becomes an overall constant function  $\chi(n)$  of the time independent global density  $n = N/V$ . Aside from this factor, the collision operator becomes the usual Boltzmann-Lorentz operator for an impurity of mass  $m_0^*$ , i.e.,  $I_E[x_0; \alpha_0 = 1, m_0^* | F(t), f(t)] \rightarrow \chi(n) I_B[\mathbf{v}_0 | F(t), f(t)]$ . Since the equation is linear it is sufficient to consider a single Fourier mode and the kinetic equation becomes

$$\partial_t \tilde{F}(\mathbf{k}, \mathbf{v}, t) = -i\mathbf{k} \cdot \mathbf{v} \tilde{F}(\mathbf{k}, \mathbf{v}, t) + \chi(n) I_B[\mathbf{v} | \tilde{F}(t), f(t)]. \quad (9)$$

This is the equation for an impurity with elastic collisions, all effects of the impurity inelasticity being contained in the effective mass  $m_0^*$ .

The condition for a steady state  $F(\mathbf{v}, t) \rightarrow F_e(\mathbf{v})$  is  $\mathbf{k} = \mathbf{0}$  and  $I_B[\mathbf{v} | F_e, f(t)] = 0$ . For an isolated system (e.g., unbounded, or periodic boundary conditions) the only solution is a Maxwellian for both the fluid and impurity distributions, at the same temperature,

$$f(\mathbf{v}, t) \rightarrow f_e(\mathbf{v}) = n(m/2\pi T)^{d/2} e^{-mv^2/2T}, \quad (10)$$

$$F_e(\mathbf{v}) = (m_0^*/2\pi T_0^*)^{d/2} e^{-m_0^*v^2/2T_0^*},$$

with  $T_0^* = T$ . The distribution for the impurity particle can be expressed in terms of its actual mass  $m_0$  by introducing the true impurity temperature  $T_0 \equiv m_0 T_0^*/m_0^* = T(1 + \alpha_0)/[2 + (1 - \alpha_0)m/m_0]$ . Thus, the impurity particle is at equilibrium (Maxwellian), just as the fluid particles, but at a lower temperature  $T_0 < T$ . This agrees with previous results [6] for the stationary state of an impurity in an equilibrium fluid.

Next, consider the fluid state to be in equilibrium,  $f = f_e$ , and study the approach of the impurity to its equilibrium distribution from a general initial state. For this purpose write

$$F(\mathbf{r}, \mathbf{v}, t) = F_e(\mathbf{v})[1 + \phi(\mathbf{r}, \mathbf{v}, t)], \quad (11)$$

so the Enskog-Lorentz equation becomes (in Fourier space)

$$\partial_t \tilde{\phi}(\mathbf{k}, \mathbf{v}, t) = (-i\mathbf{k} \cdot \mathbf{v} + \bar{I}_e) \tilde{\phi}(\mathbf{k}, \mathbf{v}, t), \quad (12)$$

where  $\bar{I}_e X = \chi(n) F_e^{-1} I_B[\mathbf{v} | F_e X, f_e]$ . The spectrum of  $-i\mathbf{k} \cdot \mathbf{v} + \bar{I}_e$  has been characterized rigorously in the following sense [11]: The spectrum of  $\bar{I}_e$  is negative with an isolated point at zero (conservation of probability). The spectrum of  $-i\mathbf{k} \cdot \mathbf{v} + \bar{I}_e$  is analytic in  $\mathbf{k}$  about  $\mathbf{k} = \mathbf{0}$ , and its real part is negative. Hence the point at zero becomes one at  $-D(k)$  and remains isolated from the rest of the spectrum for sufficiently small  $k$ . In that limit  $D(k) \rightarrow Dk^2$  and represents a diffusion mode. In summary, an initial state decays rapidly to a dominant diffusion mode and subsequently approaches uniform equilibrium by relaxation of this hydrodynamic mode. This is the classical picture of ‘‘aging to hydrodynamics’’, followed by approach to equilibrium. The significance of this well-

established result is that it now applies as well to a granular impurity, through only a change in the effective mass.

If the host fluid itself is composed of granular particles with inelastic collisions then the homogeneous state is no longer equilibrium but rather the HCS [2,12]

$$f(\mathbf{v}, t) \rightarrow nc^{-d}(t) f_h(v/c(t)), \quad c(t) = \sqrt{2T(t)/m}, \quad (13)$$

where  $T(t)$  is related to the average kinetic energy in the usual way. Its time dependence is due to the continual collisional energy loss, or ‘‘cooling’’. A similar scaling solution for the impurity particle is sought of the form

$$F(\mathbf{v}, t) \rightarrow c_0^{-d}(t) F_h(v/c_0(t)), \quad c_0(t) = \sqrt{2T_0^*(t)/m_0^*}. \quad (14)$$

Here  $T_0^*(t)$  is the corresponding measure of the impurity particle’s average kinetic energy. Its time dependence is determined from the Enskog-Lorentz equation with an explicit time dependence through the host fluid temperature. If the impurity and fluid velocities are scaled with  $c_0(t)$  and  $c(t)$ , respectively, and a dimensionless time  $s$  is defined through  $ds = [c_0(t)/l]dt$ , with  $l \equiv 1/\chi(n)n\bar{\sigma}^{d-1}$ , then the Enskog-Lorentz collision operator becomes a function of time only through  $T_0^*(t)/T(t)$ . The scaling solution (14) exists, therefore, only if this ratio is constant,  $T_0^*(t)/T(t) = \gamma$ . This does not imply that the temperatures are the same, only that the cooling rates for the fluid and impurity particle are the same.

The specific form for  $F_h(v/c_0(t))$ , which is in general different from that of  $f_h(v/c(t))$ , is determined from the Enskog-Lorentz equation. In the above dimensionless units, with the cooling rate denoted by  $\zeta_0 = -\partial_s \ln T_0^*(t)$ , it becomes the time independent stationary equation

$$\mathcal{L} F_h = 0, \quad \mathcal{L} \equiv -\frac{\zeta_0}{2} \nabla_v \cdot \mathbf{v} + I. \quad (15)$$

Here,  $I X = I_B[\mathbf{v} | X, f_h]$ , except that the dimensionless relative velocity is  $\mathbf{v}_{01} = \mathbf{v}_0 - \mathbf{v}_1 \sqrt{m_0^*/m\gamma}$  and the dimensionless restituting velocities are  $\mathbf{v}_0'' = \mathbf{v}_0 - [2m/(m_0^* + m)](\mathbf{v}_{01} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}$  and  $\mathbf{v}_1'' = \mathbf{v}_1 + [2\sqrt{m_0^* m \gamma}/(m_0^* + m)] \times (\mathbf{v}_{01} \cdot \hat{\boldsymbol{\sigma}}) \hat{\boldsymbol{\sigma}}$ . In this context, it might be expected that initial states for the impurity approach this stationary HCS solution, analogous to the approach to equilibrium described above. Let us prove that this is indeed the case.

Paralleling the above analysis, define

$$F(\mathbf{r}, \mathbf{v}, t) = c_0^{-d}(t) F_h(v/c_0(t)) [1 + \phi(\mathbf{r}/l, \mathbf{v}/c_0(t), t)], \quad (16)$$

so that for a single Fourier component one has

$$\partial_s \tilde{\phi} = (-i\mathbf{k} \cdot \mathbf{v} + \bar{\mathcal{L}}) \tilde{\phi}, \quad (17)$$

$$\bar{\mathcal{L}} = -\frac{\zeta_0}{2} \mathbf{v} \cdot \nabla_v - (\bar{I}1) + \bar{I},$$

with  $\tilde{\mathcal{L}} \equiv F_h^{-1} \mathcal{L} F_h$  and  $\tilde{\mathcal{I}} \equiv F_h^{-1} \mathcal{I} F_h$ . Define a Hilbert space with scalar product  $(a, b) \equiv \int d\mathbf{v} F_h(v) a^+(\mathbf{v}) b(\mathbf{v})$ . Then, the following identity applies

$$\text{Re}(\psi, \tilde{\mathcal{L}}\psi) = \text{Re}(\psi, \tilde{\mathcal{I}}\psi) - \frac{1}{2}(\psi, \psi \tilde{\mathcal{I}}1). \quad (18)$$

Next, note the representation

$$\begin{aligned} (\varphi, \tilde{\mathcal{I}}\psi) &= \int d\mathbf{v}_0 d\mathbf{v}_1 d\hat{\boldsymbol{\sigma}} F_h(\mathbf{v}_0) f_h(\mathbf{v}_1) \Theta(\mathbf{v}_{01} \cdot \hat{\boldsymbol{\sigma}}) |\mathbf{v}_{01} \cdot \hat{\boldsymbol{\sigma}}| \\ &\times [\varphi^+(\mathbf{v}'_0) - \varphi^+(\mathbf{v}_0)] \psi(\mathbf{v}_0), \end{aligned} \quad (19)$$

where use has been made of the consequence of elastic collisions  $d\mathbf{v}_0 d\mathbf{v}_1 = d\mathbf{v}'_0 d\mathbf{v}'_1$ ,  $\mathbf{v}_{01} \cdot \hat{\boldsymbol{\sigma}} = -\mathbf{v}'_{01} \cdot \hat{\boldsymbol{\sigma}}$ , and the fact that the inverse and direct scattering laws are the same. Applying this to the right side of (18) gives the desired result

$$\text{Re}(\psi, (-i\mathbf{k} \cdot \mathbf{v} + \tilde{\mathcal{L}})\psi) \leq 0, \quad (20)$$

i.e., the generator for the dynamics is dissipative [13]. A similar analysis of  $(\varphi, \tilde{\mathcal{L}}\psi)$  shows that a constant is an eigenfunction of both  $\tilde{\mathcal{L}}$  and its adjoint, with zero eigenvalue. The null space is therefore spanned by 1. By normalization the solution  $\tilde{\phi}$  in (17) is orthogonal to 1. Consequently,

$$\partial_s \|\tilde{\phi}\|^2 = 2 \text{Re}(\tilde{\phi}, \partial_s \tilde{\phi}) < 0. \quad (21)$$

Since the inequality is strict now,  $\|\tilde{\phi}\|$  is positive, monotonically decreasing, and must go to zero.

In summary, the connection (2) obtained here presents the possibility to explore new consequences for the kinetic theory of granular impurity dynamics. This has been illustrated for the case of the Enskog-Lorentz kinetic equation. The result (12) for the equilibrium host fluid is significant since it establishes the fact that inelasticity does not affect any qualitative features of the impurity dynamics in that case. In particular, the existence of a diffusion mode, its dominance at long times, and approach to equilibrium still apply. In the more interesting case of a granular host fluid, the result (21) is significant in showing that the nontrivial scaling solution  $F_h$  is universal in the same sense as the Maxwellian for normal fluids. Further study of the inhomogeneous generator  $-i\mathbf{k} \cdot \mathbf{v} + \tilde{\mathcal{L}}$  is needed to answer such questions as: do spatial perturbations exhibit a diffusive mode? If so, does the diffusive mode exist and dominate at long times even for strong dissipation? Formally, the diffusion mode can be identified by assuming spectral isolation and analyticity in  $\mathbf{k}$  for a perturbation expansion of the zero eigenvalue of  $\tilde{\mathcal{L}}$  [14]. However, analysis in the large mass limit suggests that the answers may be conditional. In that limit it has been shown [5] that diffusion requires that the cooling rate of the host fluid not be too large compared to the impurity-fluid collision rate. More complete characterization of the spectrum of the generators

of dynamics for inhomogeneous states seems to be limited at present to idealized models [14,15].

Kinetic theory for granular fluids and its domain of validity remain topics of intense debate. In practice, limitations due to approximate implementations can become confused with those of the theory itself. In this context, precise results for restricted systems (e.g., an impurity particle) can provide instructive benchmarks for important conceptual issues. This is one of the objectives of the present analysis.

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