Hydrodynamic equations for one-dimensional systems of inelastic particles

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Using a different method, the balance equations of mass, momentum, and kinetic energy are derived for an arbitrary one-dimensional system of inelastic particles from its kinematic description. The failure of the hydrodynamic equations for such dissipative systems must be attributed to the inconsistency of constitutive relations with the microscopic structure of the system. Among the constitutive relations, the Fourier law of heat conduction is the most inappropriate. [S1063-651X(97)06505-7]

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Recently, Du, Li, and Kadanoff [1] have shown that with the introduction of a very small dissipation in the microscopic dynamics, the usual hydrodynamics approach for granular flows fails to give a correct picture for a many-particle system. They have numerically simulated the one-dimensional motion of N sizeless inelastic particles of identical mass, confined by two walls of infinite mass. If this system is driven by collisions with the boundary walls, most of the particles become squeezed in a small ''clump'' and move with a smaller velocity than the other particles. This result is independent of how the energy is pumped in at the boundaries. Contrary to the prediction of the usual hydrodynamic equations, the clump does not disappear as the dissipation tends to zero. In fact, the particles in the clump are squeezed into a smaller space and move with slower speed. A similar phenomenon has been reported in the cooling of inelastic particle systems [2–4].

In this paper we investigate the reason for the hydrodynamics breakdown for this corpuscular system. The hydrodynamic description of a continuum consists of two parts. The first is a set of balance equations for local macroscopic fields modeling fundamental physical quantities (mass, momentum, energy, entropy, etc.) [5]. The balance equations are postulated and have a general form and validity. In general, the number of continuous fields is greater than the number of balance equations, so additional relations are needed (e.g., the expression of the stress tensor for a specified material). In continuum mechanics, such relations are referred to as ''constitutive relations'' [6] and represent the second part of the hydrodynamic description. Thus the hydrodynamic equations always consist of balance equations and constitutive relations. The constitutive relations describe the macroscopic properties of the material and are related to the specific microscopic structure of the corpuscular system.

The balance equations are valid for any conserved physical quantity [5,7,8]. If the physical quantity is not conserved, then the balance equations are supplemented with the supply and production densities for the physical quantity, for instance, the entropy production for irreversible processes in a continuum. The same approach works for the kinetic energy lost in inelastic collisions. Therefore, the contradiction between the numerical results in [1] and the solution of the usual hydrodynamic equations cannot be associated with the balance equations, but with constitutive relations inadequate to the microscopic structure.

Du, Li, and Kadanoff [1] have used the constitutive relations for relatively dense granular materials in high shear flow derived in [9,10]. In that case the flux of the kinetic energy is proportional to the gradient of the kinetic temperature (the Fourier law) and the dissipation rate of the kinetic energy is proportional to the kinetic temperature to $\frac{3}{2}$power. But the Fourier law is not valid for the corpuscular system in [1]. Indeed, the fast particle running between the left wall and the ''clump'' transports the energy gained from the collision with the wall and loses it during the inelastic collision with the neighboring particle. This nonvanishing energy flux near the wall corresponds to a vanishing gradient of the kinetic temperature, because in this region only the fast particle can move and its average state does not depend on position.

The numerical experiment in [1] contains only 100 particles and an unquestionable continuum macroscopic interpretation of the results is difficult to obtain. In this paper we use a simplified form of a more general approach valid for three-dimensional systems as well [11]. A space-time coarse-grained average for an arbitrary physical quantity attached to the particles is defined. Its first-order partial derivatives are almost everywhere continuous. For an arbitrary number of particles, we prove that this space-time average satisfies a relation of the same form as the balance equations. If the temporal and spatial averaging intervals can be chosen such that the discontinuities of the partial derivatives vanish or become negligible, the usual continuous fields and balance equations are obtained.

Our approach has the advantage that the macroscopic continuous description does not depend on the number of the particles or the microscopic dynamical laws. The space-time coarse-grained averages can be defined and satisfy a balance equation even for a single particle. Also, we can analyze the macroscopic properties of the corpuscular system without a

direct study of the dynamical system associated with the particles. For instance, Du, Li, and Kadanoff's corpuscular system does not verify the equipartition of energy, but we do not need to find out the cause of this behavior. First we derive the balance equations of mass, momentum, and kinetic energy for the same system as in [1]. Then we apply our method to a very simple situation such that all the terms in the balance equations can be explicitly determined. The constitutive relations are directly tested and we prove that in this case the Fourier law of heat conduction is not valid.

Consider N identical sizeless particles of mass m. We study the evolution of the system during the time interval $I=[0,T]$. The particles are confined within the spatial interval [0,1] by collisions with two walls of infinite mass. The collisions between particles are inelastic and are characterized by the numerical parameter $\epsilon=(1-r)/2$. The restitution coefficient r is defined in terms of the particles velocities after and before the collision by $v_1'-v_2'=-r(v_1-v_2)$. The particles interact only when they collide and there are no external forces acting on the particles, except that due to the collisions with the walls. We assume that the system kinematics is known, i.e., the position of each particle $i\leqslant N$ is a given function of time $x_i: \quad I\rightarrow[0,1]$. When a collision occurs, the corresponding velocities $\xi_i=\dot{x}_i$ undergo jumps and between collisions the motion is uniform. We suppose that the total number of collisions during I is finite.

Let $\varphi_i(t)$, $t\in I$, be the real function of time describing the variation of an arbitrary physical quantity φ attached to the ith particle. In the following, φ_i will represent only the mass (m), the momentum $(m\xi_i)$, and the kinetic energy $(m\xi_i^2/2)$. Since the only variations of the velocity ξ_i are the jumps from one constant value to another, the temporal derivative of φ_i identically vanishes $\dot{\varphi}_i\equiv 0$ almost everywhere. Consider two real parameters $0<\tau<T/2$ and $a>0$ and define the function

$$\langle\varphi\rangle(x,t)=\frac{1}{4\tau a}\sum_{i=1}^{N}\int_{t-\tau}^{t+\tau}G_i(x,t')dt', \tag{1}$$

where

$$G_i(x,t)=\varphi_i(t)H(a-|x_i(t)-x|), \tag{2}$$

and H is the left continuous Heaviside function. A nonvanishing contribution to $\langle\varphi\rangle$ is due only to particles lying in the spatial interval $(x-a,x+a)$ during the temporal interval $(t-\tau,t+\tau)$. Therefore, $\langle\varphi\rangle(x,t)$ characterizes the mean distribution of φ about the point x and the time t. It is a coarse-grained average over the space and time intervals defined by a and τ, i.e., the density of φ. Obviously, $\langle\varphi\rangle$ also depends on the parameters a and τ, but we do not explicitly write this dependence. The average $\langle\varphi\rangle$ is nonvanishing only if $x\in(-a,1+a)$ and the integral interval in Eq. (1) is contained in I only if $t\in(\tau,T-\tau)$.

For a given x, the integrand (2) is a continuous function, except at a finite number of points where it has discontinuities of jump type. Hence G_i is Riemann integrable and the partial derivative with respect to t of $\langle\varphi\rangle$ is

$$\partial_t\langle\varphi\rangle=\frac{1}{4\tau a}\sum_{i=1}^{N}[G_i(x,t+\tau)-G_i(x,t-\tau)]. \tag{3}$$

The function $\langle\varphi\rangle$ depends on x through the instants u when the ith particle enters or leaves the interval $(x-a,x+a)$. These instants are given by the zeros of the equations

$$x_i(u)-x\pm a=0,$$

and using the implicit function theorem we obtain $du/dx=1/\xi_i(u)$. If $u\in(t-\tau,t+\tau)$, then u occurs as the integration limit in Eq. (1) and the derivative of $\langle\varphi\rangle$ with respect to x is

$$\partial_x\langle\varphi\rangle=\frac{1}{4\tau a}\sum_{i=1}^{N}\left[\sum_{u\in U_i'}\frac{\varphi_i(u)}{\xi_i(u)}-\sum_{u\in U_i''}\frac{\varphi_i(u)}{\xi_i(u)}\right], \tag{4}$$

where U_i' (U_i'') is the set containing the instants when the ith particle leaves (enters) the interval $(x-a,x+a)$ during the interval $(t-\tau,t+\tau)$. One can prove that the partial derivatives (3) and (4) are almost everywhere continuous [11].

Relation (3) shows that $\partial_t\langle\varphi\rangle$ is related to the change of G_i from $t-\tau$ to $t+\tau$. Since $\dot{\varphi}_i\equiv 0$ and $\dot{H}\equiv 0$ almost everywhere, the changes of G_i are only jumps. When the ith particle enters [leaves] the interval $(x-a,x+a)$, the change of G_i is $+\varphi_i(u)$ $[-\varphi_i(u)]$. According to Eq. (4), the corresponding part of $\partial_t\langle\varphi\rangle$ is equal to $-\partial_x\langle\varphi\xi\rangle$. The change of G_i due to φ_i occurs when the particles collide inside the interval $(x-a,x+a)$. The collision part of $\partial_t\langle\varphi\rangle$ is

$$\delta_c\varphi=\frac{1}{4\tau a}\sum_{i=1}^{N}\sum_{s\in V_i}[\varphi_i(s-0)-\varphi_i(s+0)], \tag{5}$$

where V_i is the set containing the instants s when the ith particle collides inside $(x-a,x+a)$ during $(t-\tau,t+\tau)$, $\varphi_i(s+0)$ is the limit to the left, and $\varphi_i(s-0)$ is the limit to the right. We deduce that the relation

$$\partial_t\langle\varphi\rangle+\partial_x\langle\varphi\xi\rangle=\delta_c\varphi \tag{6}$$

is always true. In the following we show that this identity is the general form of the balance equations for the corpuscular system considered.

First we apply the identity (6) for mass, i.e., $\varphi_i=m$. The space-time average (1) becomes the mass density $\langle m\rangle$. Since the masses of the particles are identical, we have $\langle m\rangle=mc$, where $c=\langle 1\rangle$ is the particle number density or the concentration obtained from Eq. (1), for $\varphi_i\equiv 1$. The mean velocity field v is defined by $\langle\xi\rangle=cv$ if $c\neq 0$ and is zero otherwise. (In [1] the velocity field is incorrectly defined, but this oversight has not affected the hydrodynamic equations for granular flows used in [1].) The term $\delta_c\varphi$ defined by Eq. (5) vanishes because the collisions do not imply the variation of the mass of particles or their number. Then relation (6) becomes

$$\partial_t c+\partial_x(cv)=0, \tag{7}$$

which is the continuity equation.

For momentum, we choose $\varphi_i=m\xi_i$ and then $\langle\varphi\rangle=mcv$. The second term on the left-hand side of Eq. (6) can

be written as the sum of two terms, namely, $\langle m\xi^2\rangle = mcv^2 + m\langle(\xi - v)^2\rangle$. The first term is due to the mean motion of the particles and the second one can be interpreted as the ''microscopic'' flux of momentum. The momentum is conserved when two particles collide such that $\delta_c\xi$ vanishes. But the collision with the walls induces a variation of the particle momentum and $\delta_c\xi$ is nonvanishing for $x \in (-a,a)\cup(1-a,1+a)$. In this case Eq. (6) represents the balance equation of momentum

$$\partial_t(cv) + \partial_x(cv^2) + \partial_x(c\theta) = \delta_c\xi. \tag{8}$$

Here we have introduced the kinetic temperature $\theta = \langle(\xi - v)^2\rangle/c$ (when $c \neq 0$), known for the granular materials as the granular or fluctuating temperature.

In a similar manner, for $\varphi_i = m\xi_i^2/2$ we obtain from Eq. (6) the balance equation of the kinetic energy

$$\partial_t e + \partial_x(ve) + \partial_x(2vc\theta) + \partial_x q = \delta_c\xi^2, \tag{9}$$

where $e = c(v^2 + \theta)$ is proportional to the density of the kinetic energy and $q = \langle(\xi - v)^3\rangle$ is the microscopic flux of the granular temperature. The collision term does not vanish because of the energy loss at inelastic collisions.

Relations (7)–(9) are of the same form as the usual balance equations, but they have a wider validity. We have not imposed any restriction to the number of particles N, which can be very small. Therefore, these relations also hold for simple mechanical systems not possessing statistical properties characteristic to thermodynamic systems, but they preserve the discontinuous nature of the initial corpuscular description. The first-order partial derivatives (3) and (4) have discontinuous variations when a collision occurs or when a particle enters or leaves the spatial interval $(x-a,x+a)$. For certain corpuscular systems, we can choose a and τ such that these discontinuous variations vanish or are negligible, and the smoothness specific to the continuous fields is obtained.

When $\tau \to 0$, definition (1) is reduced to an instantaneous space average. In this case $\langle\varphi\rangle$ coincides with the usual macroscopic fields if at an arbitrary time t the particles in $(x-a,x+a)$ form a near-equilibrium thermodynamic system. If the local equilibrium holds, then there is an $a_{\min}$ such that for $a > a_{\min}$ this condition is satisfied. Hence the usual balance equations are particular cases of the relations (7)–(9).

Definition (1) also contains a time average. The time integral in Eq. (1) is identical to that used in the formulation of the ergodic hypothesis. Therefore, for a nonvanishing value of τ, more microstates of the corpuscular system are included in the average $\langle\varphi\rangle$ and the smoothness of $\langle\varphi\rangle$ is improved in comparison to an instantaneous space average. The upper limit of τ is given by the requirement that the time averaging should not distort the time evolution of the local fields $\langle\varphi\rangle$. If the corpuscular system is in a steady state, we can take $\tau \to \infty$ and then the space averaging can be reduced even to a point $(a \to 0)$.

Relations (6)–(9) are either identities or equations, according to the available information on the microscopic structure. If the motion of each particle is explicitly known, then Eqs. (6)–(9) are simple identities containing only known functions. Otherwise, they become the balance equations for the averages $\langle\varphi\rangle$, which now are unknown functions, and to obtain a solvable problem, the constitutive relations are needed. To obtain some information on the inadequate constitutive relations in [1], we consider a very simple case of Du, Li, and Kadanoff's corpuscular system such that the motion of the particles is known and the averages $\langle\varphi\rangle$ can be determined.

The system contains only two particles. The simplest periodic motion occurs if the following restrictive conditions are imposed: $0 < \epsilon < \frac{1}{3}$; the left wall returns the first particle with constant velocity $v_0 = 1$; the collision of the second particle with the right wall is perfectly elastic. The collisions of the two particles always take place at the same point $x_c = \frac{1}{2} - \epsilon^2/(1-2\epsilon-\epsilon^2)$ and the velocity of the first particle after the collision is $v_1' = (1-3\epsilon)/(1+\epsilon)$. The velocity modulus of the second particle is the same $|v_2| = (1-\epsilon)/(1+\epsilon)$ before and after the collision. The period of the motion is $(1-\epsilon^2)/(1-2\epsilon-\epsilon^2)$.

Usually, in continuum mechanics, the spatial average is taken over a volume microscopic in comparison to the macroscopic scale of the continuous phenomenon. For our approach this corresponds to $a \to 0$. First we take the average (1) over a spatial interval much smaller than the system length, i.e., $a \ll 1$, and then we study the limit case. For a more condensed description we distinguish five spatial regions. Each of the two boundary regions $(-a,a)$ and $(1-a,1+a)$ contains one wall and the particles can move only within a subdomain of the averaging spatial interval $(x-a,x+a)$. In the transition region (x_c-a,x_c+a) both particles contribute to the average (1). The transition region and the boundary regions bound two ''uniform'' regions (a,x_c-a) and $(x_c+a,1-a)$.

This is a simple mechanical system and the averages $\langle\varphi\rangle$ could present discontinuous variations. The periodicity of the motion allows one to completely eliminate these discontinuities, although the local equilibrium assumption is not satisfied. For a fixed, the necessary smoothness is obtained if 2τ is equal to the period of the motion. Then Eq. (3) implies that all the temporal derivatives vanish and we could say that the system is in a ''steady'' state.

We estimate the quantities in the balance equations (7)–(9). The mean velocity field identically vanishes $v \equiv 0$ because $\langle\xi\rangle \equiv 0$. In the uniform regions the concentration c takes two constant values $c_1 = (1-\epsilon)/\tau(1-3\epsilon)$ and $c_2 = (1+\epsilon)/\tau(1-\epsilon)$. In the boundary and transition regions c has a linear variation between these constant values and the exterior null value. The granular temperature θ has a linear variation only in the transition region between the constant values $\theta_1 = (1-3\epsilon)/(1+\epsilon)$ and $\theta_2 = (1-\epsilon)^2/(1+\epsilon)^2$. We notice that θ has the same value in a uniform region and the adjacent boundary region.

In the hydrodynamic equations used by Du, Li, and Kadanoff [1], the other quantities are given by constitutive relations: $\delta_c\xi = 0$, $q = -\partial_x(C_1\theta^{3/2})$, and $\delta_c\xi^2 = -C_2\epsilon c^2\theta^{3/2}$ with C_1 and C_2 numerical constants. In our case, they can be calculated from the microscopic motion of the corpuscular system. In the left uniform region, q has the constant value $q_1 = 4\epsilon(1-\epsilon)/\tau(1+\epsilon)^2$. In the transition region and the left boundary region it has a linear variation, while for $x > x_c + a$ it vanishes. The momentum is not conserved when the particles collide with the walls, such that in the boundary regions $\delta_c\xi = \pm(1-\epsilon)/2a\tau(1+\epsilon)$. For x

$\in(a,1-a)$, we have $\delta_c\xi=0$. The kinetic energy is conserved for the elastic collision with the right wall and the nonvanishing values of the corresponding collision term are $\delta_c\xi^2 = \pm 2\epsilon(1-\epsilon)/a\tau(1+\epsilon)^2$ if $x\in(-a,a)$ or $x\in(x_c-a,x_c+a)$. It is easy to test that the balance equations (7)–(9) are identically satisfied, while all the constitutive relations for granular materials used in [1] are incorrect.

The limit $a\to 0$ simplifies the above continuous description. The boundary regions disappear and the domain of definition of the continuous fields becomes (0,1). The transition region is reduced to the collision point x_c separating the two uniform regions. In these uniform regions, all the terms of the balance equations (7)–(9) are equal to zero. However, the values of the continuous fields correspond to a state that is analogous to that described in [1]. Indeed, there are two distinct regions with different concentrations and temperatures. Because $c_1>c_2$ and $\theta_1<\theta_2$, the ''denser'' and ''colder'' clump is composed by the first particle near the left wall. In [1] the clump occurred near the right wall. This difference appears because in our case, after the collision, the first particle loses kinetic energy, while the kinetic energy of the second particle is conserved.

Now we can study the validity of the constitutive relations in [1]. The first, $\delta_c\xi=0$, is identically satisfied. But the constitutive relations concerning the granular temperature θ remain inappropriate. In particular, the proportionality of the kinetic-energy flux to the temperature gradient, i.e., the Fourier law, is contradicted. Indeed, although θ is constant for $x\in(0,x_c)$, $q=q_1$ is nonvanishing. This flux really exists because the first particle transports the energy gained from the collision with the left wall and loses it during the inelastic collision with the second particle. The energy dissipation is described by $\delta_c\xi^2$, which is proportional to the Dirac function $-\delta(x-x_c)$. Therefore, in [1] the constitutive relations for q and $\delta_c\xi^2$ must be modified. The validity of other constitutive relations can be tested by applying our method to the results of numerical simulations.

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