Towards unequal partition of energy?

A tantalizing simulation of simple colliding particles in one dimension reveals a clumping tendency in which energy is by no means equally shared among them. The bearing of this on three-dimensional hydrodynamics is another matter.

Now for something conceptually simple, the problem of relating the macroscopic behaviour of some object to the behaviour of its constituent parts, ultimately of the atoms of which it consists. Versions of the problem are well rehearsed in the most elementary of physics textbooks.

The shape taken by a string suspended between two points and hanging freely under gravity? Simple; a piece of string, by definition, can exert a force on the piece to which it is attached only along the line joining them, which is the tangent to the familiar catenary curve. And the same with the usual conundrums of bending beams; on the assumption that the applied forces are not so great that the longitudinal integrity of the structure is destroyed (or that the beam does not snap), the forces to which one part of the beam is subjected consist of torques or bending moments exerted by its neighbour pieces and by the downward force of gravity.

Classical physics, in other words, is a way of representing the microscopic forces between atoms and molecules with plausible patterns of macroscopic forces. That, for example, is the case for the simple calculation of the vibration of a string under tension, or of the velocity of sound in a gas (where it is simply necessary to know the equation of state and the ratio of specific heats at constant volume and pressure respectively). Then, simple calculation will yield a plausible result. Hardly anybody would dream of tackling such a problem by starting with a distribution function for the position and velocity of the constituent molecules and then allowing for their mutual collisions (but, among other excellent things, Chapman and Cowling did just that in their classical monograph, *The Mathematical Theory of Non-Uniform Gases*).

Hydrodynamics more generally is based on the same principles. People speak of infinitesimal elements of fluid, which are supposed to obey the laws of mechanics. Because they have internal structure, the same particles are allowed to have thermodynamic properties as well. (The velocity of sound in a gas is a particular case.) Frictional forces are allowed, and lead to the dissipation of energy. But how generally valid is the supposition that microscopic behaviour can be described in macroscopic terms?

Leo P. Kadanoff from the University of Chicago, with Yunson Du and Hao Li, has now, a little subversively, set out to demonstrate that there are exceptions to the rule by means of one of the simplest systems there could be — a set of classical particles moving in one dimension in a simple confining box, capable of colliding with each other and in such a way that energy may be lost in the process (*Phys. Rev. Lett.* **74**, 1268–1271; 1995). The objective is to follow the collisions of the particles individually and to compare the behaviour of the system they constitute with the appropriate macroscopic hydrodynamic equations.

A deliciously school-textbook notion then arises, the "coefficient of restitution", which is a number between 0 and 1 representing the fraction of the relative velocity of two particles retained in a collision. Think of bouncing a ball vertically onto the floor; if the impact velocity is v, the velocity on rebound will be $-rv$, where r is the coefficient (and the minus sign allows for the rebound of the ball in an opposite direction).

Evidently, such a system will not remain in motion indefinitely. Because energy is lost at each collision, the point will be reached at which there is no kinetic energy left, and all the particles will be at rest. To avoid that trivial outcome, the authors specify appropriately the boundary conditions at the walls of the box. Collisions at one wall are supposed to be perfectly elastic; the rebound velocity is equal to the impact velocity, but in the opposite direction. But at the other wall, energy is fed into the system of colliding particles. This may be notionally arranged in various ways. One is to return each impacting particle into the collision space with a fixed velocity, another is to return the particle with a velocity taken from some random distribution, yet another is to suppose that the wall is vibrating and that particles collide with it elastically. Whatever the arrangement, one wall feeds energy into the system to compensate for that lost in collisions between particles.

The end result appears to be more or less inescapable, whatever the starting distribution of the particles in their one-dimensional box. Because the particles can only collide with each other, and cannot pass through one another, the particle nearest the wall that serves as a source of energy will move very quickly, but the other particles will tend to huddle near the other wall as if they were sheep penned in by dogs.

The authors argue that this condition is robust in that it is reached from all conceivable starting conditions. In the case in which the energetic wall provides the particle reaching it with variable velocity, the particles clumped together near the other wall may burst out of their confinement, only to be returned to it when the free particle is given a greater velocity.

When both walls are sources of energy, most of the particles clump together away from the walls, but support runners on either side of them will fetch and carry energy. In the case in which the wall that is the source of energy returns all particles reaching it with a finite speed, and in which the other particles start with zero velocity, the centre of gravity of the clump moves rhythmically, and the range over which the particles within it are spread increases (and decreases) in unison.

Cynics will say that all this simulation is just a way of occupying inventive people on tasks with which they are familiar when there is nothing more useful in their minds, but that would be a mean *canard*. For the truth is that the simulations demonstrate a direct contravention of what is called the theorem of the 'equipartition of energy' — the doctrine that in a system of interacting particles, energy will be distributed, on the average, equally between all of them. And that is the basis of classical hydrodynamics and much else.

A further feature of the simulation is that the results are quite different when collisions between the particles are elastic (or the coefficient of restitution is equal to unity). Then, in the long run, there is no penning of the majority of particles into clumps, energy (on the average) is equally shared between all of them and the equations of classical hydrodynamics can be expected faithfully to apply.

So where is the snag? The concluding sentence of Du *et al.* is "it remains to be seen whether such a behaviour persists in a driven system in higher dimensions". That may be the crux of this affair. The trouble with a one-dimensional system is that it provides a natural hierarchy for the interaction between one particle and its neighbours; only the next nearest matters. That, in other contexts, is the reason why long-range order cannot exist in one-dimensional systems on the basis of interactions between next-nearest neighbours alone. But it will be interesting to learn what the two-dimensional simulations now implicitly promised will show. A similar result would indeed be subversive. That outcome seems improbable, but it is important that it should be attempted. And soon.

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