

Uniting mechanics and statistics

An adventurous scheme which seeks to incorporate thermodynamics into the quantum laws of motion may end arguments about the arrow of time — but only if it works.

THE logical relationship between the laws of mechanics and those of thermodynamics deserves more attention than it usually receives. Thermodynamics and statistical mechanics are ways of describing the behaviour of macroscopic systems made from components whose behaviour is determined by the laws of mechanics, classically those of Newton (as amended), but otherwise the equations of motion of quantum mechanics. Where the first law of thermodynamics is concerned, there is no difficulty. In both classical and quantum mechanics, total energy is a constant of the motion and is thus always conserved, at least in a closed system.

The difficulty arises chiefly with the second law of thermodynamics, and not only because there is such a variety of ways in which this principle can be defined. But now a group of three theoreticians has put forward an intriguing way in which the laws of quantum mechanics may be modified so as to incorporate the second law from what appears to be the outset (Beretta, C. P., Gyptopoulos, E. P. & Park, J. L., *Il Nuovo Cimento B* **87**, 77–97; 1985). Whether the modification proposed is sufficient, only time will tell, but the objective seems well worth the trouble Beretta *et al.* have taken.

The difficulty is well illustrated by the way in which some kind of correspondence is established between the mechanical behaviour of a system and its thermodynamic properties. For more than a century, people have been brooding on the paradox that while the laws of classical (and, for that matter, quantum) mechanics are symmetrical with respect to time inversion, the second law selects from all possible trajectories of motion only those corresponding to a continual increase of the entropy. The arrow of time is conjured like a rabbit from a hat.

The definition of entropy in terms of the mechanical properties of the constituents of a system is similarly clouded. The classical model is Boltzmann's *H*-theorem (1872), which shows that the rate of change with time of a certain mathematical construct from the probability distribution of single particles in phase space will always be zero or negative. So Boltzmann argued, his quantity *H* is admirably suited to be the negative of what is known in thermodynamics as entropy. This is argument by analogy, but none the worse for that — if it works.

Since Boltzmann's time, there has

accumulated a rich literature on the implied paradox of the conflict between the irreversibility of macroscopic processes and the reversibility (in time) of the laws of mechanics and thus of microscopic processes. Indeed, the argument was begun by Loschmidt in 1976, but now even elementary text-books of thermodynamics reckon to give some kind of account of it.

The standard explanation is that the apparent paradox is not a paradox at all, but a confusion about timescales. Any measure of entropy, that derived from Boltzmann's *H* or otherwise, will fluctuate (and so decrease as well as increase on a short timescale), which is not inconsistent with the notion that the average value of the entropy should increase steadily over long periods of time (or remain unchanged when the system is in equilibrium).

Much the same is said of the recurrence paradox, based on the observation due to Poincaré that the point in phase space (momentum as well as position) representing the state of a classical system will return to more or less the same place after a sufficient length of time. On the face of things, that means that non-equilibrium states of a system will repeatedly recur. The standard resolution of that paradox is the observation that, for any realistic system, the interval of time between recurrences will be huge, much greater than, say, the age of the Universe. Again there is nothing wrong with these arguments, but they are far from being rigorous.

So why not take the bull by the horns, and build irreversibility into the laws of mechanics? That is the point from which Beretta *et al.* start. Properly, they acknowledge that they are not the first to tread this path. They work with quantum statistical mechanics, where the formalism is easier. They start from the equation of motion for the operator representing the state of a physical system, say *m*, which is, in operator language, $dm/dt = -i/\hbar[\mathbf{H}, \mathbf{m}]$, where *t* is time, *H* the Hamiltonian operator of the system and *i* and \hbar the square route of minus one and Planck's constant (divided by 2π) respectively. The quantity in square brackets is the commutator of its two components, $\mathbf{mH} - \mathbf{Hm}$.

The natural way to proceed is to assume that this equation is modified in such a way that the right-hand side is some other function of the state operator *m* than in the standard form. The objective is to find a form of the function which is compatible

both with what is known of the evolution of thermodynamic systems and, perhaps more important, the dynamics of real microscopic systems. Beretta *et al.* have convinced themselves that the function they are seeking cannot be a linear function of *m*. What they propose is the addition to the right-hand side of the quantum equation of motion of a particular function of *m* which, by including both the square root and the logarithm of the state operator of the system, is non-linear enough to satisfy anybody's taste.

Almost magically, the system has some of the obviously necessary properties. For example, for a system in a pure quantum state, say that represented by a solution of Schrodinger's equation, the extra terms vanish and the simple form of the equation of motion applies. Similarly, constants of the motion in the new system are also constants of the motion determined by the simpler equation of motion.

What can be said about the entropy? In reality, the state operator *m* is the equivalent of what is called the density matrix in quantum statistical mechanics, which is why Beretta *et al.* define entropy in terms of the operator $m \log m$, where the logarithm is the natural logarithm of the operator *m*. Specifically, the entropy of the negative of the trace of this operator multiplied by Boltzmann's constant; the authors are able to show that it increases (or does not increase) in the course of time.

So is this a demonstration that the laws of mechanics and of thermodynamics can indeed be combined? Not quite. For one thing, there are various mathematical problems that make some of the steps in the argument conjectural. Worse still, some of the operator functions in the formalism are sometimes undefined. But the system does have the merit of hanging together — the paper now published extends to composite systems the treatment of one-component systems published a year ago.

None of this implies that the arguments about the reconciliation between microscopic reversibility and macroscopic irreversibility will now be stilled. Indeed, while for as long as the present justification of the basis of statistical mechanics holds water, there will be many who say that what Beretta *et al.* have done is strictly unnecessary. But this is a field in which the proof of the pudding is in the eating.

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