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LETTER TO THE EDITOR

Successive derivatives of H for a solution of Boltzmann's equation do not alternate

A J M Garrett

Cavendish Laboratory, University of Cambridge, UK

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Abstract. The conjecture that successive time derivatives of the Boltzmann entropy alternate in sign during free thermal relaxation governed by the nonlinear Boltzmann equation is shown to be false: the Bobylev–Krook–Wu solution of this equation is an explicit counter-example.

The Boltzmann entropy H for an evolving system of similar particles described by a velocity distribution function $f(\boldsymbol{v}, t)$ in d dimensions is given by

$$H = \int \ldots \int f \ln f \, \mathrm{d}^d \boldsymbol{v}. \tag{1}$$

For solutions of Boltzmann's nonlinear integrodifferential equation for the evolution of f in the absence of external force fields and spatial inhomogeneities, the H theorem states that H always decreases, and thereby guarantees that the system relaxes to thermal equilibrium. It has been conjectured (McKean 1966) that the theorem can be generalised to the statement that H is completely monotonic in the sense of Widder (1941):

$$(-\mathrm{d}/\mathrm{d}t)^n H \geqslant 0 \qquad \forall n \geqslant 0. \tag{2}$$

In the same paper McKean also conjectured that property (2) singles out one particular functional as the physical entropy for the system; indeed Harris (1968a, b) was moved by such considerations to use a definition of entropy different from (1). Clarification of these issues is therefore of considerable importance. Property (2) has been studied for various model kinetic equations; the references are given by Ziff *et al* (1981). However, the question of whether (2) holds for the Boltzmann entropy (1) when the evolution is governed by Boltzmann's nonlinear integrodifferential equation has, until now, remained open. There seems little prospect of checking (2) directly from (1) and the Boltzmann equation when n is large: indeed, it does not appear to have been done beyond $n = 1$ (the H theorem). The present paper shows that (2) is *not* valid under these circumstances: this disproof is achieved by finding a specific counter-example. The example considered is the Bobylev–Krook–Wu (BKW) solution of Boltzmann's equation for particles which interact with each other with a differential collision cross section inversely proportional to collision speed (Bobylev 1975, Krook and Wu 1976). This solution is isotropic in velocity space, and describes the relaxation to thermal equilibrium of a particular class of initial velocity distribution functions. It was previously supposed on the basis of numerical studies that the Boltzmann entropy for the BKW solution did satisfy (2) (Ziff *et al* 1981).

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The method of disproof is as follows: it is obviously a sufficient condition for H to be completely monotonic that it is expressible as the Laplace transform of a non-negative definite function. For if

$$H(t)=\int_0^\infty \psi(s)\exp(-st)\,\mathrm{d}s, \qquad \psi(s)\geqslant 0 \text{ in } s\geqslant 0 \tag{3}$$

then

$$(-\mathrm{d}/\mathrm{d}t)^n H=\int_0^\infty s^n\psi(s)\exp(-st)\,\mathrm{d}s\geqslant 0. \tag{4}$$

Implicit in (4) is the condition that the integrals converge. Now it is a mathematical result that the condition is necessary as well as sufficient (Bernstein 1928, Widder 1941, theorem 12b, p 161). We show that, for the BKW solution, H is either not expressible as a Laplace transform, or if it is then the corresponding function ψ is not non-negative definite. Although only one of these possibilities can be true, the truth of either suffices to disprove (2) in view of the necessity of (3) to hold for H to be completely monotonic; consequently we do not pursue the matter further. It is necessary to use the Laplace–Stieltjes transform, or equivalently here to allow $\psi(s)$ to be distribution valued; hc♠ever Widder's result still holds in that case.

The BKW solution in d dimensions is

$$f(v,t)=(2\pi\beta)^{-d/2}\exp(-v^2/2\beta)[1+\beta^{-1}(1-\beta)(v^2/2\beta-\tfrac{1}{2}d)] \tag{5}$$

where

$$\beta(t)=1-(1+\tfrac{1}{2}d)^{-1}\exp(-t) \tag{6}$$

and is given in the original references of Bobylev (1975), Krook and Wu (1976). Both velocity and time have been scaled appropriately, the former by the second (energy) moment of (5), which is conserved, and the latter by an integrated moment of the angular dependence of the collision cross section. It is necessary for f to be non-negative at all velocities and successive times that $t\geqslant 0$: this differs from the convention of Ziff *et al* (1981) by a time translation of $\ln(1+\tfrac{1}{2}d)$. By substituting (5) into (1), performing the angular integrations, changing the scalar variable of integration to $v^2/2\beta$, integrating by parts to remove the logarithm, and finally differentiating with respect to time (which causes much simplification on use of standard properties of the functions involved),

$$-\mathrm{d}H/\mathrm{d}t=\gamma(\gamma-1)[\gamma\exp(t)-1]^{-2}U(2,2-\gamma,\gamma[\exp(t)-1]) \tag{7}$$

where

$$\gamma=1+\tfrac{1}{2}d \tag{8}$$

(Ziff *et al* 1981). The function U in (7) is a confluent hypergeometric function (Abramowitz and Stegun 1965, ch 13). We now use its asymptotic expansion for large argument:

$$U(2,2-\gamma,z)\sim z^{-2}[1-2(1+\gamma)z^{-1}+3(2+\gamma)(1+\gamma)z^{-2}-\dots] \tag{9}$$

to expand (7) in the first few inverse powers of $\exp(t)$:

$$\begin{aligned}-\mathrm{d}H/\mathrm{d}t=\gamma^{-3}(\gamma-1)[&\exp(-4t)\\ &+\gamma^{-2}(5+3\gamma)\exp(-6t)-14\gamma^{-3}(1+\gamma)\exp(-7t)+R(t)]\end{aligned} \tag{10}$$

where the remainder $R(t)$ is given, tautologically, by subtracting (7) from (10):

$$R(t)=\gamma^4[\gamma\exp(t)-1]^{-2}U(2,2-\gamma,\gamma[\exp(t)-1])$$
$$-\exp(-4t)-\gamma^{-2}(5+3\gamma)\exp(-6t)+14\gamma^{-3}(1+\gamma)\exp(-7t). \qquad (11)$$

From (9),

$$R(t) \text{ is } \mathrm{O}[\exp(-8t)] \qquad \text{as } t\to\infty. \qquad (12)$$

We now consider the possibility of writing (10) as a Laplace transform; from (4) we see that if this is feasible, (10) is none other than the Laplace transform of $s\psi(s)$. It is possible that $R(t)$ cannot be written as a Laplace transform: this would be the case, for example, if it contained terms falling off more quickly than any power of $\exp(-t)$. It would follow from (10) and (4) that H could not be written as a Laplace transform. On the other hand, if $R(t)$ *can* be written as a Laplace transform of a function $\phi(s)$, then from (12)

$$\phi(s)=0 \qquad \text{for } s<8. \qquad (13)$$

From (10) and (4) it follows that the function ψ of which H is the Laplace transform,

$$\psi(s)=\gamma^{-3}(\gamma-1)[\tfrac{1}{4}\delta(s-4)+\tfrac{1}{6}\gamma^{-2}(5+3\gamma)\delta(s-6)-2\gamma^{-3}(1+\gamma)\delta(s-7)+s^{-1}\phi(s)], \qquad (14)$$

is not non-negative definite, since in view of (13) and (14) it has a negative spike at $s=7$. The result that (2) is not true now follows from the argument based on Bernstein's work given below (4).

Why is there no sign of this breakdown in the numerical studies of Ziff *et al* (1981), who considered $1\leqslant d\leqslant 6$, $0\leqslant n\leqslant 30$ and $0<t<4.5$? The explanation cannot lie in an insufficient range of d, for either $R(t)$ cannot be written as a Laplace transform for any d, or if it can then a glance at (14) shows the spike at $s=7$ is negative for all d. Nor is the problem likely to reside in an insufficient range of t, as the graphs presented there ($d=3$, $n\leqslant 20$) seem by $t=4.5$ to have settled down to their predicted large-time exponential decay (although successively higher derivatives take successively longer to settle down). A function different from H is used as a calculational vehicle by these authors, but the statement still holds. On the other hand, it can be shown analytically that any violation of the alternating derivative property cannot happen before $n=7$, and is most unlikely to occur for at least several values beyond that. It therefore seems that the calculation of an insufficient number of derivatives led Ziff *et al* to the opposite conclusion. The argument is set out below.

From Leibnitz' theorem it can be verified that the product of two completely monotonic functions is itself completely monotonic. Now $[\gamma\exp(t)-1]^{-1}$ is completely monotonic since it is the Laplace transform of the non-negative definite function

$$\sum_{p=1}^{\infty}\gamma^{-p}\delta(s-p). \qquad (15)$$

Therefore, from (7), it suffices to prove that $U(2,2-\gamma,z)$, where

$$z=\gamma[\exp(t)-1], \qquad (16)$$

has alternating time derivatives up to $n=N$ in order to demonstrate the same property for H up to at least $n = N+1$ (Ziff *et al* 1981). Now

$$U(2, 2-\gamma, z) = \int_0^\infty x(1+x)^{-1-\gamma} \exp(-zx)\, dx \tag{17}$$

(Abramowitz and Stegun 1965, formula 13.2.5) and so

$$-\frac{d}{dt} U(2, 2-\gamma, z) = -\frac{dz}{dt}\frac{d}{dz} U(2, 2-\gamma, z) \tag{18}$$

$$= (\gamma + z) \int_0^\infty x^2(1+x)^{-1-\gamma} \exp(-zx)\, dx \tag{19}$$

$$= \int_0^\infty x(2+x+\gamma x^2)(1+x)^{-2-\gamma} \exp(-zx)\, dx, \tag{20}$$

integrating (19) by parts to remove the factor of z. Since the integrand in (20) is positive definite, dU/dt is negative, and so H has alternating derivatives up to $n = 2$. By successive differentiations and integrations by parts it may further be shown that

$$(-d/dt)^m U(2, 2-\gamma, z) = \int_0^\infty x P_{2m}(x)(1+x)^{-m-1-\gamma} \exp(-zx)\, dx \tag{21}$$

where the polynomials $P_{2m}(x)$ are given by

$$P_{2m}(x) = \sum_{r=0}^{2m} b_r^{(m)} x^r \tag{22}$$

and the γ-dependent coefficients $\{b\}$ obey the recurrence relation

$$b_r^{(m+1)} = (r+2)b_r^{(m)} + (r-m)b_{r-1}^{(m)} + \gamma b_{r-2}^{(m)}, \qquad b_q^{(m)} = 0 \text{ if } q > 2m \text{ or } < 0 \tag{23}$$

with starting condition

$$b_r^{(0)} = \delta_{r0}. \tag{24}$$

Direct but tedious evaluation now shows that all $b_r^{(m)}$ are non-negative for $0 \leqslant m \leqslant 3$, and so P_0, P_2, P_4 and P_6 are certainly positive definite in $x \geqslant 0$. For $m = 4, 5$ the only negative coefficients occur when $r = 1$; by considering the lowest three powers of x in P_8 and P_{10} and completing the square, these polynomials can also be demonstrated to be positive definite in $x \geqslant 0$. From (21) derivatives of $U(2, 2-\gamma, z)$ therefore alternate in t up to at least $m = 5$. Furthermore, since the operation $-d/dt$ on (21) merely introduces a positive definite further factor $x(\gamma + z)$ into the integrand (before integration by parts) the result can be extended one value further to $m = 6$. Alternation of derivatives of H is therefore assured in (2) at least up to $n = 7$. Moreover, the 'margin of safety' by which P_{2m} is positive definite is large, at least up to $m = 5$, and the violation seems unlikely to occur for at least several values of m beyond this: it is not only necessary that P_{2m} be non-positive definite, but, more strongly, that (21) be negative for some z. That the violation is not surprising from this outlook can be seen by solving (23) for lower values of r:

$$b_0^{(m)} = 2^m, \qquad b_1^{(m)} = (m+1)2^m - 3^m. \tag{25}$$

These can be confirmed by substitution in (23): the coefficient $b_1^{(m)}$ becomes progressively more negative as m increases. The recurrence relation (23) is not solved here for arbitrary r.

Since H is completely monotonic for $t \ll 1$ (from (17), since $z \propto t$ for $t \ll 1$, and $U(2, 2-\gamma, z)$ is the Laplace transform of a positive definite function) and for $t \gg 1$ (from (10)) and tends to zero in the latter case, the number of zeros in $(-\mathrm{d}/\mathrm{d}t)^{n+1}H(t)$ either equals the number in $(-\mathrm{d}/\mathrm{d}t)^n H$ or exceeds it by an even number. The reader can quickly be convinced of this by drawing graphs of functions with these properties. Consequently if $(-\mathrm{d}/\mathrm{d}t)^N H$ is found to be positive for all time $t(\geqslant 0)$, it must be so for all $n < N$. This fact is of potential use in a numerical search for the lowest n for which violation of (2) occurs; such a study would be of considerable interest.

Finally we note that the McKean conjecture (2) is likely to be incompatible with the Krook–Wu conjecture that many solutions of the Boltzmann equation relax by first tending rapidly to the BKW mode, which then evolves according to (5). This mechanism would be likely to cause maxima and minima in the second (or higher) derivatives of the Boltzmann entropy near the time at which the transition from rapid to BKW relaxation occurs, and consequently violates (2). Although the Krook–Wu conjecture has been largely discredited (Ernst 1981) the clash is still noteworthy.

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