Extension of the Boltzmann H theorem

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I show that the Bobylev-Krook-Wu solution of the Boltzmann equation violates the inequality $(-d/dt)^n H \geq 0$ for $n \geq 102$. Thus the conjectured "super-H theorem" does not hold.

The H theorem of Boltzmann states that, for any solution $f(\vec{v},t)$ of the Boltzmann equation, the function

$$H(t;f) \equiv \int f(\vec{v},t) \ln f(\vec{v},t) d\vec{v} \tag{1}$$

will decrease monotonically with time: $dH/dt \leq 0$. This suffices to prove that any initial distribution will evolve towards an equilibrium solution as $t \to \infty$.

A possible extension of the H theorem, first discussed by McKean[1] and Harris,[2] states that *all* derivatives of $H(t)$ approach their equilibrium value of zero monotonically, e.g., that

$$\frac{(-d)^n H}{dt^n} \geq 0 \; . \tag{2}$$

Until now this very strong statement has neither been proven nor has a counterexample been found. Very recently Ziff *et al.*[3] considered in this journal the verification of (2) for one of the few available exact solutions to a realistic Boltzmann equation, namely, the Bobylev-Krook-Wu (BKW) solution[4,5] for a system of Maxwell molecules (and its generalization to d-dimensional space[6-8]). They found the expression

$$\frac{-dH}{dt} = m(m+1) \int_0^\infty dx \left[\frac{x e^{mx}}{(1+x)^{2+m}} \right] Y^2 e^{-x/Y} \tag{3}$$

[where $m = d/2$, $Y = (e^t - 1)^{-1}$, and $t > \ln(m+1)$] and were, with the help of numerical calculations, able to verify the inequality (2) for $n \leq 30$ and $1 \leq d \leq 6$.

This "physicist's induction" gives strong support for the belief that (2) must be true for all n. I therefore set out to provide a rigorous proof of (2) for all n, but found to my agony that there was always a loophole in my induction arguments, although it is fairly straightforward to show that $(-d)^n H/dt^n$ is the integral of a positive function up to $n = 25$ for all $d \geq 1$. After a while I began to suspect that the theorem was not true at all, but that one was confronted with a diabolic counterexample where it fails only for very large n. I was thus led to consider asymptotic expansions valid for large times (and all values of n). From these one easily deduces that $(-d)^n H/dt^n$ must take alternating signs when n is sufficiently large. I find this first to occur when n is greater than a critical value $n_c(d)$, where $n_c(d)$ is about 100 for small dimensionalities d.

In the remaining of this note I shall first outline the analytic proof of (2) for $n \leq 25$, and then derive the asymptotic expansions which disproves it for large n.

I. PROOF FOR $n \leq 25$

By use of the identity

$$\frac{-d(Y^n e^{-x/Y})}{dt} = \left[n - x \frac{d}{dx} \right] (Y^{n+1} + Y^n) e^{-x/Y} \tag{4}$$

and a partial integration one can prove by induction that

$$\frac{(-d)^{n+1} H}{dt^{n+1}} = \sum_{k=0}^{n} \sum_{l=2}^{2+n} A_{k,l}^n \int_0^\infty dx \, \rho_k(x) Y^l e^{-x/Y} , \tag{5a}$$

where $A_{k,l}^n \geq 0$, and where

$$\rho_k(x) \equiv [P_k(x) e^{mx}/(1+x)^{2+m+k}] = \left[3 + x \frac{d}{dx} \right]^k [x e^{mx}/(1+x)^{2+m}] \; . \tag{5b}$$

Therefore, if $P_k(x) \geq 0$ for $k \leq N-1$ (and $x \geq 0$), then the inequality (2) must be true for $n \leq N$. By direct evaluation

$$P_1(x)=4x+2x^2+mx^3\,,$$
$$P_2(x)=16x+14x^2+(4+10m)x^3+5mx^4+m^2x^5\,, \tag{6a}$$
$$\ldots$$

up to P_7, only positive terms occur. But

$$P_8(x)=65\,536x-125\,890x^2+(1\,682\,258+4\,907\,776m)x^3+\cdots\,, \tag{6b}$$

where the ellipses represents positive terms. However, by completing squares one can easily show that $P_8(x)\geq 0$ for $x\geq 0$. With further analysis one also finds $P_k(x)\geq 0$ for $k=9$, 10, and 11. Alas, setting $m=0$, it turns out that $P_{12}(x)$ becomes negative over a certain interval. For positive dimensions ($d=2m$) P_{12} is still positive, but when we continue the process to sufficiently high k the method again fails. For instance, with $d=1$ we find that $P_k(x)\geq 0$ for $k\leq 17$, but that $P_{18}(x)$ does take negative values.

In this way one can show that only positive quantities A,ρ will occur in Eq. (5a) up to $n=17$ (for $d\geq 1$).

This proves that the generalized H theorem (2) holds up to $n=18$, and this does not quite exhaust our resources. We set $n=17$ in Eq. (5a) and continue to differentiate, now using the identity

$$\frac{-d(Y^l e^{-x/Y})}{dt}=[lY^{l+1}+(l+x)Y^l+xY^{l-1}]e^{-x/Y}\,. \tag{7}$$

Repeated applications of this leads to an expression

$$\frac{(-d)^{n+18}H}{dt^{n+18}}=\sum_{k=0}^{17}\sum_{l=2}^{19}A_{k,l}^n\int_0^\infty dx\,\rho_k(x)Q_n^l(x,Y)e^{-x/Y}\,, \tag{8a}$$

where $A_{k,l}^n\geq 0$, $\rho_k(x)\geq 0$, and where

$$Q_n^l(x,Y)=e^{x/y}\frac{(-d)^n Y^l e^{-x/Y}}{dt^n} \tag{8b}$$

is a polynomial in x and a rational function in Y. Thus, as long as all the Q_n^l are positive, only positive terms will occur in (8a) and (2) must be true. Now it is obvious from the recursion (7) that $Q_n^l\geq 0$ for $n\leq l+1$ and that $Q_n^2\geq 0$ implies $Q_{n+k}^{2+k}\geq 0$. It is therefore sufficient to investigate $Q_n^2(x,Y)$, which must be positive at least up to $n=3$. By direct evaluation we find that Q_4^2 and Q_5^2 contain only terms with positive coefficients. Proceeding to Q_6^2 this is no longer true, since

$$Q_6^2(x,Y)=x^6Y^{-4}+(-3x^5+6x^5)Y^{-3}+(5x^4-3x^5+15x^6)Y^{-2}+\cdots\,, \tag{9}$$

where again the ellipsis represents positive terms, but a short analysis shows that this expression is still positive. The same holds true for Q_7^2. However, $Q_9^2(x,Y)$ is found to take negative values, and then this method breaks down. (Q_8^2 I have not analyzed completely.) Combined, the two methods prove (2) for $n\leq 25$ for all $d\geq 1$ and with still some room left for improvement.

II. DISPROOF FOR LARGE n

However, having twice seen the failure of physicist's induction, one looses some faith in the general validity of (2). Since it follows from the recursion (7) that only those terms in Q_n^l which contain negative powers of Y can be negative, the conjecture seems most likely to fail for small values of Y, i.e., for large times. This suggests that one study the asymptotic expansions of $(-d)^nH/dt^n$ in the large-t region for all values of n. I first find the asymptotic series for the integral (3), and by use of the recursion (7) it is straightforward to derive the general expansion. I have done so explicitly up to order Y^{13}, and find it to be of form

$$\frac{(-d)^{n+1}H}{dt^{n+1}}=m(m+1)Y^4\{4^n-4^{n+1}Y+[(8+3m)6^n+10\cdot 4^n]Y^2-[(28+14m)7^n+\cdots]Y^3+[(201+129m+15m^2)8^n+\cdots]Y^4-[(1424+1072m+180m^2)9^n+\cdots]Y^5+\cdots+(-)^l[a_l(3+l)^n+b_l(2+l)^n+\cdots]Y^l+\cdots\}\,, \tag{10}$$

where $a_l, b_l, \ldots$ are polynomials in m with positive coefficients. If one evaluates this series at the point $Y = \exp[-n/(3+k)]$, i.e., for a time of order n, and then let $n \rightarrow \infty$, one finds that the term with $l = k$ will dominate the sum, giving the leading order result

$$\frac{(-d)^{n+1}H}{dt^{n+1}} \simeq m(m+1)[(-1)^k a_k (3+k)^n \times e^{-nk/(3+k)}] \quad (11)$$

when $t \simeq n/(3+k)$. This shows that when n becomes larger and larger, the derivative series (10) must become an increasingly oscillating function of time, in violation of the inequality (2).

It is also of interest to find the lowest value of n for which $(-d)^n H/dt^n$ becomes negative. Clearly, one can trust the series (10) only in the asymptotic region, but I have reason to believe that this is precisely where the first zero occurs.

A first estimate can be found by considering the balance between the terms with $l = 2$, 3, and 4. By analyzing this quadratic form, one finds that it takes negative values only when

$$(\tfrac{49}{48})^{n-1} \geq \frac{(8+3m)(201+129m+15m^2)}{(14+7m)^2}, \quad (12)$$

which leads to the estimate $n_{cr} \simeq 108$ for $d = 3$. This formula also gives a mathematical explanation for why the inequality (2) breaks down only for such a very large n.

In order to get accurate results I have evaluated the series (10) numerically, taking into account all terms up to order $l = 9$. This predicts the critical value to be $n_{cr} = 97$, 98, 100, 102, 105, 107, and 109 when the dimension $d = 2m = 0$, 1, 2, 3, 4, 5, and 6, respectively. In Fig. 1 I also plot $(-d)^n H/dt^n$ in the relevant region of time for $n = 102$ and $d = 3$ (i.e., the original BKW solution). The expansion (10) seems to be very accurate in this region, the last term (for $l = 9$) giving a contribution of relative order 10^{-7}. One can therefore have good

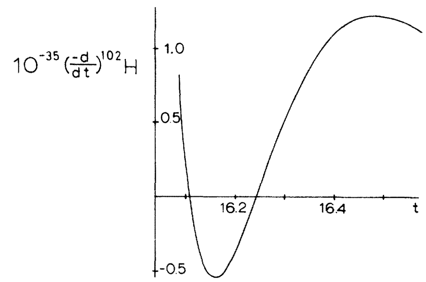

FIG. 1. The 102nd derivative of H plotted as a function of t for $d = 3$.

faith in the results predicted by (10).

In conclusion, I have shown for the (generalized) BKW solutions:

(i) that they satisfy the extended H theorem (2) for all $n \leq 25$ and $d \geq 1$ (rigorous proof),

(ii) that they violate it when n exceeds a critical value $n > n_{cr}(d)$. [For complete rigor one must provide error bounds for the asymptotic series (10), but that is certainly possible.];

(iii) that $n_{cr}(d) \geq 98$ for $d \geq 1$, and increases with d. (This depends upon the unproven assertion that the first zero will develop inside the validity region of the asymptotic series.)

Thus, the "super-H theorem" is disproven, but (although mathematically explained) it still remains a puzzle why it holds to such a very high value of n. Is this a general property of *all* solutions to the Boltzmann equation? In future work one must settle for less ambitious goals: Can an extended H theorem (2) be proven, in general, for values of n greater than 1? Can one find new counterexamples with lower critical values n_{cr}?

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