Journal of Statistical Physics, Vol. 32, No. 1, 1983

The Entropy of the BKW Solution

Christian J. Tourenne[1]

Received August 27, 1982; revised February 1, 1983

The entropy of the d-dimensional generalization of the BKW solution of the homogeneous Boltzmann equation is calculated and expressed for $d = 3$ in terms of error functions. It is verified that the McKean conjecture cannot hold in most of the time domain where the d-dimensional BKW solution is defined.

KEY WORDS: Boltzmann entropy; BKW solution; hypergeometric function; McKean conjecture.

1. INTRODUCTION

A few years ago, Bobylev[1] and Krook and Wu[2] found an exact analytical solution (the BKW solution) of the full nonlinear Boltzmann equation for the case where the intermolecular differential cross section is inversely proportional to the molecular relative velocity. As discussed by Ernst,[3] the BKW solution has caused an enormous revival of interest in the field of the kinetic theory of gases, because it describes the manner in which a dilute gas of Maxwell molecules approaches equilibrium.

More recently, Ernst[4] and Ziff[5] obtained a d-dimensional generalization of the BKW solution given by

$$f(v,t) = A\exp(-Bv^2/2)(C + Dv^2/2) \tag{1}$$

where $A = 1/(2\pi\beta^2\kappa)^p$, $B = 1/\kappa\beta^2$, $C = [\kappa + (\kappa - 1)p]/\kappa$, $D = (1-\kappa)/\beta^2\kappa^2$, $\kappa = 1 - e^{-t}$, $\beta^2 = kT/m$, and $p = d/2$. The time t has been scaled by a constant which depends upon the angular dependence of the differential scattering cross section. The requirement that $f(v,t)$ be positive implies that $t \geqslant \ln[(d+2)/2]$.

---

[1] Physics Department, Maharishi International University, Fairfield, Iowa 52556.

According to Boltzmann's H-theorem, the approach to equilibrium for any solution of the Boltzmann equation is accompanied by a monotonic increase in the value of the Boltzmann dimensionless entropy

$$S(t) = -H(t) = -\int f(v,t) \ln f(v,t)\, d\mathbf{v} \tag{2}$$

Therefore Boltzmann's H-theorem states that $dS/dt \geqslant 0$, the equality holding at equilibrium. McKean[6] and Harris[7] have conjectured that $S(t)$ is a completely monotonic and therefore uniquely defined function, and all of its derivatives alternate in sign

$$(-1)^n d^n S/dt^n \leqslant 0 \qquad \text{for all } n \tag{3}$$

and approach their zero equilibrium value with no change in sign.

A few years ago, the validity of the alternating derivative property (the McKean conjecture) was shown to hold for any solution of the linearized Boltzmann equation,[8-10] which is valid close to equilibrium, but does not hold for a solution of the Bhatnager–Gross–Krook (BGK) equation for Maxwell molecules.[11]

Because, until recently, no general proof of (3) or counterexample had been found for a spatially homogeneous solution of the Boltzmann equation, the investigation of whether the McKean conjecture would hold for the BKW solution was undertaken. Rouse and Simons[12] showed that for $d = 3$, the second time derivative of the Boltzmann entropy of the BKW solution remains negative during the passage to equilibrium. The integrals involved in the calculation of d^2S/dt^2 were computed numerically but no direct calculation of $S(t)$ or dS/dt appeared in their paper.

More recently, Ziff *et al.*[13] noticed that the integrals contained in the explicit expression of the Boltzmann entropy of the d-dimensional BKW solution could not be evaluated in a closed form. They were, however, able to express dS/dt as a hypergeometric function; the same result was obtained by Garret.[14] Ziff *et al.* computed numerically higher derivatives of $S(t)$ showing that (3) holds for n up to 30 and $1 \leqslant d \leqslant 6$.

By using a theorem on the properties of completely monotonic functions, Lieb[15] recently showed that the McKean conjecture cannot hold for the d-dimensional generalization of the BKW solution. The result was confirmed by Olaussen,[16] who, by an asymptotic analysis, showed for $d = 3$ that (3) breaks down for $n = 102$ and for $t = 15$.

In this paper, we start from the d-dimensional BKW solution and define from it a function of a parameter λ whose λ derivative evaluated at $\lambda = 0$ equals the Boltzmann entropy. This trick is also used in the replica method.[17,18] We calculate the parametric function in Section 2. In Section 3, we show how the entropy of the three-dimensional BKW solution can be derived in a closed form by using error functions. In Section 4, we calculate the time derivative of the d-dimensional BKW entropy from the parametric function and show that it is identical to the one calculated by Ziff *et al.*[13] and Garret.[14] In Section 5, we derive an expression for the BKW entropy valid for most of the domain where the d-dimensional BKW solution is defined, and check that for $t > \ln[(d+4)/2]$ and for all d, the McKean conjecture cannot be true.

2. PARAMETRIC FUNCTION FOR THE d-DIMENSIONAL BKW DISTRIBUTION FUNCTION

Considering a nonequilibrium distribution function $f(v,t)$, we define the following parametric function:

$$\Phi(\lambda) = \int \left[f(v,t) \right]^{1-\lambda} d\mathbf{v} \tag{4}$$

where $0 \leqslant \lambda < 1$. The Boltzmann entropy can be easily calculated by taking the derivative of $\Phi(\lambda)$

$$S(t) = -\int f(v,t) \ln f(v,t)\, d\mathbf{v} = \left[\partial\Phi(\lambda)/\partial\lambda \right]_{\lambda=0} \tag{5}$$

When $f(v,t)$ is the d-dimensional generalization of the BKW solution, the corresponding parametric function $\phi(\lambda)$ can be written as

$$\Phi(\lambda) = (2\pi)^p/\Gamma(p) A^{1-\lambda} \int_0^\infty u^{p-1} (C + Du)^{1-\lambda} e^{-B(1-\lambda)u}\, du$$

where $u = v^2/2$ and $2\pi^p/\Gamma(p)$ is the surface area of a d-dimensional unit sphere. By performing the change of variable $z = B(1-\lambda)u$ and writing $X = BC/D$, the integral becomes a simple confluent hypergeometric function and the parametric function is represented by

$$\Phi(\lambda) = CX^p (AC)^{-\lambda} U\{p, p+2-\lambda, X(1-\lambda)\} \tag{6}$$

3. THE ENTROPY OF THE BKW SOLUTION

Using the definition of the confluent hypergeometric function in terms of Γ functions

$$U(a,b,z) = \frac{\pi}{\sin(\pi b)} \frac{1}{\Gamma(a)\Gamma(1+a-b)} \times \sum_{k=0}^{\infty} \left[\frac{\Gamma(k+a) z^k}{\Gamma(k+b)\Gamma(k+1)} - \frac{\Gamma(1+a-b+k) z^{k+1-b}}{\Gamma(2-b+k)\Gamma(k+1)} \right]$$

It is easy to derive the following expansion for the confluent hypergeometric function contained in (6) when p takes on half-integer values:

$$
\begin{aligned}
U\{p, p+2-\lambda, X(1-\lambda)\}
&= U(p, p+2, X) + (-1)^{p+1/2}\pi\lambda \\
&\times \left\{ \frac{M(p,p+2,X)}{\Gamma(p+2)} - \sum_{k=0}^{\infty} \frac{X^{k+1-p}}{(k+1)(k+2)\Gamma(p)\Gamma(k-p+2)} \right. \\
&\quad + \frac{X^{-p-1}[\ln X - \Psi(-p) - p - 1]}{\Gamma(p)\Gamma(-p)} \\
&\quad \left. - \frac{X^{-p}[\ln X + \Psi(1-p) - p + 1]}{\Gamma(p)\Gamma(1-p)} \right\} + O(\lambda^2)
\end{aligned} \tag{7}
$$

When p takes on integer values, it is still possible to expand $U\{p, p+2-\lambda, X(1-\lambda)\}$ as a function of λ, although the expansion is more complicated and is not of much interest for this paper.

We now intend to find an explicit expression for the BKW entropy when $p = 3/2$. By using (6) and (7), it is possible to derive the following expansion:

$$
\begin{aligned}
\Phi(\lambda) = 1 + \lambda \Bigg\{ \Bigg[\left(\frac{8\sqrt{\pi}}{15} \right) M\left(\frac{3}{2}, \frac{7}{2}, X \right) \\
- 2\sqrt{\pi} \sum_{k=0}^{\infty} \frac{X^{k-1/2}}{(k+1)(k+2)\Gamma(k+1/2)} \Bigg] C X^{3/2} \\
+ \ln\left(\frac{X}{AC} \right) + \left(\frac{2C}{X} \right) + \gamma + 2\ln 2 - \frac{3}{2} \Bigg\} + O(\lambda^2)
\end{aligned} \tag{8}
$$

where $M(3/2, 7/2, X)$ is a hypergeometric Kummer function. By then using three of its properties contained in standard tables,[19] it can be transformed into

$$
\begin{aligned}
M(3/2, 7/2, X) \\
= (5/2X)[(9/2)M'(1/2, 3/2, X) - (3/2)M(1/2, 3/2, X)]
\end{aligned} \tag{9}
$$

On the other hand, it is easy to show that

$$
M(1/2, 3/2, X) = (1/2)[(\pi/X)^{1/2}] e^X I[W(\sqrt{X})] \tag{10}
$$

where $I[W(\sqrt{X})]$ represents the imaginary part of the complex error function $W(\sqrt{X})$.[19] By taking the derivative of (10) and then using (9) and

(10), we get

$$M(3/2,7/2,X) = (15/8)X^{-3/2}e^X \times \left\{(3/2\sqrt{\pi})X^{-1/2} - (\sqrt{\pi}/C)I\left[W(\sqrt{X})\right]\right\} \quad (11)$$

We now transform the series in (8) into a closed form; for that purpose, let us look at the following series:

$$\sum_{k=0}^{\infty} \frac{X^{k+2}}{(k+1)(k+2)\Gamma(k+1/2)} = -\frac{1}{2}\sum_{k=0}^{\infty}\frac{X^{k+2}}{(k+1)\Gamma(k+3/2)} + \frac{3}{2}\sum_{k=0}^{\infty}\frac{X^{k+2}}{(k+2)\Gamma(k+3/2)} \quad (12)$$

The first series in (12) can be written

$$X\sum_{k=0}^{\infty}\frac{X^{k+1}}{(k+1)\Gamma(k+3/2)} = f(X)$$

By differentiating both sides of the last equation, we find a first-order differential equation that can be easily solved by using error functions. We get

$$f(X) = \sqrt{\pi}XI\left[W(\sqrt{X})\right]\left(e^X \operatorname{erf}\sqrt{X} - \sqrt{X}\right) + Xe^X \quad (13)$$

The second series in (12) can be transformed and expressed in terms of $f(X)$:

$$\sum_{k=0}^{\infty}\frac{X^{k+2}}{(k+2)\Gamma(k+3/2)} = \sqrt{X}\,e^X \operatorname{erf}\sqrt{X} - \frac{\frac{1}{2}f(X)}{X} - \frac{X}{\sqrt{\pi}} \quad (14)$$

Putting the results (13) and (14) back into (12), rearranging terms, and using (8), we find the Boltzmann entropy of the BKW solution:

$$\begin{aligned} S(t) &= \gamma + 2\ln 2 - 3/2 + \ln(X/AC) + (2C/X)\left[1 + (3/2)X\right] \\ &\quad + \pi I\left[W(\sqrt{X})\right]\left[C\left(e^X\operatorname{erf}\sqrt{X} - \sqrt{X}\right)(1 + 3/2X) - e^X\right] \\ &\quad + e^X\left\{\sqrt{\pi}\,C\left[1 + 3/2X - (3\sqrt{X})\operatorname{erf}\sqrt{X}\right] + 3C/2\sqrt{X}\right\} \end{aligned} \quad (15)$$

4. THE TIME DERIVATIVE OF THE *d*-DIMENSIONAL BKW ENTROPY

The interest of Eq. (15) is in showing that the entropy of the BKW solution can be expressed in closed form, which was thought to be impossible by Rouse and Simons[12] and Ziff *et al.*[13] because of the logarithmic integrals in (2).

Starting now from the parametric function (6) for the d-dimensional BKW distribution, which can be more easily handled and which is more general than (15), we intend to find the time derivative of the entropy; from (6), it is straightforward to derive

$$\begin{aligned} S(t) &= \{\partial\Phi(\lambda)/\partial\lambda\}_{\lambda=0} \\ &= -\ln AC + p(1 + D/B) - CX^p\{(\partial/\partial\lambda)U(p, p+2-\lambda, X)\}_{\lambda=0} \end{aligned} \tag{16}$$

Now, replacing A, B, C, D as functions of t, taking the time derivative of $S(t)$ and transforming the confluent hypergeometric function by using some of its properties[19] we find after rearranging terms

$$\begin{aligned} dS/dt &= \left[-p/(e^t-1)^2\right] + \left[e^t/(e^t-1)^2\right]X^p \\ &\quad \times \{(\partial/\partial\lambda)[U(p+1, p+2-\lambda, X) - pU(p, p+1-\lambda, X)]\}_{\lambda=0} \end{aligned}$$

If we integrate the integral form of $U(p+1, p+2-\lambda, X)$ by parts, the λ derivatives cancel out and the time derivative of the entropy takes the form

$$\frac{dS}{dt} = \frac{-p}{(e^t-1)^2} + \frac{e^t}{\Gamma(p)(e^t-1)^2}\int_0^\infty \frac{u^p e^{-u}}{(u+X)}\,du$$

which can be rearranged by again integrating by parts, and lead us to the result

$$\frac{dS}{dt} = \frac{1}{\Gamma(p)(e^t-1)^2}\int_0^\infty \frac{u^{p+1}e^{-u}}{(u+X)^2}\,du \tag{17}$$

in accordance with the results of Garret[14] and Ziff *et al.*[13]

5. d-DIMENSIONAL BKW ENTROPY AND MCKEAN CONJECTURE

From the definition of the confluent hypergeometric function

$$U(a,b,z) = \frac{z^{-a}}{\Gamma(a)}\int_0^\infty s^{a-1}\left(1+\frac{s}{z}\right)^{b-a-1} e^{-s}\,ds$$

it is possible to show that in the following expansion

$$\begin{aligned} U(a,b,z) = z^{-a}\Bigg[&\sum_{n=0}^{N}(-1)^n (a)_n \frac{(a-b+1)_n}{n!}\frac{1}{z^n} \\ &+ \frac{1}{\Gamma(a)}\int_0^\infty s^{a-1}R_N(s,z)e^{-s}\,ds\Bigg] \end{aligned} \tag{18}$$

where

$$(a)_n = a(a+1)(a+2)\cdots(a+n-1)$$

$$(a-b+1)_n = (a-b+1)(a-b+2)\cdots(a-b+n)$$

and

$$R_N(s,z) = \frac{(b-a-1)(b-a-2)\cdots(b-a-N)}{N!}\left(1+\frac{s}{z}\right)^{b-a-1} \times \int_0^{s/z} r^N(1+r)^{a-b}\,dr$$

the integral contained in (18) is of the order of $1/z^{N+1}$ and converges when $|z| > 1$, for real z, and when $N + a - 1 > 0$.[20] Therefore, for $p > 0$ and for $X > 1$ $\{t > \ln[(d+4)/2]\}$, we can expand $U(p, p+2-\lambda, X(1-\lambda))$ in the following series:

$$U\{p, p+2-\lambda, X(1-\lambda)\} = X^{-p}\sum_{k=0}^{\infty}\frac{p(p+1)(p+2)\cdots(p+k-1)}{k!} \times \frac{[1+1/(\lambda-1)][1+2/(\lambda-1)]\cdots[1+(k-1)/(\lambda-1)]}{X^k} \tag{19}$$

By inserting (19) into (6), expanding $\Phi(\lambda)$ in terms of λ, we get an expression for the BKW entropy valid for all p and for all $t > \ln[(d+4)/2]$

$$\begin{aligned} S(t) &= \left\{\frac{\partial\Phi(\lambda)}{\partial\lambda}\right\}_{\lambda=0} \\ &= p - \ln A_0 + (p+1)\ln(1-e^{-t}) - \ln[1-(p+1)e^{-t}] \\ &\quad + \frac{X}{e^t-1}\sum_{k=2}^{\infty}(-1)^{k+1}\frac{a_k}{X^k} \end{aligned} \tag{20}$$

where $A_0 = 1/(2\pi\beta^2)^p$ and $a_k = p(p+1)(p+2)\cdots(p+k-1)/k(k-1)$.

It is easy to verify that $S_{\text{eq}} = p - \ln A_0$ represents the equilibrium value of a d-dimensional generalization of a Maxwell Boltzmann distribution, because, from (20), it is obvious that

$$\lim_{t\to\infty}[S(t) - S_{\text{eq}}] = 0$$

If we now expand (20) in powers of e^{-t} and separate the even from the odd terms in the series contained in (20), we can write the nth derivative in respect to time of the d-dimensional BKW entropy as

$$(-1)^n \frac{d^nS}{dt^n} = \sum_{q=1}^{\infty} a_{2q} e^{-2qt} \Bigg[b_{2q}(2q)^n + b_{2q+1}(2q+1)^n e^{-t} + \sum_{m=0}^{\infty} c_m(2q) e^{-mt} \times \Big((m+2q+1)^n (m+2q)\alpha(q) e^{-t} - (m+2q)^n + \sum_{m'=0}^{\infty} p e^{-(m'+1)t} \big[(m+m'+2q+1)^n - (m+m'+2q+2)^n \times (m+2q)\alpha(q) e^{-t} \big] \Big) \Bigg] \tag{21}$$

where $b_{2q} = [(p+1)/2q][(p+1)^{2q-1} - 1)$, $c_m(2q) = (p+1)^m(2q)(2q+1)\cdots(2q+m-1)/m!$ and $\alpha(q) = (p+2q)(2q-1)/[(2q)(2q+1)]$.

We can think of two simultaneous conditions that, if obeyed, would lead to a violation of the McKean conjecture:

$$\frac{t - \ln[Y\alpha(q)]}{\ln[(Y+1)/Y]} < n < \frac{[t - \ln(Y\alpha(q))]}{\ln[(Y+2)/(Y+1)]} \tag{22}$$

where $Y = m + 2q$; the couple of conditions in (22) would, then, make the sums over m and m' in (21) both positive. Considering that $\alpha(q) \to 1$ when q increases, we immediately see that the two functions of Y on both sides of n in (22) will admit a maximum for $Y = Y_M$, Y_M being a little bit less than e^t in both cases. The two maxima being close from each other, we can expect that, for $Y > Y_{M1}$ (Y_{M1} being the maximum of the function of Y on the left), the first condition on the left in (22) will continue to be satisfied but that the second inequality will not.

For $Y > Y_{M1}$, therefore, we have to find another set of conditions in order for the two sums over m and m' in (21) to be positive. For that, let us look at the following group of terms:

$$\sum_1 (Y) = p \sum_{m'=0}^{\infty} e^{-(m'+1)t} (Y+m'+1)^n - Y^n = Y^n \left[p \sum_{m'=0}^{\infty} S(m', Y) - 1 \right] \tag{23}$$

where

$$S(m', Y) = e^{-(m'+1)t}\left[1 + \frac{n(m'+1)}{Y} + \frac{n(n-1)(m'+1)^2}{Y^2 2!} + \cdots\right]$$

Now, let us consider the following group of terms:

$$\sum_2 (Y) = \alpha(q) Y e^{-t}\left[(Y+1)^n - p \sum_{m'=0}^{\infty} e^{-(m'+1)t}(Y + m' + 2)^n\right]$$

which can be written

$$\sum_2 (Y) > \alpha(q) Y e^{-t}(Y+1)^n\left[1 - p \sum_{m'=0}^{\infty} S(m', Y)\right] \tag{24}$$

By combining (23) and (24), we have

$$\begin{aligned}\sum (Y) &= \sum_1 (Y) + \sum_2 (Y)\\ &> \left[\alpha(q) Y e^{-t}(Y+1)^n - Y^n\right]\left[1 - p \sum_{m'=0}^{\infty} S(m', Y)\right]\end{aligned}$$

By approximating the series, we find

$$\sum (Y) > \left[\alpha(q) Y e^{-t}(Y+1)^n - Y^n\right]\left[1 - p/(e^{t-n/Y} - 1)\right] \tag{25}$$

We can see that $\sum(Y)$ is equal to the sum of terms in m of (21); it is easy to check now that the only set of conditions that would make $\sum(Y)$ positive and that would be compatible with the first condition on the left of (22) are

$$\frac{t - \ln[Y\alpha(q)]}{\ln[(Y+1)/Y]} < n < Y[t - \ln(p+1)] \tag{26}$$

It is obvious that the second condition on the right of (26) can be satisfied for all $Y > Y_{M1}$. Therefore, if n satisfies (26) with $Y = Y_{M1}$, we can predict that the McKean conjecture will be violated for all $t > \ln(p+2)$.

6. CONCLUSION

This work contributes to and confirms some already known results concerning the BKW solution. We have been able to express the Boltzmann entropy of the BKW solution in closed form in terms of error functions. The calculation of the entropy for integer values of p should also be interesting since it includes for $p = 1$, the Tjon–Wu model;[21] it will be done in a separate publication. The series expansion of the nth derivative in respect to time of the d-dimensional BKW entropy also confirms Lieb's result,[15] showing that this particular Boltzmann entropy is not a completely monotonic function.

REFERENCES

1. A. V. Bobylev, *Sov. Phys. Dokl.* **20**:820 (1976).
2. M. Krook and T. T. Wu, *Phys. Rev. Lett.* **36**:1107 (1976).
3. M. H. Ernst, in *Fundamental Problems in Statistical Mechanics V*, E.G.D. Cohen, ed. (North Holland, Amsterdam, 1980).
4. M. H. Ernst, *Phys. Lett.* **69A**:390 (1979).
5. R. M. Ziff, *Phys. Rev. A* **23**:916 (1981).
6. H. P. McKean, *Arch. Ration. Mech. Anal.* **21**:343 (1966).
7. S. Harris, *J. Math. Phys.* **8**:2407 (1967).
8. S. Harris, *J. Chem. Phys.* **48**:4012 (1968).
9. S. Simons, *J. Phys.* **A2**:12 (1969).
10. S. Simons, *Phys. Lett.* **33A**:154 (1970).
11. S. Simons, *J. Phys.* **A5**:1537 (1972).
11. S. Rouse and S. Simons, *J. Phys.*, **A11**:423 (1978).
13. R. M. Ziff, S. D. Merajver, and G. Stell, *Phys. Rev. Lett.* **47**:1493 (1981).
14. G. Garret, *J. Phys.* **A15**:L351 (1982).
15. E. H. Lieb, *Phys. Rev. Lett.* **48**:1057 (1982).
16. K. Olaussen, *Phys. Rev. A* **25**:3393 (1982).
17. D. Sherrington and S. Kirkpatrick, *Phys. Rev. Lett.* **35**:1792 (1975).
18. V. J. Emery, *Phys. Rev. B* **11**:239 (1975).
19. M. Abramowitz and I. Stegun, *Handbook of Mathematical Formulas* (US Government Printing Office, Washington, D.C., 1965).
20. E. T. Whittaker and G. N. Watson, *A Course of Modern Analysis* (Cambridge University Press, Cambridge, 1963).
21. J. Tjon and T. T. Wu, *Phys. Rev. A* **19**:883 (1979).