Journal of Statistical Physics, Vol. 41, Nos. 1/2, 1985

A Method to Calculate Boltzmann Entropy

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Received January 11, 1985; revision received May 20, 1985

A method is proposed to calculate the Boltzmann non equilibrium entropy as a Taylor series expansion in terms of the successive moments of the velocity distribution function. As a first application, the entropy of the BKW solution of the Boltzmann equation is calculated for both even and odd dimensions. The properties of the entropy of the Tjon Wu model ($d=2$) are studied and a quantitative condition is derived, showing that the McKean conjecture is incorrect. As a second application of the method, the entropy of one of the solutions of the very hard particle model for the Boltzmann equation is also derived.

KEY WORDS: Boltzmann entropy; BKW solution; McKean conjecture; VHP model.

1. INTRODUCTION

The Boltzmann nonequilibrium dimensionless entropy for an evolving system of similar particles described by a velocity distribution $f(v, t)$ in d dimensions is given by

$$S(t) = -H(t) = -\int f(v, t) \ln f(v, t)\, d^d v \tag{1}$$

From the knowledge of $S(t)$ it is possible to analyze the process of a system relaxing toward equilibrium and to study near equilibrium states.[1] 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 entropy ($dS/dt \geqslant 0$). A possible extension of the H theorem, first discussed by McKean[2] and Harris[3]

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0022-4715/85/1000-0335$04.50/0

states that all derivatives of $S(t)$ approach their equilibrium value of zero monotonically:

$$(-1)^n \, d^nS/dt^n \leqslant 0 \tag{2}$$

implying an "infinitely smooth" approach to equilibrium. This alternating derivative property (known in the literature as the McKean conjecture) has stimulated some controversy. It was shown to hold for any solution of the linearized Boltzmann equation[4–6] but not to hold for a solution of the Bhatnager–Gross–Krook (BGK) equation for Maxwellian molecules.[7] Because, until recently, no general proof of (2) had been found, investigations into whether or not the McKean conjecture would hold for an exact solution of the full nonlinear Boltzmann equation (BE) were undertaken. In recent years some exact solutions of the nonlinear BE have indeed been found for two kinds of homogeneous systems described, respectively, by the Maxwell and very hard particle models.[8] A few years ago Bobylev[9] and Krook and Wu[10] found an exact analytical solution (the BKW solution) of the nonlinear BE for the case where the intermolecular differential cross section is inversely proportional to the molecules' relative velocity. More recently, Ernst[11] and Ziff[12] obtained a d-dimensional generalization of the BKW solution given by

$$f(v, t) = \exp(-v^2/2\alpha)[(2\alpha - d + d\alpha)/2\alpha + v^2(1-\alpha)/2\alpha^2]/(2\pi\alpha)^{d/2} \tag{3}$$

where $\alpha = 1 - e^{-t}$ and is valid for $t \geqslant \ln[(d+2)/2]$. The time, t, has been scaled by a constant which depends upon the angular dependence of the differential cross section.

For $d = 3$, Rouse and Simons[13] have found that the second time derivative of the BKW solution remains negative in approaching equilibrium. The integrals involved in the calculation of d^2S/dt^2 were evaluated numerically, but no direct calculation of $S(t)$ or dS/dt appeared in their paper. Ziff *et al.*[14] were able to express the first time derivative of the d-dimensional BKW solution in a closed form, but they said in their paper that the logarithmic integral contained in $S(t)$ could not be calculated in closed form. They computed numerically higher derivatives of $S(t)$ showing that the McKean conjecture holds for n up to 30 and for $1 \leqslant d \leqslant 6$.

Contrary to the above studies, Lieb[15] recently showed, by using a theorem on the properties of completely monotonic functions, that the McKean conjecture cannot hold for the d-dimensional BKW solution. The result was confirmed by an asymptotic analysis by Olaussen,[16] who showed that for $d = 3$, (2) breaks down for $n = 102$ and for $t = 15$. For all d, the same conclusion was obtained analytically by Garrett.[17] The last three papers contain a derivation of the first time derivative of $S(t)$ as a starting point, but none of these authors was able to derive $S(t)$ in closed form for the d-dimensional BKW solution. Recently, however, the author,[18] using error functions, has been able to calculate in closed form the Boltzmann entropy of the BKW solution for $d = 3$. Garrett's result with regard to the violation of the McKean conjecture was also analytically confirmed for all dimensions.

As Garrett mentioned in his paper,[17] the numerical search for the lowest n, for which violation of the McKean conjecture occurs, would be of considerable interest. No such evaluation has ever been found yet. Also, the calculation in closed form of the Boltzmann entropy of the BKW solution still remains to be done for all d.

In this paper, a general method to calculate Boltzmann non-equilibrium entropy is presented. The entropy is expanded in a Taylor series as a function of the successive moments of the velocity distribution function. This method is general enough to be applicable to a large class of distribution functions and could give the entropy in closed form every time the infinite series obtained converges. As a first application of the method, the entropy of the d-dimensional BKW solution is calculated in closed form (valid for $t > \ln[(d+4)/2)]$ with two different results for odd and even values of d. A simple expression for the entropy of the Tjon–Wu model ($d = 2$) is derived and as a way of checking the result, dS/dt is calculated and compared to previous results. An approximate but sufficient condition is derived for which the McKean conjecture is necessarily violated for $d = 2$ and an approximate value of n for which this occurs is calculated; the method can be easily extended to all values of d. Then, as a second application of the entropy calculation method, the entropy of a particular exact solution of the VHP model is calculated for which the initial distribution function is a superposition of two Maxwellians.

2. BOLTZMANN ENTROPY AS A MOMENT SERIES EXPANSION

For any nonequilibrium distribution function $f(v, t)$, the function $g(v, t) = \ln[f(v, t)]$ is defined and it is expanded around a particular value of the velocity (a) in a Taylor series:

$$g(v, t) = \sum_{k=0}^{\infty} \left(\frac{\partial^k g}{\partial v^k}\right)_a \frac{(v-a)^k}{k!}$$

The Boltzmann entropy $S(t)$ can be expressed

$$S(t) = -\sum_{k=0}^{\infty} \left(\frac{\partial^k g}{\partial v^k}\right)_a \frac{1}{k!} \int f(v, t)(v-a)^k \, d^d v$$

which, for $a = 0$, takes the form

$$S(t) = -\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{\partial^k g}{\partial v^k}\right)_0 m_k(t) \tag{4}$$

where $m_k(t)$ is the moment of order k of $f(v, t)$.

In this paper it is shown that in certain cases, Eq. (4) gives a useful method to calculate the Boltzmann entropy whenever the logarithmic integral contained in (1) cannot be found in standard tables.[19,20]

3. THE BKW SOLUTION

The d-dimensional BKW solution is written

$$f(v, t) = A(C + Dv^2/2) \exp(-Bv^2/2) \tag{5}$$

in which $A = 1/(2\pi\alpha)^p$, $B = 1/\alpha$, $C = (\alpha - p + p\alpha)/\alpha$, $D = (1-\alpha)/\alpha^2$, and $p = d/2$. The corresponding function $g(v, t)$ is then

$$g(v, t) = \ln A - Bv^2/2 + \ln(C + Dv^2/2) \tag{6}$$

The successive derivatives of $g(v, t)$ with respect to v, evaluated at $v = 0$, can easily be calculated; the odd derivatives are zero and the even derivatives are found to be

$$\begin{aligned} \left(\frac{\partial^2 g}{\partial v^2}\right)_0 &= -B + \frac{D}{C} \\ \left(\frac{\partial^{2k} g}{\partial v^{2k}}\right)_0 &= (-1)^{k+1}\, 2(2k-1)! \Big/ \left(\frac{2C}{D}\right)^k, \qquad k \geqslant 2 \end{aligned} \tag{7}$$

The even moments of (5) are defined

$$m_{2k}(t) = \int A(C + Dv^2/2)\, v^{2k} \exp(-Bv^2/2)\, d^d v$$

Transforming to the variable $u = v^2/2$ the following expression is obtained:

$$\begin{aligned} m_{2k}(t) &= (2\pi)^p/\Gamma(p) \int_0^{\infty} 2^k A u^{k+p-1} e^{-Bu}(C + Du)\, du \\ &= 2^k A (2\pi)^p/\Gamma(p)[C\Gamma(k+p)/B^{k+p} + D\Gamma(k+p+1)/B^{k+p+1}] \end{aligned} \tag{8}$$

Using (4), (6), (7), and (8), the entropy of the d-dimensional BKW solution can be expressed as the following infinite series:

$$\begin{aligned} S(t) = &-\ln AC + (2\pi)^p/[\Gamma(p)]\, ABC\Gamma(p+1)[1+(p+1)\, D/BC]/B^{p+1} \\ &- (2\pi)^p\, AC/[\Gamma(p)\, Bp] \sum_{k=1}^{\infty} (-1)^{k+1}/k \\ &\times [\Gamma(k+p)/(BC/D)^k + \Gamma(k+p+1)/(BC/D)^{k+1}] \end{aligned} \tag{9}$$

The series contained in equation (9) can now be evaluated in closed form in two different ways, depending if p is half-integer (odd d) or integer (even d).

4. THE ENTROPY OF THE BKW SOLUTION FOR ODD DIMENSIONS

The incomplete γ function can be expanded in the following infinite series[20]:

$$\Gamma(a, X) = X^{a-1} e^{-X} \sum_{k=0}^{\infty} \Gamma(1-a+k)/[X^k \Gamma(1-a)] \tag{10}$$

valid when $X > 1$. With $1 - a = p$, equation (10) can be written

$$\sum_{k=0}^{\infty} (-1)^k\, \Gamma(p+k)/X^k = \Gamma(p)\, X^p e^X \Gamma(1-p, X) \tag{11}$$

Using this result, the first infinite series contained in the entropy (9) can be transformed in the following way ($X = BC/D$):

$$\begin{aligned} S_1 &= \sum_{k=1}^{\infty} (-1)^{k+1}\, \Gamma(k+p)/(kX^k) \\ &= \int (1/X) \left[\sum_{k=0}^{\infty} (-1)^k\, \Gamma(k+p)/X^k - \Gamma(p) \right] dx \\ &= \Gamma(p) \int X^{p-1} e^X \Gamma(1-p, X)\, dX - \Gamma(p) \ln X \end{aligned} \tag{12}$$

Equations (6-5-3) and (6-5-12) from Abramowitz and Stegun[20] are used to express the integrand of (12) as

$$X^{p-1} e^X \Gamma(1-p, X) = X^{p-1} e^X \Gamma(1-p) - M(1, 2-p, X)/(1-p) \tag{13}$$

where $M(1, 2-p, X)$ is a hypergeometric Kummer function. Replacing (13) into (12) and using equation (6-5-4)[20] leads to

$$S_1 = (-1)^{2p}\,\Gamma(p)^2\,\Gamma(1-p)\,\gamma^*(p, -X) - \Gamma(p)\ln X$$
$$+ \Gamma(p-1)\int M(1, 2-p, X)\,dx \tag{14}$$

The integral contained in the last equation can be calculated by expending the Kummer function in power series (for $X > 1$); the result of the integration gives rise to a generalized hypergeometric function:

$$\int M(1, 2-p, X)\,dX = X + X^2/[2(2-p)]\,{}_2F_2(1, 2; 3, 3-p; X) \tag{15}$$

The second infinite series in Eq. (9) can be expressed as a function of S_1in the following manner:

$$S_2 = \sum_{k=1}^{\infty} (-1)^{k+1}\,\Gamma(k+p)(k+p)/kX^{k+1}$$
$$= (1/X)\sum_{k=1}^{\infty} (-1)^{k+1}\,\Gamma(k+p)/X^k + (p/X)\sum_{k=1}^{\infty} (-1)^{k+1}\,\Gamma(k+p)/kX^k$$
$$= \Gamma(p)/X - \Gamma(p)\,X^{p-1}e^X\Gamma(1-p, X) + (p/X)\,S_1 \tag{16}$$

The using Eq. (9), (14), (15), and (16), and rearranging terms, the following expression is obtained for the Boltzmann entropy of the BKW solution for odd dimensions:

$$S(t) = -\ln AC + (2\pi)^p\,AC/(B^p)\{(p-1)\,D/BC$$
$$+ (BC/D)^{p-1}\,e^{BC/D}\Gamma(1-p, BC/D) + [1 + p/(BC/D)]$$
$$\times [p - (-1)^{2p}\,\Gamma(1-p)\,\Gamma(p)\,\gamma^*((p, -BC/D)) - (BC/D)/(p-1)$$
$$+ \ln(BC/D) + (BC/D)^2/[2(p-1)(p-2)]\,{}_2F_2(1,2;3,3-p;BC/D)]\} \tag{17}$$

5. THE ENTROPY OF THE BKW SOLUTION FOR EVEN DIMENSIONS

The entropy obtained in equation (17) is obviously undefined for even dimensions; it is necessary to find a different expression for $S(t)$ when p is not an integer. In fact, S_1 can be transformed in a different way $(X = BC/D)$:

$$S_1 = \sum_{k=1}^{\infty} (-1)^{k+1} \Gamma(k+p)/kX^k$$
$$= \sum_{k=1}^{\infty} (-1)^{k+1} \Gamma(k+p-1)/X^k + (p-1) \sum_{k=1}^{\infty} (-1)^{k+1} \Gamma(k+p-1)/kX^k$$

This last step is repeated p times [taking (11) into account] to obtain

$$S_1 = (1/X) \sum_{n=0}^{p-1} \Gamma(p)/[\Gamma(p-n)] \sum_{k=0}^{\infty} (-1)^k \Gamma(p+k-n)/X^k$$
$$= \Gamma(p)\, e^X \sum_{n=0}^{p-1} X^{p-n-1} \Gamma(n-p+1, X) \tag{18}$$

The same procedure can be used to evaluate S_2 and it can easily be shown that

$$S_2 = \Gamma(p+1)\, e^X \sum_{n=0}^{p} X^{p-n-1} \Gamma(n-p, X) \tag{19}$$

The entropy of the BKW solution, for even dimensions, can now be expressed in closed form, in terms of incomplete gamma functions; taking (9), (18), and (19) into account and rearranging terms, we get

$$S(t) = -\ln AC + (2\pi)^p AC/(B^p)(p\{1 + (D/BC)[p - e^{BC/D}\Gamma(0, BC/D)]\}$$
$$- e^{BC/D} \sum_{n=0}^{p-1} n(BC/D)^{p-n-1} \Gamma(n-p, BC/D)) \tag{20}$$

6. THE ENTROPY OF THE TJON–WU MODEL

The results (17) and (20) show that the entropy of the BKW solution can be found, in closed form, for all dimensions. Rouse and Simons[13] and Ziff *et al.*[14] considered that the logarithmic integrals contained in Eq. (1) precluded such a result. However, it should be emphasized that these results are only defined for $BC/D > 1\,[t > \ln((d+4)/2)]$.

The expression of $S(t)$ for $d = 3$ was derived in a previous paper.[18] Instead of deriving it again from Eq. (17), it is of some interest to consider the entropy of the Tjon–Wu model $(d = 2)$ and study some of its properties.

This entropy is calculated from the general result (20) as a function of time; by taking (5) into account, the following result is obtained:

$$S(t) = \ln 2\pi + (1 - 2e^{-t})/(1 - e^{-t}) - \ln(1 - 2e^{-t}) + e^{-t}/[(1 - e^{-t})][1 - e^{(e^t - 2)}\Gamma(0, e^t - 2)] \quad (21)$$

As a way of checking the validity of this result, the first time derivative of the entropy is calculated. A straightforward time differentiation of Eq. (21) leads to

$$dS/dt = 1/(e^t - 1) + e^t(2 - e^t)\, e^{(e^t - 2)}\Gamma(0, e^t - 2)/(e^t - 1)^2$$

Taking the following result into account[20]:

$$e^{(e^t - 2)}\Gamma(0, e^t - 2) = U(1, 1, e^t - 2)$$

The first time derivative is expressed as

$$dS/dt = 1/(e^t - 1) + e^t(2 - e^t)\, U(1, 1, e^t - 2)/(e^t - 1)^2$$

Then using one of the transformation properties of the confluent hypergeometric function (equation 13-4-19 of Ref. 20) and the following result:

$$U(1, 1, z) = \int_0^\infty e^{-zt}/(1 + t)\, dt = 1/z - U(1, 0, z)/z$$

(where $z = e^t - 2$), it is found that

$$dS/dt = 2U(2, 0, e^t - 2)/(e^t - 1)^2 \quad (22)$$

in accordance with the results of Garrett[17] and Ziff *et al.*[14]

7. THE ENTROPY OF THE TJON–WU MODEL AND THE MCKEAN CONJECTURE

In a previous paper[18] an inequality was derived showing that the McKean conjecture is violated by the d-dimensional BKW distribution function. Neither the present attempt nor the one by Garrett[17] gives an approximate numerical value of n for which the McKean conjecture is untrue. Also, the question of whether (2) is violated for times greater than a critical value or for a finite time domain is not clarified in the current literature on the subject. The derivation which follows sheds some light on the question. The following development is done for the Tjon–Wu model but can be generalized for any value of d.

Starting from equation (22) dS/dt is expanded in successive powers of e^{-t}. The first factor $2/(e^t-1)^2$ can be expanded easily:

$$2/(e^t-1)^2 = \sum_{k=2}^{\infty} (2k-2)\, e^{-kt} \tag{23}$$

The confluent hypergeometric function can also be expanded, provided that $t > \ln 3$:

$$U(2, 0, e^t-2) = (e^t-2)^{-2} \sum_{k=0}^{\infty} (-1)^k (2)_k (3)_k [k!(e^t-2)^k]^{-1} \tag{24}$$

A systematic and careful evaluation of the terms up to e^{-12t}, using the expansions (24) and (25) into equation (22), gives

$$\begin{aligned} dS/dt = {} & 2e^{-4t} + 22e^{-6t} - 84e^{-7t} + 690e^{-8t} \\ & - 5352e^{-9t} + 48638e^{-10t} - 486684e^{-11t} \\ & + 5362378e^{-12t} \cdots \end{aligned} \tag{25}$$

Differentiating $(n-1)$ times with respect to t and expressing the result as a limited Taylor series, as a function of the variable $X = e^{-t}$, leads to

$$(-1)^n\, d^nS/dt^n = -2(4)^{n-1} e^{-4t} - 22(6)^{n-1} e^{-6t} + 84(7)^{n-1} e^{-7t} + R_7 \tag{26}$$

where the remainder R_7 is equal to

$$\begin{aligned} R_7 = {} & -690(8)^{n-1} e^{-8t} + e^{-8t}[9!(5352/1!\,8!)(9)^{n-1}\, \theta e^{-t} \\ & - 10!(48638/2!\,8!)(10)^{n-1}(\theta e^{-t})^2 \\ & + 11!(486684/3!8!)\, 11^{n-1}(\theta e^{-t})^3 \\ & - 12!(5362378/4!\,8!)(12)^{n-1}(\theta e^{-t})^4 + \cdots] \end{aligned}$$

and where $0 < \theta < 1$.

A series of conditions for the quantity in brackets to be always positive is

$$e^t > 5(48638/5352)(10/9)^{n-1}\, \theta \tag{27}$$

$$e^t > 3(5362378/486684)(12/11)^{n-1}\, \theta \tag{28}$$

$$\vdots$$

It is easy to verify, in general, that condition (27) is sufficient and includes all the following conditions above. As a result

$$R_7 > -690(8)^{n-1} e^{-8t} \tag{29}$$

Then, from (26) and (29), it is obvious that the McKean conjecture (2) will be violated if both condition (27) and the following condition are satisfied:

$$84(7)^{n-1} e^{-7t} - 2(4)^{n-1} e^{-4t} - 22(6)^{n-1} e^{-6t} - 690(8)^{n-1} e^{-8t} > 0 \tag{30}$$

In order for the last condition to be satisfied, it can be expected that n will have to be big and therefore that the term in e^{-4t} will be negligible (for n big) with respect to the other three; as a result, the following condition will probably be enough for the McKean conjecture to be untrue:

$$22(6)^{n-1} e^{2t} - 84(7)^{n-1} e^{t} + 690(8)^{n-1} < 0 \tag{31}$$

The condition for the above polynomial in e^t to have real roots can be found to be

$$n > 105.38 \tag{32}$$

and inequality (31) will be satisfied, in the approximation of n big, if

$$(76695/9702)(8/7)^{n-1} < e^t < (42/11)(7/6)^{n-1} \tag{33}$$

It is obvious that inequality (33) becomes sufficient and that (27) can be forgotten. Conditions (32) and (33) are then approximate conditions for the McKean conjecture to be violated; condition (30) is instead a strong, sufficient condition.

8. THE BOLTZMANN ENTROPY OF ONE OF THE SOLUTIONS OF THE VERY HARD PARTICLE MODEL

In the literature, many kinetic models with a stochastic mechanism have been studied, in which momentum is not conserved, but total number of particles and total energy are.[22] Binary collisions are described in terms of a transition rate that depends only on the total energy of the two colliding particles and not on the energies of the separate particles. When the transition rate has the specific form of a δ function, the product of the relative velocity and the differential cross section increases linearly with the energy and the nonlinear BE leads to the very hard particle (VHP) model.[23] For this model, the BE gives an exact solution in closed form. The study of this solution has brought out a very interesting point: the description of the approach to equilibrium by the linearized BE is not adequate for the high-energy tail of the distribution function.[8] This raises questions about the range of validity of the local equilibrium hypothesis, essential in the formulation of irreversible thermodynamics,[24] when one has to study the relaxation to equilibrium. Also, this raises questions about the range of validity of the Gibbs relation in evaluating the entropy production for a system close to equilibrium, and when one wants to study how the entropy production evolves toward equilibrium. It seems therefore very important to know exact solutions of the nonlinear BE and to be able to calculate the entropy of these distribution functions in order to be able to accurately describe the approach to equilibrium.

In this section, is calculated the Boltzmann entropy of the following energy distribution function solution of the VHP model[8]:

$$F(X, t) = A_1 e^{z_1 X} + A_2 e^{z_2 X} \tag{34}$$

where $X = v^2/2$ and A_1, A_2, z_1, and z_2 are functions of time. This function corresponds to an initial $(t = 0)$ distribution function which is a superposition of two Maxwellians:

$$F(X, 0) = \alpha_1 e^{-\beta_1 X} + \alpha_2 e^{-\beta_2 X}$$

in which $\beta_1 < \beta_2$. When $t \to \infty$, $A_1 \to 1$, $z_1 \to -1$, $A_2 \to 0$, $z_2 \to -\infty$ and the function (34) converges to a Maxwell–Boltzmann type of distribution function:

$$F(X, \infty) = e^{-X}$$

It is straightforward to show that, when $f(v, t)$ is replaced by the energy distribution function $F(x, t)$, Eq. (4) is replaced by

$$S(t) = -\sum_{k=0}^{\infty} (\partial^k g/\partial X^k)_0 \, M_k(t)/k! \tag{35}$$

where

$$g(x, t) = \ln[\Gamma(p)(2X)^{1-p} F(x, t)/(2\pi) \, p] \tag{36}$$

in which $p = d/2$ and where

$$M_k(t) = \int_0^{\infty} F(x, t) \, X^k \, dx \tag{37}$$

$S(t)$ will now be calculated in two dimensions in order to simplify the problem, but the calculation in any dimension could be done by evaluating the $\partial^k g/\partial v^k$ at $v=\bar{v}$ for instance. From (36), with $p=1$, $A=A_1$, $B=A_2/A_1$, $\alpha=-z_1$ and $\beta=z_1-z_2$, the following expression is obtained:

$$g(x,t)=\ln(A/2\pi)-\alpha X+\ln(1+Be^{-\beta X})$$

The logarithm can be expanded in a Taylor series, because $B<1$; then, it is easy to verify that

$$(\partial^k g/\partial X^k)_0=\sum_{\gamma=1}^{\infty}(-1)^{\gamma+1}(-\gamma\beta)^k B^\gamma/\gamma \tag{38}$$

where a term $-\alpha$ has to be added to (38) for $k=1$. From (38) and (34), the moments are found to be

$$M_k(t)=A\Gamma(k+1)[1/\alpha_{k+1}+B/(\alpha+\beta)^{k+1}] \tag{39}$$

Now, use of (35), (38), (39) leads to the result

$$\begin{aligned}S(t)=&-\ln(A(1+B)/2\pi)+A[1/\alpha+B\alpha/(\alpha+\beta)^2]\\&-(A/\alpha)\sum_{j=1}^{\infty}(-1)^{j+1}(B^j/j)\sum_{k=1}^{\infty}(-j\beta/\alpha)^k\\&-[AB/(\alpha+\beta)]\sum_{j=1}^{\infty}(-1)^{j+1}(B^j/j)\sum_{k=1}^{\infty}[-j\beta/(\alpha+\beta)]^k\end{aligned} \tag{40}$$

In this last equation, the infinite sums over k can easily be written in closed form to give

$$\begin{aligned}S(t)=&-\ln(A(1+B)/2\pi)+A[1/\alpha+B\alpha/(\alpha+\beta)^2]\\&-(A\beta/\alpha)\sum_{\gamma=1}^{\infty}(-B)^j/(\beta j+\alpha)-[AB\beta/(\alpha+\beta)]\\&\times\sum_{\gamma=1}^{\infty}(-B)^j/(\beta j+\alpha+\beta)\end{aligned} \tag{41}$$

The following infinite series,

$$f(B)=\sum_{\gamma=1}^{\infty}(-B)^j/(aj+b)$$

can be calculated by differentiating both sides with respect to B and solving the obtained first-order differential equation:

$$f(B)=-(1/a)(B)^{b/a}\int[(B)^{-b/a}/(1+B)]\,dB \tag{42}$$

in which the integral can be expressed with an incomplete β function:

$$\int (-B)^{-b/a}(1+B)^{-1}\,dB = \mathscr{B}_{B/(B+1)}(1-b/a, b/a) \tag{43}$$

When the results (42) and (43) are inserted into (41), the entropy of the VHP model distribution function (34), for $p=1$, can be expressed in closed form:

$$\begin{aligned} S(t) = &-\ln(A(1+B)/2\pi) + A[1/\alpha + B\alpha/(\alpha+\beta)^2] \\ &+ [A(B)^{\alpha/\beta}/\alpha]\,\mathscr{B}_{B/(B+1)}(1-\alpha/\beta, \alpha/\beta) \\ &+ [A/(\alpha+\beta)](B)^{2+\alpha/\beta}\,\mathscr{B}_{B/(B+1)}(-\alpha/\beta, 1+\alpha/\beta) \end{aligned} \tag{44}$$

9. CONCLUSION

This paper both improves and concludes a previous attempt[18] to evaluate the entropy of the BKW solution. The method used here is apparently more powerful, because, except for the moments of the non-equilibrium distribution, no integral calculus is needed and if the infinite series (4) converges and can be expressed in closed form, the non-equilibrium entropy can be obtained without having to calculate the logarithmic integrals contained in (1). In this paper, the entropy of the BKW solution has been calculated for all dimensions, obtaining two different expressions in closed form for odd and even values of $p = d/2$. Particular attention was given to the study of the entropy of the Tjon–Wu model ($p = 1$). A minimum value of n was obtained as well as a condition for which the McKean conjecture is violated within certain time intervals depending on n itself. Although condition (31) is sufficient, it is approximate and a value of n slightly smaller than (33) would be expected. In view of the interest in the VHP model in the literature,[8] the present method was used to calculate the Boltzmann entropy of one of its exact solutions. Knowledge of the entropy of distribution functions that are exact solutions of the BE are of great interest to the study of the approach to equilibrium in nonequilibrium thermodynamics, particularly since the solutions of the linearized BE apparently give inadequate descriptions of the process.

REFERENCES

1. M. Mareschal, *Phys. Rev. A*, **29**(2):926 (1984).
2. H. P. McKean, *Arch. Ration. Mech. Anal.* **21**:343, (1966).
3. S. Harris, *J. Math. Phys.* **8**:2407 (1967).

4. S. Harris, *J. Chem. Phys.* **48**:4012 (1968).
5. S. Simons, *J. Phys.* **A2**:12 (1969).
6. S. Simons, *Phys. Lett.* **33A**:154 (1970).
7. S. Simons, *J. Phys* **A5**:1537 (1972).
8. M. Ernst, in *Non Equilibrium Phenomena I, The Boltzmann Equation,* J. L. Lebowitz and E. W. Montroll, eds. (North-Holland, Amsterdam, 1983).
9. A. V. Bobylev, *Sov. Phys. Dokl.* **20**:820 (1976).
10. M. Krook and T. T. Wu, *Phys. Rev. Lett.* **36**:1107 (1976).
11. M. H. Ernst, *Phys. Lett.* **69A**:390 (1979).
12. R. M. Ziff, *Phys. Rev. A* **23**:916, (1981).
13. S. Rouse and S. Simons, *J. Phys.* **All**:423 (1978).
14. R. M. Ziff, S. D. Merajver, and G. Stell, *Phys. Rev. Lett.* **47**:1493 (1981).
15. E. H. Lieb, *Phys. Rev. Lett* **48**:1057 (1982).
16. K. Olaussen, *Phys. Rev. A* **25**:3393 (1982).
17. A. J. M. Garrett, *J. Phys.* **A15**:L351 (1982).
18. C. J. Tourenne, *J. Stat. Phys.* **32**:1, (1983).
19. I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series and Products* (Academic Press, New York, 1965).
20. M. Abramowitz and I. Stegun, *Handbook of Mathematical Functions* (National Bureau of Standards, Washington, D. C., 1965).
21. J. Tjon and T. T. Wu, *Phys. Rev. A* **19**:883 (1979).
22. M. H. Ernst, *Phys. Rep.* **78**:1 (1981).
23. M. H. Ernst and E. M. Hendriks, *Phys. Lett.* **70A**:183 (1979).
24. H. J. Krenzer, *Non Equilibrium Thermodynamics and Its Statistical Foundations* (Clarendon Press, Oxford, 1981).
25. J. O. Vigfusson and A. Thellung, *Phys. Lett.* **91A**:9, 435 (1982).
26. J. O. Vigfusson, *J. Phys. A* **16**:L352 (1983).