

The Bobylev Approach to the Nonlinear Boltzmann Equation

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The Bobylev approach to the nonlinear Boltzmann equation is reviewed. The linearized problem is discussed and it is shown that eigenfunctions decaying like a negative power of the velocity are possible with Maxwell molecules only. The relaxation to equilibrium according to the nonlinear equation is discussed and the Krook–Wu conjecture on the status of the BKW mode is shown to be false in general. The buildup of the high-energy tails is considered and a phenomenon observed by Tjon is given a simple explanation. Finally, the method is illustrated with numerical calculations performed for two sets of initial conditions.

KEY WORDS: Nonlinear Boltzmann equation; relaxation to equilibrium; high-energy tails.

1. INTRODUCTION

During the last two decades significant progress has been made in our understanding of higher density effects in kinetic theory. The great collective effort at unravelling the mysteries *beyond* the Boltzmann equation might leave the impression that the properties of the Boltzmann equation itself have been completely clarified. This, however, is not quite the case.

It is true, of course, that we know a great deal about the Boltzmann equation, and that the body of knowledge is growing. Our knowledge is, nevertheless, limited, and, in particular, exact solutions are rare indeed. It was therefore a remarkable coincidence when, in 1976, Bobylev⁽¹⁾ and, independently, Krook and Wu⁽²⁾ published an exact solution (the BKW

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mode) of the *nonlinear* Boltzmann equation for a spatially uniform gas of Maxwell molecules with an isotropic velocity distribution. The discovery of this exact solution has on the one hand triggered a search for similar models for which exact solutions can be found⁽³⁻⁵⁾ (for a review, see Ernst⁽⁶⁾), while, on the other hand, several authors have investigated, numerically^(7,8) and analytically,^(9,10) the status of the BKW mode and the related problem of the buildup of the high-energy tails in the equilibrium distribution.

In this paper we shall review and advocate the Bobylev method⁽¹⁾ as, in our opinion, the most effective realization of the simplifications inherent in models with a velocity-independent collision frequency. We restrict ourselves to the classical case of Maxwell molecules in three dimensions (repulsive interaction potential proportional to the inverse fourth power of intermolecular distance). We shall mainly use the method to examine the status of the BKW mode and to study the problem of the high-energy tails.

Bobylev's basic trick is a Fourier transformation in velocity space of the *nonlinear* Boltzmann equation. With Maxwell molecules this leads to a considerable simplification of the equation. We recall Bobylev's derivation in Section 2.

In Section 3 we again follow Bobylev, who rederived the standard solution of the linearized equation and, in addition, found an infinite class of eigenfunctions that decay asymptotically like a negative power of the velocity. In the Appendix we show that such *eigenfunctions* are only possible with Maxwell molecules. Nevertheless, velocity distributions of this kind are perfectly acceptable from a physical point of view.

The derivation of a recursion scheme defining the Bobylev class of similarity solutions characterized by a single relaxation rate is given in Section 4. The BKW mode is a member of this class. A generalization to classes characterized by a finite number of relaxation rates is indicated.

The general solution of the nonlinear initial value problem was given recursively by Ernst,^(11,12) who showed that his recursion scheme is closely related to Maxwell's moment equations. As we shall need it in later sections, we present the general recursion scheme in Section 5.

A problem of special interest has been the status of the BKW mode. Krook and Wu⁽²⁾ conjectured it to be a crucial one in that an arbitrary initial state will relax to equilibrium via the BKW mode. This conjecture is shown⁽¹⁰⁾ to be essentially false in Section 6.

The second problem on which much interest has been focused is that of the high-energy tails. The tail of the BKW mode approaches the equilibrium Maxwellian from below. Tjon,⁽⁸⁾ however, observed that for certain initial states there is a crossover to overpopulated tails that decay to equilibrium from above. This phenomenon is explained⁽¹⁰⁾ in Section 7.

Finally, the general recursion scheme is solved to eighth order for two types of initial conditions in Section 8, where also the rate of convergence of this procedure is discussed.

2. THE BOBYLEV TRANSFORMATION

In this section we summarize the Bobylev transformation.⁽¹⁾ The Boltzmann equation for the one-particle distribution $f(\mathbf{r}, \mathbf{v}, t)$ reads

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} \right) f(\mathbf{r}, \mathbf{v}, t) = \int d\mathbf{w} d\hat{\mathbf{n}} \sigma(\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}; u) u [f(\mathbf{w}')f(\mathbf{v}') - f(\mathbf{w})f(\mathbf{v})] \quad (1)$$

Here $\sigma(\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}; u)$ is the differential cross section for the collision process $(\mathbf{v}, \mathbf{w}) \rightarrow (\mathbf{v}', \mathbf{w}')$, $\mathbf{u} = \mathbf{w} - \mathbf{v}$ is the relative velocity (with magnitude $u = |\mathbf{u}|$) before the collision, and $\hat{\mathbf{u}}$ and $\hat{\mathbf{n}}$ are the unit vectors in the direction of \mathbf{u} and \mathbf{u}' , respectively. Since energy and momentum conservation give $u' = u$ and $\mathbf{v}' + \mathbf{w}' = \mathbf{v} + \mathbf{w}$, one has

$$\mathbf{v}' = \frac{1}{2}(\mathbf{v} + \mathbf{w}) - \frac{1}{2}u\hat{\mathbf{n}}; \quad \mathbf{w}' = \frac{1}{2}(\mathbf{v} + \mathbf{w}) + \frac{1}{2}u\hat{\mathbf{n}} \quad (2)$$

With repulsive power-law potentials $U(r) = \text{const} \cdot r^{-s}$, the dependence of the differential cross section on u can be determined explicitly,^(13,14) and one has

$$\sigma(\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}; u) = g_s(\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}) u^{1-4/s} \quad (3)$$

For Maxwell molecules ($s = 4$) the dependence on u cancels. Hard spheres correspond to $s \rightarrow \infty$.

We now follow Bobylev and introduce a Fourier transformation in velocity space

$$\varphi(\mathbf{r}, \mathbf{k}, t) = \int d\mathbf{v} [\exp(-i\mathbf{k} \cdot \mathbf{v})] f(\mathbf{r}, \mathbf{v}, t) \quad (4)$$

giving

$$\frac{\partial \varphi}{\partial t} + i \frac{\partial^2 \varphi}{\partial \mathbf{k} \cdot \partial \mathbf{r}} = S(\varphi, \varphi) \quad (5)$$

where

$$S(\varphi, \varphi) = \int d\mathbf{v} d\mathbf{w} d\hat{\mathbf{n}} [\exp(-i\mathbf{k} \cdot \mathbf{v})] g_s(\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}) u^{1-4/s} \times [f(\mathbf{w}')f(\mathbf{v}') - f(\mathbf{w})f(\mathbf{v})] \quad (6)$$

The collision term $S(\varphi, \varphi)$ is clearly invariant under the operation $(\mathbf{v}, \mathbf{w}) \rightleftharpoons (\mathbf{v}', \mathbf{w}')$. But so are the following quantities separately: u , $\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}$, $d\mathbf{v} d\mathbf{w} d\hat{\mathbf{n}}$. The first term in (6) can then be transformed such that the f 's depend on

unprimed velocities, and using (2), one finds

$$S(\varphi, \varphi) = \int dv d\mathbf{w} f(\mathbf{v})f(\mathbf{w}) \{ -\exp[\frac{1}{2}i\mathbf{k} \cdot (\mathbf{v} + \mathbf{w})] \} u^{1-4/s} F(\mathbf{u}, \mathbf{k}) \quad (7)$$

with

$$F(\mathbf{u}, \mathbf{k}) = \int d\hat{\mathbf{n}} g_s(\hat{\mathbf{u}} \cdot \hat{\mathbf{n}}) [\exp(\frac{1}{2}i\mathbf{k} \cdot \hat{\mathbf{n}}\mathbf{u}) - \exp(\frac{1}{2}i\mathbf{k} \cdot \mathbf{u})]$$

Since F is a scalar, it can at most be a function of the scalars $\mathbf{u} \cdot \mathbf{k}$, $\mathbf{k} \cdot \mathbf{k}$, and $\mathbf{u} \cdot \mathbf{u}$. Inspection of its explicit form shows that F depends on $\mathbf{u} \cdot \mathbf{k}$ and the combination uk only. Thus $F(\mathbf{u}, \mathbf{k}) = F(\mathbf{k}, \mathbf{u})$. Changing the order of integrations, one can then write

$$S(\varphi, \varphi) = \int d\hat{\mathbf{n}} g_s(\hat{\mathbf{k}} \cdot \hat{\mathbf{n}}) \int dv d\mathbf{w} f(\mathbf{v})f(\mathbf{w}) u^{1-4/s} \\ \times \{ \exp[-\frac{1}{2}i\mathbf{v} \cdot (\hat{\mathbf{k}} + \hat{\mathbf{n}})k] \exp[-\frac{1}{2}i\mathbf{w} \cdot (\hat{\mathbf{k}} - \hat{\mathbf{n}})k] - \exp(-i\mathbf{k} \cdot \mathbf{v}) \} \quad (8)$$

For $s \neq 4$ this form does not represent a major simplification, although it can, as we shall see, be useful for certain purposes. With $s = 4$, however, the integrations over velocities decouple, and one arrives at the equation

$$\frac{\partial \varphi}{\partial t} + i \frac{\partial^2 \varphi}{\partial \mathbf{k} \cdot \partial \mathbf{r}} = \int d\hat{\mathbf{n}} g_4(\hat{\mathbf{k}} \cdot \hat{\mathbf{n}}) \left[\varphi\left(\frac{k}{2}(\hat{\mathbf{k}} + \hat{\mathbf{n}})\right) \varphi\left(\frac{k}{2}(\hat{\mathbf{k}} - \hat{\mathbf{n}})\right) - \varphi(\mathbf{k})\varphi(0) \right] \quad (9)$$

This is the Bobylev form of the Boltzmann equation for Maxwell molecules. It represents a drastic simplification of the equation. Previously known results can be rederived in a very simple manner, and important steps forward can be taken.

We shall simplify matters further by restricting ourselves to the case of a spatially uniform system with an isotropic velocity distribution. In that case φ is a function of $k^2/2 = x$ and t only, i.e., $\varphi(\mathbf{k}, \mathbf{r}, t) = \bar{\varphi}(x, t)$. For simplicity we drop the bar on $\bar{\varphi}$ and the subscript $s = 4$ on $g_4(\hat{\mathbf{k}} \cdot \hat{\mathbf{n}})$.⁴ Then Eq. (9) reduces to

$$\frac{\partial \varphi(x, t)}{\partial t} = 2\pi \int_{-1}^1 d\mu g(\mu) [\varphi(x_+) \varphi(x_-) - \varphi(x)\varphi(0)] \quad (10)$$

In (10), the notation $\hat{\mathbf{k}} \cdot \hat{\mathbf{n}} = \mu$ and $x_{\pm} = \frac{1}{2}x(1 \pm \mu)$ has been introduced, and the integration over the azimuthal angle performed.

3. THE LINEARIZED EQUATION

For convenience we shall choose units such that the equilibrium distribution is of the form $f_{\text{eq}}(v) = (2\pi)^{-3/2} \exp(-v^2/2)$, i.e., $\langle v^2 \rangle = \frac{3}{2}$. In

⁴ We shall not need the explicit form of the somewhat complicated function $g(\mu)$ in this paper. For details, see, e.g., Ref. 19.

the Fourier variable $x = \frac{1}{2}k^2$ the equilibrium distribution then reads $\varphi_{\text{eq}}(x) = e^{-x}$. We write

$$\varphi(x, t) = e^{-x} [1 + h(x, t)] \quad (11)$$

Since $x_+ + x_- = x$, the factor e^{-x} cancels when (11) is inserted into (10). Linearization in the deviation h from equilibrium then yields

$$\frac{\partial h(x, t)}{\partial t} = 2\pi \int_{-1}^1 d\mu g(\mu) [h(x_+, t) + h(x_-, t) - h(x, t) - h(0, t)] \quad (12)$$

The corresponding eigenvalue problem follows when one writes $h(x, t) = h(x) \exp(-\Lambda t)$:

$$\Lambda h(x) = 2\pi \int_{-1}^1 d\mu g(\mu) [h(x) + h(0) - h(x_+) - h(x_-)] \quad (13)$$

Clearly $h_0 = 1$ and $h_1 = x$ are eigenfunctions with zero eigenvalue, reflecting conservation of particle number and energy, respectively. But also all other eigenfunctions and eigenvalues are immediately found! They are ($p \neq 0$)

$$h_p(x) = x^p; \quad \Lambda_p = 2\pi \int_{-1}^1 d\mu g(\mu) \left[1 - \left(\frac{1+\mu}{2} \right)^p - \left(\frac{1-\mu}{2} \right)^p \right] \quad (14)$$

Fourier transformation of the eigenfunctions gives, when one writes $f(v) = f_{\text{eq}}(v) + \delta f(v)$,

$$\begin{aligned} \delta f_p(v) &= \frac{1}{(2\pi)^3} \int d\mathbf{k} [\exp(i\mathbf{k} \cdot \mathbf{v} - \frac{1}{2}k^2)] \left(\frac{k^2}{2} \right)^p \\ &= \frac{1}{\pi^2 \sqrt{2}} \Gamma\left(p + \frac{3}{2}\right) \left[\exp\left(-\frac{v^2}{2}\right) \right] {}_1F_1\left(-p; \frac{3}{2}; \frac{v^2}{2}\right) \end{aligned} \quad (15)$$

where ${}_1F_1$ is the confluent hypergeometric function.⁽¹⁵⁾ For $p = n = \text{integer}$ it reduces to

$${}_1F_1\left(-n; \frac{3}{2}; \frac{v^2}{2}\right) = \frac{n! \Gamma(3/2)}{\Gamma(n + 3/2)} L_n^{(1/2)}\left(\frac{v^2}{2}\right) \quad (16)$$

where $L_n^{(1/2)}$ is the associated Laguerre polynomial.⁽¹⁵⁾ Thus

$$\delta f_n(v) = f_{\text{eq}}(v) n! L_n^{(1/2)}(v^2/2) \quad (17)$$

The eigenfunctions (17) and the corresponding eigenvalues (14) were first found by Wang Chang and Uhlenbeck.⁽¹⁶⁾ However, as Bobylev pointed out, these are not the only ones. There is nothing preventing us from choosing a noninteger p in (14) (in fact, p could even be complex). For noninteger real p the large- v asymptotic behavior of $\delta f_p(v)$ is⁽¹⁵⁾

$$\delta f_p(v) \underset{v \gg 1}{\simeq} \frac{1}{(2\pi)^{3/2}} \frac{\Gamma(p + 3/2)}{\Gamma(-p)} \left(\frac{v^2}{2} \right)^{-p-3/2} \quad (18)$$

The only physical requirement restricting p is the existence of energy, which dictates that $p > 1$ (or, more generally, $\text{Re } p > 1$).

At first sight the continuum of possible values for p seems to contradict the usual notion of a discrete spectrum with the corresponding Laguerre functions as a complete set. The contradiction is only apparent, however, since completeness here refers to a Hilbert space which makes the usual linearized Boltzmann operator self-adjoint, and in which the norm is defined by⁽¹⁴⁾

$$\|\delta f\|^2 = \int dv \frac{|\delta f(v)|^2}{f_{\text{eq}}(v)} \quad (19)$$

Clearly all eigenfunctions with noninteger p , i.e., with asymptotics given by (18), live *outside* this Hilbert space.

A natural question is then: do eigenfunctions of this kind exist for interaction potentials different from that of Maxwell molecules? We show in the Appendix that the answer is *no*: when the Boltzmann collision operator, appropriately linearized, acts on a function with asymptotic decay $\sim v^{-2p-3}$, the result is a function decaying like v to the power $[-2(p - \frac{1}{2} + 2/s) - 3]$. As a consequence, eigenfunctions decaying like a power of v are only possible for $s = 4$, i.e., for Maxwell molecules.

How an initial state with asymptotics v^{-2p-3} decays to equilibrium with, say, hard-sphere interactions seems to be an open problem.

In this connection one should note that although the above problem is mathematically well defined in the context of the linearized equation, it is *not* clear that linearization is meaningful with such states.

4. THE BKW MODE

We return to the nonlinear Boltzmann equation for Maxwell molecules in the form (10). This equation has the following invariance properties, which are easily verified: (i) If $\varphi(x, t)$ is a solution, then $e^{ax}\varphi(x, t)$ is also a solution. [The constant a is arbitrary except for conditions resulting from existence and positivity of $f(v, t)$.] (ii) If $\varphi(x, t)$ is a solution, then $\varphi(ax, t)$ is also a solution.

Let us define $\psi(x, t)$ by

$$\varphi(x, t) = e^{-x}\psi(x, t) \quad (20)$$

By property (i), ψ obeys Eq. (10). Choose the normalization of φ as $\varphi(0, t) = 1$. Then $\psi(x, t)$ has to fulfill the conditions: (a) $\psi(0, t) = 1$ (normalization); (b) $\lim_{x \rightarrow 0} [\psi(x, t) - 1]/x = 0$ (the energy is fixed by e^{-x}); (c) $\psi(x, t \rightarrow \infty) = 1$ (approach to equilibrium). These conditions and the invari-

ance property (ii) motivate a search for solutions of the type⁵

$$\psi(x, t) = \psi(xe^{-\lambda t}) \tag{21}$$

where λ is a relaxation rate.

As observed by Bobylev, insertion of (21) into (10) for $t = 0$ shows that initial conditions leading to solutions of the form (21) must obey the equation

$$-\lambda x \psi'(x) = 2\pi \int_{-1}^1 d\mu g(\mu) [\psi(x_+) \psi(x_-) - \psi(x)] \tag{22}$$

This equation determines a whole class (the Bobylev class) of solutions. A member of this class is characterized by a decay to equilibrium according to a single decay rate, as shown in (21). Assume that the behavior of ψ for small x is given by

$$\psi_p(x) = 1 + c_p x^p + \dots \tag{23}$$

Here p does not have to be an integer, but is restricted to $p > 1$ by condition (b). Insertion of (23) into (22) shows that the corresponding relaxation rate is

$$\lambda_p = \Lambda_p / p \tag{24}$$

where Λ_p is the eigenvalue of the linearized equation given by (14). Insistence that (22) should be obeyed to every order in x uniquely determines the higher coefficients in terms of c_p (except for an arbitrariness due to the “accidental” degeneracy $\lambda_2 = \lambda_3$).

We note in passing that this approach is easily generalized. The next class of exact solutions of the nonlinear equation has the form $\psi = \psi(xe^{-\lambda_a t}, xe^{-\lambda_b t})$, where $\psi(x_a, x_b) - 1$ is given as a double power series with positive powers (larger than 1) only. This class is thus characterized by two relaxation rates λ_a and λ_b . The steps analogous to (22)–(24) lead to a (somewhat complicated) recurrence scheme which uniquely determines the relaxation rates and the solution, modulo (in general) two arbitrary constants. Generalization to exact solutions with any finite number of relaxation rates is straightforward, but tedious.

Even the exact solutions in the Bobylev class must be determined recursively, and the coefficients of the terms beyond c_p depend, in general, on an infinite sequence of μ -integrals. However, one particular member of the Bobylev class can be written down *explicitly*. One verifies by insertion that

$$\psi_{\text{BKW}}(x) = e^{bx} (1 - bx) \tag{25}$$

does indeed solve (22) with $\lambda = \lambda_2 = \frac{1}{2} \Lambda_2$. It is remarkable that this solution was found (all these years after Maxwell and Boltzmann!) at essentially the

⁵ For a deeper motivation, see Ref. 1.

same time, and independently, by Bobylev and by Krook and Wu (using a different method). We accordingly call the solution (25) the BKW mode.

In expanded form the BKW mode reads

$$\psi_{\text{BKW}}(x) = 1 - \frac{1}{2}b^2x^2 - \frac{1}{3}b^3x^3 - \frac{1}{8}b^4x^4 - \dots \quad (26)$$

According to (21), the time dependence is incorporated when one writes

$$b = b_0 e^{-\lambda_2 t} = b_0 e^{-\Lambda_2 t/2} \quad (27)$$

Fourier transformation of (25) yields the BKW mode in velocity space. With $R(v, t) = f(v, t)/f_{\text{eq}}(v)$ one finds

$$R_{\text{BKW}}(v, t) = \frac{\exp[-bv^2/2(1-b)]}{(1-b)^{3/2}} \left[1 - \frac{3b}{2(1-b)} + \frac{bv^2}{2(1-b)^2} \right] \quad (28)$$

Roughly speaking, the BKW mode is a Maxwellian with too low a temperature, dressed with a first-order polynomial in v^2 so that the energy is kept at the prescribed value of $\frac{1}{2}\langle v^2 \rangle = \frac{3}{2}$. The requirement of a nonnegative-definite f for all t restricts b_0 to the interval $0 < b_0 < \frac{2}{5}$.

5. THE GENERAL SOLUTION

The *general* solution of the nonlinear equation

$$\frac{\partial \psi(x, t)}{\partial t} = 2\pi \int_{-1}^1 d\mu g(\mu) [\psi(x_+) \psi(x_-) - \psi(x)] \quad (29)$$

can be constructed recursively, as shown by Ernst.⁽¹¹⁾ For simplicity we restrict ourselves to the conventional Hilbert space, i.e., to functions $\psi(x, t)$ that can be expanded in a Taylor series in x :

$$\psi(x, t) = 1 + \sum_{n=2}^{\infty} c_n(t) x^n \quad (30)$$

With the requirement that (29) should be fulfilled to every order in x , insertion of (30) yields the following infinite set of equations for the coefficients $c_n(t)$:

$$\begin{aligned} \frac{dc_n(t)}{dt} + \Lambda_n c_n(t) &= \sum_{m=2}^{n-2} c_{n-m}(t) c_m(t) \\ &\times 2\pi \int_{-1}^1 d\mu g(\mu) \left(\frac{1+\mu}{2} \right)^{n-m} \left(\frac{1-\mu}{2} \right)^m \end{aligned} \quad (31)$$

The integrals on the right-hand side can be expressed as linear combinations of eigenvalues. We shall come back to this in Section 8. Note that the two first equations ($n=2, 3$) in the recursion scheme (31) are *linear*. Nonlinear corrections appear for $n \geq 4$.

For the arguments of the next section we shall need the general

solution of the first three equations, which are readily found to be

$$\begin{aligned} c_2(t) &= c_2(0)e^{-\Lambda_2 t} \\ c_3(t) &= c_3(0)e^{-\Lambda_3 t} = c_3(0)e^{-3\Lambda_2 t/2} \\ c_4(t) &= -\frac{1}{2}c_2^2(0)e^{-2\Lambda_2 t} + [c_4(0) + \frac{1}{2}c_2^2(0)]e^{-\Lambda_4 t} \end{aligned} \tag{32}$$

The fact that $\Lambda_3 = \frac{3}{2}\Lambda_2$ is easily verified from the definition (14). One can also prove that $\Lambda_4 < 2\Lambda_2$. Numerically, Alterman *et al.*⁽¹⁷⁾ found that $\Lambda_4/\frac{1}{2}\Lambda_2 = 3.6844 \dots$

Having determined the time dependence of the coefficients $c_n(t)$, one can use (17) and return to v space:

$$R(v, t) = \frac{f(v, t)}{f_{\text{eq}}(v)} = 1 + \sum_{n=2}^{\infty} c_n(t)n!L_n^{(1/2)}\left(\frac{v^2}{2}\right) \tag{33}$$

6. THE KROOK-WU CONJECTURE

Krook and Wu conjectured that the BKW mode has a special status among all states relaxing toward equilibrium. Their conjecture reads⁽²⁾: “An arbitrary initial state tends first to relax towards a state characterized by the similarity solution [the BKW mode]. The subsequent stage of relaxation is essentially represented by the similarity solution with appropriate phase.”

In order to test the validity of this conjecture, Tjon and Wu⁽⁷⁾ solved the nonlinear Boltzmann equation numerically for a set of initial conditions. Their results seemed to lend support to the conjecture. Later, however, Tjon⁽⁸⁾ found initial states that seemed to contradict it.

We shall now show,⁽¹⁰⁾ by three classes of counterexamples, that the Krook-Wu conjecture is false. The phenomenon observed by Tjon will be discussed in Section 7.

Class I. Let $\psi_p(xe^{-\lambda_p t})$ be an exact solution of the nonlinear equation in the Bobilev class discussed in Section 4. Let $1 < p < 2$. From (14) and (24) it is easily seen that λ_p decreases monotonically when p decreases from 2 to 1. As p approaches 1 from above, $\lambda_p \simeq \text{const} \cdot (p - 1)$, i.e., $\lambda_p \rightarrow 0$. The fact that solutions with arbitrarily small relaxation rates exist contradicts the Krook-Wu conjecture, since the BKW mode relaxes at the finite rate given by $\lambda_2 = \frac{1}{2}\Lambda_2$.

The states in the Bobilev class with $1 < p < 2$ are, however, rather special, even if they are perfectly acceptable physically, as discussed in Section 3. We therefore turn to states for which a Taylor expansion in x exists.

Class II. Let the initial state be of the form

$$\psi(x) = \psi_{\text{BKW}}(x) + \delta c_3 x^3 + \delta c_4 x^4 + \dots \tag{34}$$

By Eqs. (26) and (27) this implies that the parameter b_0 is adjusted so that

$c_2(0) = -\frac{1}{2}b_0^2$. This is clearly possible if $c_2(0) < 0$. The deviations δc_3 and δc_4 are, from (26)

$$\delta c_3 = c_3(0) + \frac{1}{3}b_0^3 \quad (35)$$

$$\delta c_4 = c_4(0) + \frac{1}{8}b_0^4 = c_4(0) + \frac{1}{2}c_2^2(0)$$

Appealing to the general solution (32), one finds that the δc_3 term decays at precisely the same rate as the corresponding term in the BKW mode, namely $e^{-3\Lambda_2 t/2}$. The δc_4 term, however, decays like $e^{-\Lambda_2 t}$, which is *slower* than the corresponding BKW term, decaying like $e^{-2\Lambda_2 t}$.

A similar situation prevails in higher orders. The x^n term will decay with a spectrum of relaxation rates. The fastest one, $n\Lambda_2/2$, is that of the corresponding BKW term, whereas the slowest is Λ_n , the linear relaxation rate. An arbitrary initial state of class II will therefore *not* approach the BKW mode term by term.

However, states of class II *do* relax toward equilibrium via the BKW mode in the following trivial sense: The slowest term is clearly x^2 , decaying like $e^{-\Lambda_2 t}$. This term belongs to the BKW mode.

Any state with negative $c_2(0)$ can be written in the form (34). Positivity of $f(v, t)$ implies that $\langle (v^2 - \langle v^2 \rangle)^2 \rangle \geq 0$. As a consequence, $c_2(0) \geq -\frac{1}{5}$. Comparison with (26) and (28) shows that positivity of the corresponding BKW mode amounts to the more stringent condition $c_2(0) = -\frac{1}{2}b_0^2 \geq -2/25$. When $-5 < 25c_2(0) < -2$, the corresponding BKW mode f_{BKW} will therefore only be positive after a certain time has elapsed.

Class III. States of class II were restricted by the requirement $-\frac{1}{5} \leq c_2(0) < 0$. There is no physical argument, however, that restricts $c_2(0)$ to negative values in general. As we shall see in Section 7, perfectly reasonable initial states have $c_2(0) > 0$. Clearly these states do not relax to equilibrium via the BKW mode.

These three classes of counterexamples show that the Krook–Wu conjecture is false in general. The only case where it contains an element of truth is that of class II, as discussed above.

7. THE TJON PHENOMENON

A problem of central interest in the context of the nonlinear Boltzmann equation is that of the buildup of the high-energy tails in the Maxwellian from initial states where particles of high energy are rare or absent. The BKW mode represents such a state and the approach to the equilibrium form of the high-energy tail can be read off from (28). Clearly $R_{\text{BKW}} < 1$ for $v^2 \gg 1$ and $0 < b \ll 1$, i.e., the high-energy tails are approached from below. The approach is nonuniform, and the characteristic time to reach equilibrium increases essentially logarithmically with energy.

Tjon⁽⁸⁾ solved numerically the nonlinear Boltzmann equation for a

Maxwell-like model in two dimensions, with initial conditions of the type (in discretized version)

$$f(v, 0) = c_\alpha \delta(v^2 - \alpha) + c_\beta \delta(v^2 - \beta) \quad (36)$$

Normalization and the requirement $\langle v^2 \rangle = 3$ uniquely determine c_α and c_β . Positivity of f restricts the energies $\frac{1}{2}\alpha, \frac{1}{2}\beta$ to be on either side of the mean, $\frac{3}{2}$. When the high-energy peak (at $\frac{1}{2}\beta$) is located at moderate energies, Tjon found that the equilibrium distribution is approached from below, in accordance with the behavior of the BKW mode. For larger β , however, a crossover was observed to overpopulated high-energy tails that decayed to the equilibrium distribution from above. As we shall see, this phenomenon has a simple explanation.

We first discuss the approach to equilibrium of the high-energy tails of states in the Bobylev class. For simplicity, we restrict the discussion to the subclass with x^2 as the leading term (it contains, but is not exhausted by, the BKW mode). From (21) and (24) the time dependence of the coefficients in (33) is then $c_n(t) = c_n(0)e^{-n\Lambda_2 t/2}$. For high energies, $\epsilon = \frac{1}{2}v^2 \gg 1$, it is tempting to replace the Laguerre polynomials in (33) by their leading terms, $n!L_n^{(1/2)}(\epsilon) \simeq (-\epsilon)^n$. It is easy to see that this is indeed consistent, provided that $e^{-\Lambda_2 t/2} \ll 1$. In that case (33) reduces to

$$\begin{aligned} R(\epsilon, \tau) &\simeq 1 + \sum_{n=2}^{\infty} c_n(0)(-\epsilon e^{-\tau})^n \\ &= \psi(-\epsilon e^{-\tau}) \end{aligned} \quad (37)$$

where we have introduced the dimensionless time $\tau = \frac{1}{2}\Lambda_2 t$. Thus the asymptotics behavior, in the sense $\epsilon \gg 1$, $e^{-\tau} \ll 1$, $\epsilon e^{-\tau} = \text{finite}$, for states in the Bobylev class is simply discussed: calculate the Fourier transform of the initial state and replace the argument x by $-\epsilon e^{-\tau}$. [Check: in (28), let $b \rightarrow 0$ with $bv^2 = \text{finite}$. The result equals (25) with appropriate change of variables.]

In the Bobylev class discussed above the n th term decays like $e^{-n\tau}$. For a general initial state this is no longer true. The decay rates for the various parts of the x^n term range in general from $n\Lambda_2/2$ to Λ_n . With Maxwell molecules in three-dimensions the asymptotic growth of the linear eigenvalues is known to be $\Lambda_n \sim n^{1/4}$, i.e., considerably slower than linear in n . The result is that a general statement like (37), uniformly valid for all initial states in the region $\epsilon \gg 1$, $e^{-\tau} \ll 1$, $\epsilon e^{-\tau} = \text{finite}$, cannot be made.

It is still true, however, that the two slowest terms in (37) remain the slowest ones for arbitrary initial states. After a "sufficiently" long time, therefore, and for $\epsilon \gg 1$, one can write, in general,

$$R(\epsilon, \tau) \simeq 1 + c_2(0)\epsilon^2 e^{-2\tau} - c_3(0)\epsilon^3 e^{-3\tau} + \dots \quad (38)$$

What "sufficiently" means here will be investigated in the context of specific initial conditions in the next section.

The asymptotic result (38) explains the origin of the Tjon phenomenon. Using the initial condition (36), one determines $c_2(0)$ to be

$$c_2(0) = -[15 - 3(\alpha + \beta) + \alpha\beta]/30 \quad (39)$$

With $\alpha = 1$ this reduces to $c_2(0) = (\beta - 6)/15$. Thus, with $\beta < 6$ the high-energy tail of the equilibrium distribution is approached from below, whereas with $\beta > 6$ there is a crossover to an overpopulated tail which relaxes to equilibrium from above. The distinction is determined by the sign of $c_2(0)$. That is, the Tjon phenomenon (when the energy is sufficiently high so that the Laguerre polynomials can be replaced by their leading term) is associated with the states of class III discussed in Section 6.

It should be noted that the nonlinearity of the Boltzmann equation does not affect the two slowest terms in (37) or (38). The Tjon phenomenon in the final decay to equilibrium is thus contained in the linearized theory. So is the logarithmic dependence on energy of the characteristic time of the final decay. The nonlinearity does, however, play a role in determining the shape of the curve from, say, the crossover time on.

8. CALCULATIONS

From a physical point of view it is of interest to know not only the final asymptotics of $R(\epsilon, \tau)$, but the complete time dependence from times of the order of the crossover time. In this section we shall illustrate the use of the recursion scheme (31) to calculate $R(\epsilon, \tau)$ with initial conditions of the type (36). The rate of convergence of this procedure will be discussed.

Fourier transformation of (36) yields

$$\psi(x, 0) = \frac{e^x}{\beta - \alpha} \left\{ (\beta - 3) \frac{\sin[(2\alpha x)^{1/2}]}{(2\alpha x)^{1/2}} + (3 - \alpha) \frac{\sin[(2\beta x)^{1/2}]}{(2\beta x)^{1/2}} \right\} \quad (40)$$

Expansion of (40) in a Taylor series in x gives the initial values of the coefficients $c_n(0)$. Calculations will be performed with $(\alpha, \beta) = (1, 9)$ and $(\alpha, \beta) = (3, 3)$.

The recursion scheme (31) involves integrals with the complicated function $g(\mu)$ in the integrand. We do not have to carry out any integrations, however, since these integrals can be expressed as linear combinations of the eigenvalues Λ_n , which have been calculated⁽¹⁷⁾ with great accuracy up to $n = 18$. Use of the definition (14) shows that the symmetric pair of terms in the sum in (31) can be expressed as

$$\begin{aligned} 2\pi \int_{-1}^1 d\mu g(\mu) \left[\left(\frac{1+\mu}{2} \right)^{n-m} \left(\frac{1-\mu}{2} \right)^m + \left(\frac{1+\mu}{2} \right)^m \left(\frac{1-\mu}{2} \right)^{n-m} \right] \\ = - \sum_{l=0}^m (-1)^l \binom{m}{l} \Lambda_{n-m+l} \end{aligned} \quad (41)$$

The right-hand side of (41) could be reduced further since odd eigenvalues can be written as linear combinations of the preceding even ones. This is useful for certain checks of consistency, but not for numerical calculations. Introducing the dimensionless time $\tau = \frac{1}{2} \Lambda_2 t$ and dimensionless eigenvalues $\bar{\Lambda}_n = \Lambda_n / \frac{1}{2} \Lambda_2$, we arrive at the final form of the recurrence scheme (31):

$$\begin{aligned} \frac{dc_n(\tau)}{d\tau} + \bar{\Lambda}_n c_n(\tau) \\ = \sum_{m=2}^{[n/2]} \left(1 - \frac{1}{2} \delta_{m,n/2}\right) c_{n-m}(\tau) c_m(\tau) \sum_{l=0}^m (-1)^l \binom{m}{l} \bar{\Lambda}_{n-m+l} \end{aligned} \quad (42)$$

In (42) the symmetry of the sum in (31) has been used, and the factor with the Kronecker $\delta_{m,n/2}$ prevents double counting. With the $\bar{\Lambda}_n$, as calculated by Alterman *et al.*,⁽¹⁷⁾ given in Table I, we have solved the recursion scheme (42) explicitly up to $n = 8$. With $c_n(\tau)$ determined from (42), insertion into (33) gives the final result in the general form

$$R(\epsilon, \tau) = 1 + \sum_{n=2}^{\infty} c_n(\tau) n! L_n^{(1/2)}(\epsilon) \quad (43)$$

We now return to a qualitative discussion of the convergence of the above procedure for various ϵ and τ . *In principle*, convergence is no problem, irrespective of ϵ and τ . We are, however, mostly interested in energies considerably larger than the thermal average $\frac{3}{2}$. And we would like to determine $R(\epsilon, \tau)$ for times down to, say, the crossover time. Large ϵ and small τ will require many terms in the expansion (43), and the rate of convergence is thus a problem *in practice*.

To get a rough idea of the difficulty, replace the Laguerre polynomials by their leading term for high energies, and use the form (37) at $\tau = 0$. In that (unrealistically conservative) case, the rate of convergence is determined by that of the Taylor expansion of $\psi(-\epsilon)$ with ψ given by (40). For $\beta \lesssim 10$, $\epsilon \gtrsim 20$ the dominating factor in this respect is $e^{-\epsilon}$. The number of

Table I. The Eigenvalues up to $\bar{\Lambda}_{18}$ According to Alterman *et al.*⁽¹⁷⁾

n	$\bar{\Lambda}_n = \Lambda_n / \frac{1}{2} \Lambda_2$	n	$\bar{\Lambda}_n = \Lambda_n / \frac{1}{2} \Lambda_2$
3	3.0	11	6.10984780
4	3.68443307	12	6.32736687
5	4.21108267	13	6.52944437
6	4.64234021	14	6.71834398
7	5.00940137	15	6.89585472
8	5.33015367	16	7.06341604
9	5.61583056	17	7.22220420
10	5.87396163	18	7.37319329

terms N one must retain in the expansion of $\psi(-\epsilon)$ is thus roughly $N \sim \epsilon$. When $n \sim \epsilon$, however, it is not a good approximation to replace $n! L_n^{(1/2)}(\epsilon)$ by $(-\epsilon)^n$. Use of the full Laguerre polynomials in (43) will improve convergence. So will inclusion of the time dependence.

As an estimate of the latter effect, disregard the improvement caused by using the full $n! L_n^{(1/2)}(\epsilon)$. The ratio of the last term (in our case $n = 8$) to the second can then be estimated by using the slowest relaxation rate $\bar{\Lambda}_8$. This ratio should be less than unity. A rough estimate of the time τ_c from which an eight-term approximation is satisfactory is then

$$\frac{c_8 \epsilon^8 \exp(-\bar{\Lambda}_8 \tau_c)}{c_2 \epsilon^2 \exp(-2\tau_c)} \sim 1 \quad (44)$$

Initial conditions of the type (40) with $(\alpha, \beta) = (1, 9)$ or $(3, 3)$ give $c_8/c_2 \sim 10^{-5}$, i.e.,

$$\tau_c \sim (6 \ln \epsilon - 11)/3.3 \quad (45)$$

For $\epsilon = 20$ this estimate indicates that an eight-term approximation gives satisfactory results for $\tau \gtrsim 2$. For $\epsilon = 50$, however, one should not expect convergence until $\tau \gtrsim 4$.

Rather than refine the above qualitative considerations, we test the stability of the numerical results by truncation after $n = 6, 7$, and 8 , respectively. The solid curves in Fig. 1 show the results for $R(\epsilon, \tau)$ with initial condition (40), $(\alpha, \beta) = (1, 9)$ [corresponding to $c_2(0) = 0.2$], and energies $\epsilon = 20$ and $\epsilon = 50$. For comparison the dashed curves in Fig. 1 give $R(\epsilon, \tau)$, truncated after $n = 8$, for the same values of ϵ , but with $(\alpha, \beta) = (3, 3)$ [i.e., $c_2(0) = -0.2$], corresponding to all particles initially having the average energy $\frac{3}{2}$. The solid curves exhibit the Tjon phenomenon, whereas the dashed curves show a behavior much closer to that of the BKW mode.

It is interesting to compare these results with the solution of the corresponding linearized problem. The linearized equation can, in addition, be used as an indication of the rate of convergence, since the troublesome slowest relaxation rates are those of the linearized theory. The eigenvalues $\bar{\Lambda}_n$ are known accurately up to $n = 18$. If one wants to go beyond this, extrapolation is necessary. We use the asymptotic formula

$$\bar{\Lambda}_n \simeq 4.31 n^{1/4} + 2.67 - 3.65 n^{-1/4} \quad (46)$$

the form of which is taken from Ref. 18.

Using Λ_2 and the form of $g(\mu)$ as found in Ref. 19, we calculated the coefficient of $n^{1/4}$ in (46) by asymptotic analysis. The two remaining coefficients in (46) were determined by linear regression analysis based upon the known values of $\bar{\Lambda}_{12}$ to $\bar{\Lambda}_{18}$. In Fig. 2 the solution of the linearized equation, truncated after $8, 18$, and 48 terms, is compared with the nonlinear solution, truncated after $n = 8$, for $(\alpha, \beta) = (1, 9)$ and $\epsilon = 20$ and 50 .

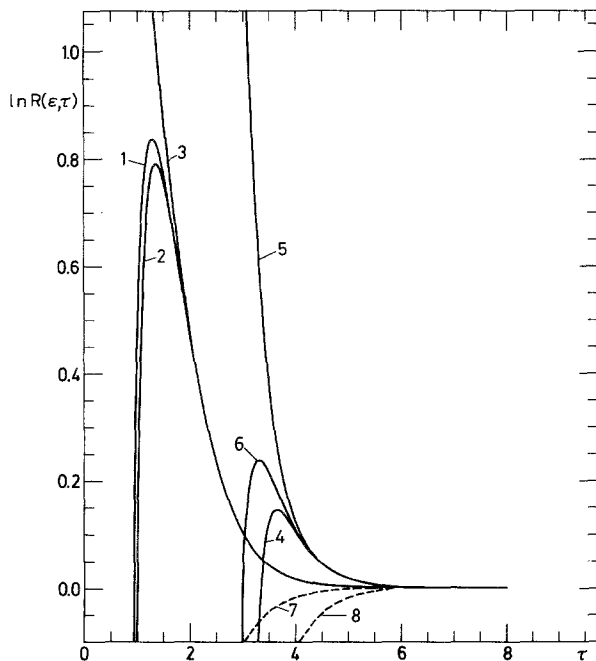


Fig. 1. The ratio $R(\epsilon, \tau)$ given by (43) as a function of τ , according to the truncated nonlinear recursion scheme (42). Solid curves refer to initial condition (40) with $(\alpha, \beta) = (1, 9)$. Curves 1–3 show $\ln R(20, \tau)$ truncated after $n = 8, 7,$ and $6,$ respectively. Curves 4–6 show $\ln R(50, \tau)$ correspondingly truncated. The dashed curves refer to an initial condition with $(\alpha, \beta) = (3, 3)$ and truncation after $n = 8$. With curve 7, $\epsilon = 20$; with curve 8, $\epsilon = 50$.

Figures 1 and 2 are in good agreement with the estimate (45). Figure 1 demonstrates clearly the sensitive dependence on τ of the convergence properties of the recursion scheme. For $\epsilon = 20$, the evidence from the linearized equation in Fig. 2 suggests that even down to the crossover time, a truncation after $n = 8$ gives results for $R(\epsilon, \tau)$ within about 10% of the exact solution. Furthermore, the linearized results in Fig. 2, truncated after $n = 18$, are indistinguishable from those truncated after $n = 48$ [with the extrapolation (46)] for $\epsilon = 20$ and 50 . This suggests that an extension of the nonlinear calculation to $n = 18$ would improve the accuracy considerably for these energies. Finally, Fig. 2 shows the effects of the nonlinearities to be relatively small in the entire time range of interest.

APPENDIX

In this appendix we show that eigenfunctions decaying asymptotically with a negative power of the velocity are only possible with Maxwell molecules.

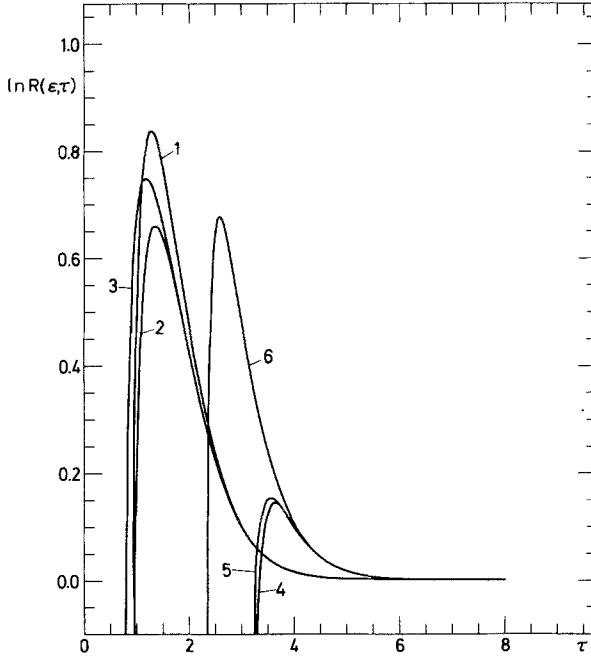


Fig. 2. Comparison with the linearized theory for $R(\epsilon, \tau)$, with $(\alpha, \beta) = (1, 9)$. With curves 1–3, $\epsilon = 20$, whereas with curves 4–6, $\epsilon = 50$. Curves 1 and 4 again give the nonlinear solutions for $\ln R(\epsilon, \tau)$ truncated after $n = 8$. Curves 2 and 5 give the correspondingly truncated linearized solutions. Curves 3 and 6 give the linearized solutions with truncation after $n = 18$. Truncation after $n = 48$ gives curves indistinguishable from curves 3 and 6.

Write for the velocity distribution and its Fourier transform

$$\begin{aligned} f(\mathbf{v}, t) &= f_{\text{eq}}(v) + \delta f(\mathbf{v}, t) \\ \varphi(\mathbf{k}, t) &= \left[\exp\left(-\frac{1}{2}k^2\right) \right] [1 + h(\mathbf{k}, t)] \end{aligned} \quad (\text{A1})$$

From Eqs. (5) and (8) in Section 2, linearization in δf yields in the spatially uniform case

$$\begin{aligned} \frac{\partial h(\mathbf{k}, t)}{\partial t} &= \frac{\exp\left(\frac{1}{2}k^2\right)}{(2\pi)^{3/2}} \int d\hat{\mathbf{n}} g_s(\hat{\mathbf{k}} \cdot \hat{\mathbf{n}}) \\ &\times \int dv dw \left[\left(\exp\left(-\frac{v^2}{2}\right) \right) \delta f(\mathbf{w}) + \left(\exp\left(-\frac{w^2}{2}\right) \right) \delta f(\mathbf{v}) \right] \\ &\times |\mathbf{v} - \mathbf{w}|^{1-4/s} \left\{ \exp\left[-\frac{i\mathbf{v}}{2} \cdot (\mathbf{k} + k\hat{\mathbf{n}}) - \frac{i\mathbf{w}}{2} \cdot (\mathbf{k} - k\hat{\mathbf{n}})\right] \right. \\ &\quad \left. - \exp(-i\mathbf{k} \cdot \mathbf{v}) \right\} \end{aligned} \quad (\text{A2})$$

Integration over the Maxwellians gives, for arbitrary s ,

$$\begin{aligned}
 \frac{\partial h(\mathbf{k}, t)}{\partial t} &= 2^{1/2-2/s} \frac{\Gamma(2-2/s)}{\Gamma(3/2)} \int d\hat{\mathbf{n}} g_s(\hat{\mathbf{k}} \cdot \hat{\mathbf{n}}) \int d\mathbf{v} \delta f(\mathbf{v}) \\
 &\times \left\{ \exp\left(-i\mathbf{k}_- \cdot \mathbf{v} + \frac{1}{2} k_-^2\right) {}_1F_1\left(-\frac{1}{2} + \frac{2}{s}; \frac{3}{2}; -\frac{v^2}{2} - i\mathbf{k}_+ \cdot \mathbf{v} + \frac{k_+^2}{2}\right) \right. \\
 &- {}_1F_1\left(-\frac{1}{2} + \frac{2}{s}; \frac{3}{2}; -\frac{v^2}{2} - i\mathbf{k} \cdot \mathbf{v} + \frac{k^2}{2}\right) \\
 &+ \exp\left(-i\mathbf{k}_+ \cdot \mathbf{v} + \frac{1}{2} k_+^2\right) {}_1F_1\left(-\frac{1}{2} + \frac{2}{s}; \frac{3}{2}; -\frac{v^2}{2} - i\mathbf{k}_- \cdot \mathbf{v} + \frac{k_-^2}{2}\right) \\
 &\left. - \exp\left(-i\mathbf{k} \cdot \mathbf{v} + \frac{1}{2} k^2\right) {}_1F_1\left(-\frac{1}{2} + \frac{2}{s}; \frac{3}{2}; -\frac{v^2}{2}\right) \right\} \quad (\text{A3})
 \end{aligned}$$

Here $\Gamma(x)$ is the gamma function, ${}_1F_1(a; b; z)$ is the confluent hypergeometric function, and $\mathbf{k}_\pm = \frac{1}{2}k(\hat{\mathbf{k}} \pm \hat{\mathbf{n}})$. The large- v asymptotics of the ${}_1F_1$ in (A3) are given by

$${}_1F_1\left(-\frac{1}{2} + \frac{2}{s}; \frac{3}{2}; -\frac{v^2}{2} + \dots\right) \simeq \frac{\Gamma(3/2)}{\Gamma(2-2/s)} \left(\frac{v^2}{2}\right)^{1/2-2/s} \quad (\text{A4})$$

Assume now that for large v , $\delta f(\mathbf{v}) \simeq v^{-2p-3}$, where p is noninteger. This corresponds to a leading noninteger power k^{2p} for small k in $h(\mathbf{k})$. The large- v contribution to the \mathbf{v} integral in (A3) reads, by (A4),

$$\begin{aligned}
 \int d\mathbf{v} v^{-2p-3+1-4/s} \left\{ \exp(-i\mathbf{k}_- \cdot \mathbf{v} + \frac{1}{2}k_-^2) - 1 \right. \\
 \left. + \exp(-i\mathbf{k}_+ \cdot \mathbf{v} + \frac{1}{2}k_+^2) - \exp(-i\mathbf{k} \cdot \mathbf{v} + \frac{1}{2}k^2) \right\} \quad (\text{A5})
 \end{aligned}$$

The leading noninteger power of k follows from (A5) after performance of the angular integral $\int d\hat{\mathbf{n}}$ in (A3) as

$$-\Lambda_{p-1/2+2/s} k^{2(p-1/2+2/s)} \quad (\text{A6})$$

That is, when the linearized operator acts on k^{2p} it generates a leading term of the form (A6). Thus an *eigenfunction* with leading noninteger power k^{2p} can only exist provided $s = 4$, i.e., with Maxwell molecules.

NOTE ADDED IN PROOF

The above argument seems to permit eigenfunctions with $p = 3/2 - 2/s$, since $\Lambda_1 = 0$. However, such eigenfunctions are excluded by energy conservation, as shown by H. Cornille and A. Gervois (to be published) for the special case of hard spheres ($s \rightarrow \infty$).

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