Boltzmann equation and the conservation of particle number

Zhang Banggu
Science Press, Beijing 100707, China
(Received 16 October 1989)

The violation of particle-number conservation by some spherical solutions of the Boltzmann equation is known to exist. The reason stems from the fact that the Boltzmann equation itself includes a contradiction: The velocity of a particle is independent of the position of the particle, but the acceleration, namely the time derivative of velocity, is related to the position. Considering the velocity as a function of position and time, we introduce a new equation. Under the same initial condition as for the Boltzmann equation, a strict solution of the new equation does not violate the particle-number conservation law.

I. INTRODUCTION

As is well known, the Boltzmann equation

$$\frac{\partial}{\partial t}f(\mathbf{v},\mathbf{r},t)+\mathbf{v}\cdot\frac{\partial}{\partial \mathbf{r}}f+\mathbf{a}\cdot\frac{\partial}{\partial \mathbf{v}}f=I_c(\mathbf{v},\mathbf{r},t) \tag{1}$$

is one of the fundamental equations in statistical mechanics;[1,2] in particular, it plays a very important role in nonequilibrium state statistics,[3] and in gas dynamics.[4–6] The distributed function $f(\mathbf{v},\mathbf{r},t)$ in (1) is the number of particles in unit volume of velocity space near $\mathbf{v}$ and unit volume of position space near $\mathbf{r}$ at time t, and $\mathbf{a}$ is the acceleration of particle.[3] Some authors write this term as $\mathbf{K}/m$, the force exerted on the unit mass of the particle. In many books the Boltzmann equation (1) is derived from the conservation of the particle number in phase space. There the corresponding term is the velocity in velocity space; therefore, the use of $\mathbf{a}$ in (1) is more direct and definite. $I_c(\mathbf{v},\mathbf{r},t)$ in (1) is the collision term[4]

$$I_c(\mathbf{v},\mathbf{r},t)=\int\int d^3v_1 d\Omega'\sigma u\,[f(\mathbf{v}')f(\mathbf{v}_1')-f(\mathbf{v})f(\mathbf{v}_1)]_{(\mathbf{r},t)}\ , \tag{2}$$

where the variables $\mathbf{r}$ and t of distributed functions in the square brackets are all the same, and the velocities are such that, after the collision of two particles with velocities $\mathbf{v}$ and $\mathbf{v}_1$, their velocities become $\mathbf{v}'$ and $\mathbf{v}_1'$, respectively. $\mathbf{u}=\mathbf{v}-\mathbf{v}_1$, $\mathbf{u}'=\mathbf{v}'-\mathbf{v}_1'$, and $d\Omega'$ is the solid angle of $\mathbf{u}'$; σ is the cross section of the collision.

II. EXPANSION OF TIME SERIES AND THE REQUIREMENT OF PARTICLE-NUMBER CONSERVATION

Because (1) is a nonlinear differential-integral equation, in general, it is difficult to find a solution of (1).[4,7] Let us only discuss an isolated particle system and find the solution with following form:

$$f(\mathbf{v},\mathbf{r},t)=\sum_{i=0}^{\infty}(C_t t)^i f_i(\mathbf{v},\mathbf{r})\ , \tag{3}$$

where C_t is a constant,

$$C_t=(2\pi m n_0 G/3)^{1/2}\ , \tag{4}$$

where m is the mass of particle, n_0 the initial density of particle number at the point $r=0$, and G is the gravitation constant.

Now let us discuss the requirement of particle-number conservation. The total particle number of the system is

$$N=\int\int d^3v\, d^3r\, f(\mathbf{v},\mathbf{r},t)\ . \tag{5}$$

From (3) we have

$$N=\sum_{i=0}^{\infty}(C_t t)^i N_i\ , \tag{6}$$

where

$$N_i=\int\int d^3v\, d^3r\, f_i(\mathbf{v},\mathbf{r})\ . \tag{7}$$

The conservation of particle number requires

$$0=\frac{dN}{dt}=\sum_{i=1}^{\infty}iC_t(C_t t)^{i-1}N_i\ , \tag{8}$$

that is,

$$N_i=0\quad(i=1,2,\ldots)\ . \tag{9}$$

III. SOME SPHERICAL SOLUTIONS OF (1) DO NOT OBEY THE CONSERVATION OF PARTICLE NUMBER

Substituting (3) into (2), we obtain

$$I_c(\mathbf{v},\mathbf{r},t)=\sum_{i=0}^{\infty}(C_t t)^i I_{ci}(\mathbf{v},\mathbf{r})\ , \tag{10}$$

where

$$I_{ci}=\int\int d^3v_1 d\Omega'\sigma u\sum_{j=0}^{i}[f_j(\mathbf{v}')f_{i-j}(\mathbf{v}_1')-f_j(\mathbf{v})f_{i-j}(\mathbf{v}_1)]_{(r)}\ . \tag{11}$$

For simplicity, we assume σ to be a constant in following calculation.

If we only discuss the isolated system in which there is gravitation interaction among particles, we have

$$\mathbf{a}=mG\int\int d^3v\, d^3r' f(\mathbf{v},\mathbf{r}',t)(\mathbf{r}'-\mathbf{r})/|\mathbf{r}'-\mathbf{r}|^3 \ . \quad (12)$$

Applying (3), we obtain

$$\mathbf{a}(\mathbf{r},t)=\sum_{i=0}^{\infty}(C_t t)^i \mathbf{a}_i(\mathbf{r}) \ , \quad (13)$$

where

$$\mathbf{a}_i(\mathbf{r})=mG\int\int d^3v\, d^3r' f_i(\mathbf{v},\mathbf{r}')(\mathbf{r}'-\mathbf{r})/|\mathbf{r}'-\mathbf{r}|^3 \ . \quad (14)$$

Substituting (3), (10), and (13) into (1), we can get a recurrence formula of $f_i(\mathbf{v},\mathbf{r})$,

$$(i+1)C_t f_{i+1}(\mathbf{v},\mathbf{r})+\mathbf{v}\cdot\frac{\partial}{\partial\mathbf{r}}f_i+\sum_{j=0}^{i}\mathbf{a}_j\cdot\frac{\partial}{\partial\mathbf{v}}f_{i-j}=I_{ci} \ . \quad (15)$$

Now let us find spherical solutions of (1) with the form (3) under some initial conditions.

(i) *Uniform initial condition.* If the initial condition is

$$f_0=f(\mathbf{v},r,t=0)=M^*(v)N(r,t=0)$$
$$=M^*(v)n_0\times\begin{cases}1 & (r\le R)\ ,\\ 0 & (r>R)\ ,\end{cases} \quad (16)$$

where $M^*(v)$ is the Maxwell velocity distribution, and n_0 and R are some constants. Applying the recurrence formula (15) twice, we can obtain $f_2(\mathbf{v},r)$, and using (7), we obtain

$$N_2=4\pi n_0 R^3/3 \ . \quad (17)$$

This result does not satisfy the condition (9) required by conservation of particle number.

Although the solution discussed here is approximate to the second order, the result of the violation of particle-number conservation by this solution is exact. That is to say, this solution does not obey the conservation of particle number, even though other N_i ($i=3,4,\ldots$) are equal to zero. This point must be emphasized.

(ii) *Some continuous initial conditions.* Instead of (16) we can take

$$f_0=M^*(v)n_0\exp(-k_1 r) \ , \quad (18)$$

where k_1 is a constant.

As for case (i), we obtain

$$N_2=4\pi n_0 k_1^{-3}(k_1/C_r)^2+7.5\neq 0 \ , \quad (19)$$

where

$$C_r=(2\pi m^2 n_0 G/3kT)^{1/2} \ , \quad (20)$$

where k is the Boltzmann constant and T is the initial absolute temperature. In other words, under the continuous initial condition (18) in all the space, the solution of the Boltzmann equation (1) still violates the conservation of particle number.

We can also discuss a more physical initial condition, assuming that the initial temperature is dependent on the radius r, i.e.,

$$f_0=[m/2kT\exp(-k_2 r)]^{3/2}\exp[-mv^2/2kT\exp(-k_2 r)]n_0\exp(-k_1 r) \ . \quad (21)$$

This time T is the initial absolute temperature at the center of the system and k_2 is a constant.

As in (19), we can obtain

$$N_2=4\pi n_0 k_1^2 C_r^{-2}(k_1+k_2)^{-3}+3n_0 k_1^{-4}k_2+36n_0 k_1^{-3}\neq 0 \ . \quad (22)$$

IV. THE CONTRADICTION OF THE BOLTZMANN EQUATION

It is well known that the Boltzmann equation (1) can be derived from the conservation of particle number in the phase space. That is to say, the velocity $\mathbf{v}$ of a particle is considered as an independent variable, irrelevant of the position $\mathbf{r}$ of the particle. But, in general, the force exerted on a particle should be dependent on the position of the particle. In fact, we can think of an isolated spherical particle group, where the force exerted on a particle at the center of the group equals zero and the force exerted on a particle at the rim of the group equals the vector sum ($-GMm\mathbf{r}/r^3$) of the forces exerted on the particle by all the particles in the group. That is to say, the acceleration of the particle, namely, the time derivative of velocity, is dependent on the position of the particle. Therefore, the Boltzmann equation (1) itself includes a contradiction. And it is this contradiction that causes the problem of the violation of the conservation of particle number by solutions of the Boltzmann equation.

The Boltzmann equation can also be derived from the Liouville equation. In that case the velocity of a particle is still considered as an independent variable, irrelevant of the position of the particle. Therefore, the contradiction still exists.

V. A NEW EQUATION

It is not difficult to see that the conservation of particle number can be guaranteed by a totally differential equation,

$$\frac{D}{Dt}f(\mathbf{v},\mathbf{r},t)=0 \ . \quad (23)$$

In fact, from (5) and (23) we have

$$\frac{dN}{dt}=\int\int d^3v\, d^3r\,\frac{D}{Dt}f(\mathbf{v},\mathbf{r},t)=0 \ . \quad (24)$$

This time we consider the velocity of a particle as a function of the position of the particle and time, i.e., we consider the relations of variables as

$$f(\mathbf{v},\mathbf{r},t)=f(\mathbf{v}(\mathbf{r}(t),t),\mathbf{r}(t),t)\ . \tag{25}$$

Then from (23) and (25) we can get

$$\frac{\partial}{\partial t}f(\mathbf{v},\mathbf{r},t)+\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}+\left[\mathbf{v}\cdot\frac{\partial \mathbf{v}}{\partial \mathbf{r}}+\frac{\partial \mathbf{v}}{\partial t}\right]\cdot\frac{\partial f}{\partial \mathbf{v}}=0\ . \tag{26}$$

Now let us solve this equation under the initial condition (16). This time, there is a new difficulty in the calculation of $\partial\mathbf{v}/\partial\mathbf{r}$. For that, we can consider the velocity $\mathbf{v}$ as a sum of the random velocity and another part. Obviously, the random velocity, i.e., the thermomotive part of the velocity, is independent of the position $\mathbf{r}$ absolutely. Only the average velocity $\bar{\mathbf{v}}$ that remains after removing the random factor is dependent on the position $\mathbf{r}$. This part of the velocity is a result of the gravitation interaction among particles. Then (26) becomes

$$\frac{\partial}{\partial t}f(\mathbf{v},\mathbf{r},t)+\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}+\left[\mathbf{v}\cdot\frac{\partial \bar{\mathbf{v}}}{\partial \mathbf{r}}+\mathbf{a}\right]\cdot\frac{\partial f}{\partial \mathbf{v}}=0\ , \tag{27}$$

where we have used $\partial\mathbf{v}/\partial t=\mathbf{a}$.

Using the method used in Ref. 8, we can obtain a strict solution of (27) without any approximation. For simplicity, here we only gave the result

$$f(\mathbf{v},r,t)=f_0\sum_{i=0}^{\infty}(C_rC_trt)^i\sum_{j=0}^{i/2}a_{ij}(C_v v\cos\alpha)^{i-2j}\ , \tag{28}$$

where the coefficients a_{ij} are

$$a_{ij}=(-1)^{i+j}2^{i-j}/(i-2j)!j!\ , \tag{29}$$

α in (28) is the angle between $\mathbf{v}$ and $\mathbf{r}$, and the constant C_v is

$$C_v=(m/kT)^{1/2}\ . \tag{30}$$

Now let us check this solution. Applying two integral formulas

$$\int M^*(v)(C_v v\cos\alpha)^{2n}d^3v=(2n-1)!!\ , \tag{31}$$

$$\int M^*(v)(C_v v\cos\alpha)^{2n-1}d^3v=0\ , \tag{32}$$

where the double factorial $(2n-1)!!$ is defined by

$$\begin{gathered}(2n-1)!!=(2n-1)(2n-3)\cdots5\times3\times1\ ,\\ (-1)!!=1,\quad m!!=0\ \text{ if } m<-1\ .\end{gathered} \tag{33}$$

We can obtain

$$\begin{aligned}\eta(r,t)&=\int d^3v\, f(\mathbf{v},r,t)\\ &=N(r,t=0)\sum_{\xi=0}(C_rC_trt)^{2\xi}\\ &\qquad\times\sum_{j=0}^{\xi}a_{2\xi,j}(2\xi-2j-1)!!\ .\end{aligned} \tag{34}$$

By means of (29) we can write the sum about j in (34) as

$$\begin{aligned}\sum_{j=0}^{\xi}a_{2\xi,j}(2\xi-2j-1)!!&=\sum_{j=0}^{\xi}(-1)^j2^{\xi}/(\xi-j)!j!\\ &=\frac{2^{\xi}}{\xi!}\lim_{x\to1}\sum_{j=0}^{\xi}(-x)^j\xi!/(\xi-j)!j!\\ &=\frac{2^{\xi}}{\xi!}\lim_{x\to1}\sum_{j=0}^{\xi}C_{\xi}^{j}(-x)^j\\ &=\frac{2^{\xi}}{\xi!}\lim_{x\to1}(1-x)^{\xi}=\frac{2^{\xi}}{\xi!}\delta_{\xi0}\ .\end{aligned} \tag{35}$$

So we get

$$\begin{aligned}\eta(r,t)&=N(r,t=0)\sum_{\xi=0}^{\infty}(C_rC_trt)^{2\xi}\frac{2^{\xi}}{\xi!}\delta_{\xi0}\\ &=N(r,t=0)\ .\end{aligned} \tag{36}$$

Considering only the gravitation among particles, we have

$$\begin{aligned}\mathbf{a}&=-\mathbf{r}Gr^{-3}4\pi\int_0^r r'^2dr'm\,\eta(r',t)\\ &=-\mathbf{r}Gr^{-3}4\pi\int_0^r r'^2dr'mN(r',t=0)\\ &=\begin{cases}-2C_t^2\mathbf{r} & (r\le R)\\ 0 & (r>R)\ .\end{cases}\end{aligned} \tag{37}$$

Noticing that $\bar{\mathbf{v}}$ is the average velocity of a single particle, and applying (31) and (32) again, we can obtain

$$\begin{aligned}\bar{\mathbf{v}}&=n_0^{-1}\int d^3v\, f(\mathbf{v},r,t)\mathbf{v}\\ &=C_v^{-1}\sum_{\xi=0}^{\infty}(C_rC_trt)^{2\xi+1}\sum_{j=0}^{\xi}a_{2\xi+1,j}(2\xi-2j-1)!!\mathbf{r}/r\\ &\qquad\qquad (r\le R)\ .\end{aligned} \tag{38}$$

As in (35), we can have

$$\sum_{j=0}^{\xi}a_{2\xi+1,j}(2\xi-2j-1)!!=-\delta_{\xi0}2^{2\xi+1}/\xi!\ . \tag{39}$$

Then, we get

$$\begin{aligned}\bar{\mathbf{v}}&=C_v^{-1}\sum_{\xi=0}^{\infty}(C_rC_trt)^{2\xi+1}(-1)\delta_{\xi0}2^{2\xi+1}\mathbf{r}/r\xi!\\ &=-2C_t^2\mathbf{r}t\quad (r\le R)\ .\end{aligned} \tag{40}$$

Applying (28), we can obtain $\partial f/\partial t$, $\partial f/\partial\mathbf{r}$, and $\partial f/\partial\mathbf{v}$ directly. Substituting them and (37) and (40) into (27) and making some appropriate readjustment, we can have

$$\frac{\partial}{\partial t}f+\mathbf{v}\cdot\frac{\partial f}{\partial \mathbf{r}}+\left[\mathbf{v}\cdot\frac{\partial \overline{\mathbf{v}}}{\partial \mathbf{r}}+\mathbf{a}\right]\cdot\frac{\partial f}{\partial \mathbf{v}}$$
$$=f_0\sum_{i=0}^{\infty}(C_rC_trt)^iC_tt\sum_{j=0}^{i/2}(C_vv_r)^{i-2j}[(i+1)a_{i+1,j+1}+2a_{i,j+1}-2(i-2j)a_{ij}]$$
$$+f_0\sum_{i=0}^{\infty}(C_rC_trt)^iC_rr\sum_{j=0}^{i/2}(C_vv_r)^{i-2j+1}[(i+1)a_{i+1,j}+2a_{ij}-2(i-2j+2)a_{i,j-1}] . \quad (41)$$

Now let us calculate the value of the expressions in the two square brackets. Using the representative (29) of a_{ij}, we get

$$[(i+1)a_{i+1,j+1}+2a_{i,j+1}-2(i-2j)a_{ij}]$$
$$=(i+1)(-1)^{i+j}2^{i-j}/(i-2j-1)!(j+1)!+2(-1)^{i+j+1}2^{i-j-1}/(i-2j-2)!(j+1)!$$
$$-2(i-2j)(-1)^{i+j}2^{i-j}/(i-2j)!j!$$
$$=(-1)^{i+j}2^{i-j}(i+1-i+2j+1-2j-2)/(i-2j-1)!(j+1)!=0 . \quad (42)$$

Similarly,

$$[(i+1)a_{i+1,j}+2a_{ij}-2(i-2j+2)a_{i,j-1}]=0 . \quad (43)$$

Now we are sure that (28) is a strict solution of Eq. (27). And from (36) we see that the solution (28) certainly obeys the conservation of particle number.

VI. CONCLUSION AND DISCUSSION

To summarize, we get the following results.

(i) The expansion of time series is a feasible method to solve differential equation with several variables.

(ii) The spherical solutions of the Boltzmann equation do not obey the particle-number conservation law.

(iii) The Boltzmann equation itself includes a contradiction. When the gravitation interaction among particles cannot be neglected, the contradiction appears.

(iv) The solution (28) of the new equation (27) obeys the particle-number conservation law.

Now let us discuss the convergence of the expansion (3) under the initial conditions (16), (18), and (21). Because the exponential functions $\exp(-v^2)$ and $\exp(-r)$ have good convergence, $f_i(\mathbf{v},\mathbf{r})$ in (3) are finite in the whole velocity space and some large position space. Equation (3) shows that the convergent region of the solution with time series is $C_tt<1$. Equation (4) indicates that C_t is a very small constant. For example, if $mn_0=1$ kg/m^3, which is the density of atmosphere near the surface of the earth, the order of C_t is 10^{-5} s^{-1} and if $mn_0=10^{-18}$ kg/m^3, the density of gas in the space among stars, the order of C_t is 10^{-14} s^{-1}. Therefore, it is meaningful to discuss the problem of particle-number conservation in the time interval $t<C_t^{-1}$.

[1]W. Pauli, *Pauli Lectures on Physics* (MIT Press, Cambridge, MA, 1973).
[2]R. H. Fowler, *Statistical Mechanics* (Cambridge University Press, Cambridge, England, 1980).
[3]I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Interscience, New York, 1962).
[4]S. Chapmann and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases*, 3rd ed. (Cambridge University Press, Cambridge, England, 1973).
[5]W. G. Vincenti and C. H. Kruger, Jr., *Introduction to Physical Gas Dynamics* (Wiley, New York, 1965).
[6]J. W. Bond, Jr., K. M. Watson, and E. A. Welch, Jr., *Atomic Theory of Gas Dynamics* (Addison-Wesley, Reading, MA, 1965).
[7]C. Cercianani, *Theory and Application of the Boltzmann Equation* (Scottish Academic, Edinburgh, 1975).
[8]Zhang Banggu, J. Phys. A **20**, L959 (1987).