Paradoxical aspects of the kinetic equations

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Abstract

Two paradoxical aspects of the prevailing kinetic equations are presented. One is related to the usual understanding of distribution function and the other to the usual understanding of the phase space. With help of simple counterexamples and direct analyses, involved paradoxes manifest themselves.

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When the Boltzmann equation, thought of as the first equation of the prevailing kinetic theory, came out, strong doubts arose, of which many were related to the fact that whereas Newton’s equations themselves were time-reversible the Boltzmann equation, as a consequence of Newton’s equations, was time-irreversible[1]. As time went by, particularly after the “rigorous” BBGKY theory was formulated in the middle of the last century[2–8], the philosophical concern of the time-reversal paradox gradually faded out, and it was believed that the ultimate understanding of the related issues had been completely established, at least in the regime of classical mechanics.

However, relatively recent developments of mathematics and physics seem to have brought new elements into the picture. In particular, the studies of fractals[9, 10] reveal that there can, at least in the mathematical sense, exist functions that have structures of self-similarity even at the infinitesimal level. Such functions are intrinsically discontinuous and cannot be described by usual differential apparatuses. Along this line, an increasing number of scientists are surmising that if any similar structures are found in realistic gases, some of conventional concepts in the standard theory need to be revised significantly.

In connection with this, we wish to present and discuss two relatively unknown aspects of the standard framework of kinetic theory. Firstly, it will be
shown that a realistic gas contains, almost always, a significant amount of particles whose distribution function does not keep invariant in the six-dimensional phase space and cannot be regarded as a continuous one. Secondly, it will be illustrated that there are inherent difficulties in formulating the particles that enter and leave an infinitesimal phase volume element during an infinitesimal time, which suggests in the sense that the phase space is more sophisticated than the customary thought assumes. By removing abstractness of the matters, all related paradoxes become surprisingly simple and straightforward. We are now convinced that if those paradoxes had been unveiled at the very beginning, kinetic theory would have been renewed several times.

The basic core of the classical kinetic theory says that if particles of a gas do not interact with each other, the distribution function describing them satisfies the collisionless Boltzmann equation

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0, \tag{1}
\]

which is, according to well-known textbooks\cite{11, 12}, equivalent to the path-invariance of collisionless distribution function

\[
\frac{df}{dt} \bigg|_{\mathbf{r}(t), \mathbf{v}(t)} = 0, \tag{2}
\]

where the subindexes \(\mathbf{r}(t)\) and \(\mathbf{v}(t)\) imply that the differentiation is taken along a particle’s path. Conceptually speaking, equation (2) can be interpreted as saying that such a gas is “incompressible” in the phase space. The standard theory further states that, if collisions between particles are more than negligible, a certain type of collisional operator needs to be introduced to replace the zero term in (1). After having the collisional operator due to Boltzmann himself, equation (1) becomes

\[
\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = \int_{\mathbf{v}_1, \Omega} [f(\mathbf{v}')f(\mathbf{v}_1') - f(\mathbf{v})f(\mathbf{v}_1)] u_{\sigma}(\Omega) d\Omega d\mathbf{v}_1, \tag{3}
\]

where the first term on the right side represents particles entering the unit phase volume element and the second term particles leaving the unit phase volume element.

Although the formulation briefed in the last paragraph seems stringent and has been accepted unanimously in the community, it is not truly sound. Ironically enough, even a simple glance at the form of the Boltzmann equation (3) offers intriguing things to ponder. On the left side there is a symmetry between \(\mathbf{r}\) and \(\mathbf{v}\) in terms of differentiation operation; whereas on the right side the position vector \(\mathbf{r}\) serves as an inactive “parameter” and all the integral operations are performed in the velocity space. (The solid angle \(\Omega\) is defined in terms of the velocities.) This disparity, while seeming a bit too schematic to be fully
convincing, should serve a motivation for us to investigate the whole issue more carefully and more thoroughly.

We first look at whether or not the collisionless Boltzmann equation (1) and the path-invariance theorem (2) make sense as they intend to.

In the mathematical sense, the picture provided by the path-invariance is quite clear and simple. Consider a sufficiently small volume element

$$\Delta x \Delta y \Delta z \Delta v_x \Delta v_y \Delta v_z$$

moving together with a certain particle in the phase space; the theorem asserts that the particle density within the element (in number herein) does not increase or decrease. In well-known textbooks, the theorem is “proved” by applying the rigorous Jacobian approach[11–13]. Here, for the purpose of this paper, we wish to illustrate the theorem and its derivation in an intuitive way. Fig. 1 describes what takes place in the two-dimensional $x$-$v_x$ subspace. As time passes from $t = 0$ to $t = T$, the particles distributed inside the rectangle $\Delta x \Delta v_x$ in Fig. 1a will be distributed inside the parallelogram in Fig. 1b. By excluding all external forces (just for simplicity), it is obvious that the area of the parallelogram is equal to that of the rectangle and the average particle density within the moving volume element keeps invariant. On the understanding that particles distribute continuously within $\Delta x \Delta v_x$ and the size of $\Delta x \Delta v_x$ can shrink to zero, the invariance of the average particle density can certainly be interpreted as the path-invariance of distribution function. The discussion above, though simplified somewhat, reflects the essence of the full theorem accurately.

It seems, at this stage, that the validity of the path-invariance (2), together with the picture of incompressible fluid in the phase space, is so solid and so clear that we should discuss it no more. But, somehow, the truth is not that simple: there exist many cases in that gases behave very differently. To get an immediate idea about such behavior, let’s look at the special arrangement shown in Fig. 2, where particles with definite velocity $v$ strike a convex solid surface and then get reflected from it elastically. (Later on, more general models about collisions between particles and boundaries will be adopted and examined.) Following a moving particle and counting particles in a definite position range $d\boldsymbol{r} \equiv dx dy dz$ and in a definite velocity range $d\boldsymbol{v} \equiv dv_x dv_y dv_z$, we find out a clear-cut fact that the reflected particles simply obey

$$\frac{df}{dt} \bigg|_{\boldsymbol{r}(t), \boldsymbol{v}(t)} < 0 \quad \text{and} \quad \frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \frac{\partial f}{\partial \boldsymbol{r}} + F \cdot \frac{\partial f}{\partial \boldsymbol{v}} < 0.$$  

That is to say, these particles diverge in the phase space. In a similar way, we can readily see that if the incident particles fall upon a concave solid surface, the reflected particles will, in some region, obey

$$\frac{df}{dt} \bigg|_{\boldsymbol{r}(t), \boldsymbol{v}(t)} > 0.$$
This tells us that the particles converge.

A sharp question arises. How can the path-invariance theorem, considered as the very core of all the kinetic equations, possibly suffer from such simple and direct counterexamples? By reviewing the derivation of the Boltzmann equation, we realize that equations (1) and (2) hold only for perfectly continuous distribution functions, while the diverging and converging particles presented above are related to none of them.

To see the point more vividly, let’s go back to the two-dimensional phase space, namely the $x$-$v_x$ space, and investigate the evolution of the particles marked with the dotted curve in Fig. 2. In the schematic sense, we may say that at $t = 0$ all these particles are distributed along the diagonal of $\Delta x \Delta v_x$ shown in Fig. 3a, rather than in $\Delta x \Delta v_x$ uniformly. After a while, at $t = T$, this diagonal is stretched and becomes longer as shown in Fig. 3b. If we set up a small, but definite, phase volume element and let it move together with one of the particles, we will certainly find that the particle density within it decreases. (For discontinuous distributions, if we allow the shape and size of measuring volume element to vary, we can get any value, drastically from zero to infinity, for the particle density.)

Now, it is in order to examine how a realistic boundary surface $S$ “reflects” realistic particles that come from all directions and with different speeds. Experimental facts inform us that the reflection cannot be truly elastic and stochastic and dissipative effects must play a certain role[14]. To express particles “produced” by such surface, it is proper (particularly if the gas is a rarefied one) to define the instant emission rate $\sigma$ on an infinitesimal surface $dS$ in such a way that

$$\sigma dt dS dv d\Omega$$

represents the number of particles ejected by the surface element in the speed range $dv$ and in the solid angle range $d\Omega$ during the time interval $dt$. By allowing the emission rate $\sigma$ to be described in probability and to have certain dependence on velocities of incident particles, it can be said that the stochastic and dissipative nature of the reflection has been included. Then, divide $S$ into $N$ surface elements. Referring to Fig. 4, we find that for the $i$th surface element $(\Delta S)_i$, the reflected particles are like ones emitted from a “point particle source” at $r_{0i}$, the position vector of $(\Delta S)_i$, and the relevant distribution function at a point $r$ in the reflection region takes the form

$$f(r, v, \Omega) = \frac{\sigma(\Delta S)_i}{|r - r_{0i}|^2 \rho^3} V_i(v) \delta(\Omega - \Omega_{r - r_{0i}}),$$

where $V_i(v)$ is a certain function of $v$ and $\delta(\Omega - \Omega_{r - r_{0i}})$ is the $\delta$-function defined on the solid angle in the velocity space. It is very obvious that, regardless of the forms of $\sigma$ and $V(v)$, this distribution function diverges in the phase space. Another interesting point about the distribution function is that it is perfectly continuous in terms of $r$ and $v$ and it is like a function defined on a single point in
terms of $\Omega$. Based on this observation, we are tempted to say that the function is on a variable domain of $4 + \epsilon$ dimensions. The total distribution function at $r$ associated with all reflected particles from $S$ is

$$f(r, v; \Omega) = \sum_{i=1}^{N} \frac{\sigma(\Delta S)_i}{|r - r_0_i|^2} v_i \delta(\Omega - \Omega_{r - r_0_i}).$$  \hspace{1cm} (9)$$

Though the distribution function expressed by (9) can, as $N \to \infty$, be regarded as a sum of an infinitely large number of $(4 + \epsilon)$-dimensional functions, it is not a continuous function defined in the phase space. Actually, with help of this expression, we can analytically or numerically prove that the particle number within a given moving volume element $d\mathbf{r}d\mathbf{v}$ is capable of decreasing, increasing or keeping invariant. As a limiting case, we may assume $S$ to be relatively small, or the distance $|\mathbf{r} - \mathbf{r}_0|$ to be relatively large, and find that expression (9) is reduced to expression (8) and the particles related to it always diverge in the phase space.

The above investigation, though formally simple, provides us with a very new picture on gas dynamics. Rather than as a continuous medium or an incompressible fluid in the phase space, a gas should be considered as a special collection of discrete particles, whose distribution function can change from continuous one to discontinuous one, as well as from discontinuous one to continuous one. Another notable fact, which may very much interest scientists carrying out practical studies, is that the changeovers aforementioned occur dramatically near interfaces between fluids and solid boundaries.

We now turn our attention to the validity of the collisional operator on the right side of (3). A widely accepted concept is that in order to formulate collisional effects we are supposed to focus ourselves on a fixed six-dimensional phase volume element and study how particles leave and enter the element due to collisions. In what follows, it will be shown that such concept is, much to our surprise, deceptive.

Firstly, particles leaving a phase volume element $d\mathbf{r}d\mathbf{v}$ during a time interval $dt$ are of interest. According to the standard theory, if a particle collides with another within the volume element $d\mathbf{r}d\mathbf{v}$ during $dt$, it should be considered as one that leaves the volume element during the time interval because of the velocity change caused by the collision (see Fig. 5). This intuitive, seemingly very reasonable, picture can be challenged in the following way. In deriving kinetic equations, a necessary step is to let $dt$, $d\mathbf{r}$ and $d\mathbf{v}$ approach zero independently. If it is assumed, in the limiting processes, that the length scale $|d\mathbf{r}|$ is much smaller than $|vdt|$, then virtually all the particles, initially within $d\mathbf{r}d\mathbf{v}$, will leave $d\mathbf{r}d\mathbf{v}$ at the end of $dt$, irrespective of suffering collisions or not. If we still want to say that the standard consideration, concerning how many particles stay inside $d\mathbf{r}d\mathbf{v}$ without involving collisions and how many particles get out of $d\mathbf{r}d\mathbf{v}$ with collisions involved, holds its significance, we have no choice but to assume that $|d\mathbf{r}| >> |vdt|$. An unfortunate fact is that no sound reason can be
found out for that we can prefer this assumption to its converse.

Secondly, particles entering a phase volume element \(d\mathbf{r}d\mathbf{v}\) during \(dt\) are under examination. In the standard treatment, two beams with velocities \(v'\) and \(v'^1\) are assumed to collide within a volume element \(d\mathbf{r}\) during \(dt\) and to give contribution to the particles expressed by \(f(\mathbf{r}, v, t)d\mathbf{r}d\mathbf{v}\), as shown in Fig. 6. Ironically enough, this treatment involves not one but many paradoxes. As one thing, particles produced by collisions in a small spatial region, like ones emitted from a point particle source, will diverge in the phase space and cannot be treated as an ordinary contribution to \(f(t, \mathbf{r}, \mathbf{v})d\mathbf{r}d\mathbf{v}\). As another thing, we again need to let \(dt\), \(d\mathbf{r}\) and \(d\mathbf{v}\) approach zero. If \(|d\mathbf{r}| \ll |vdt|\), all produced particles will “instantly” leave \(d\mathbf{r}d\mathbf{v}\) and only an insignificant fraction of them can be treated as a contribution to \(f(\mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v}\). See Ref. 16 to get more paradoxes.

In summary, two paradoxical aspects of the standard kinetic theory have been presented. The first aspect is related to the distribution function. A tacit assumption of the existing kinetic equations is that distribution functions, though describing discrete particles, must be mentally and practically continuous. The discussion of this paper, however, shows that distribution functions of realistic gases have, in general, complex local structures and they cannot be described by continuous distribution functions. The second aspect is related to the phase space. A usual concept in the standard theory is that the position space and the velocity space can be separated mentally and practically. The discussion of this paper, however, shows that whenever we investigate the time dynamics of particles in the velocity space we should keep an eye on what takes place in the position space, and vice versa.

A variety of fundamental questions can be raised, of which many are beyond the scope of this brief paper. In some of our recent works, we make more analyses and put forward alternative approaches[15, 16]. With help of a development in quantum mechanics[17], some of the discussion in this paper can also be extended to the regime of quantum statistical physics.

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Fig. 1: A moving phase volume element (a) at an initial time $t = 0$ and (b) at a later time $t = T$.

Fig. 2: Schematic of reflected particles from a solid surface. It is interesting to note that whether or not the involved collisions are elastic will not alter this picture significantly.

Fig. 3: Schematic of how the particles marked in Fig. 2 spread in the $x - v_x$ space. (a) These particles are distributed along one diagonal of the rectangle $\Delta x \Delta v_x$ at $t = 0$, and (b) the diagonal is stretched at $t = T$. 
Fig. 4: Particles reflected from a small surface element of realistic boundary.

Fig. 5: A particle involving a collision in a phase volume element.

Fig. 6: Two beams of particles collide with each other and produce particles with velocity $\mathbf{v}$. 