A path-integral approach to the collisionless Boltzmann gas

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Abstract: On contrary to the customary thought, the well-known “lemma” that the distribution function of a collisionless Boltzmann gas keeps invariant along a molecule’s path represents not the strength but the weakness of the standard theory. One of its consequences states that the velocity distribution at any point is a condensed “image” of all, complex and even discontinuous, structures of the entire spatial space. Admitting the inability to describe the entire space with a microscopic quantity, this paper introduces a new type of distribution function, called the solid-angle-average distribution function. With help of the new distribution function, the dynamical behavior of collisionless Boltzmann gas is formulated in terms of a set of integrals defined by molecular paths. In the new formalism, not only that the difficulties associated with the standard theory are surmounted but also that some of practical gases become calculable in terms of today’s computer.

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1 Introduction

The Boltzmann gas, by which we mean a gas in that molecules are subject to binary short-range interparticle forces, is usually studied by means of the Boltzmann equation\([1][2]\). The conventional wisdom assumes that if a sufficiently large supercomputer were available, a finite-difference scheme could be employed to construct solutions of the Boltzmann equation and many realistic gases would become completely analyzable.

Some of difficulties related to the solution-construction scheme of the Boltzmann equation are relatively well-known\[3\]. They include the following. (i) Seven variables have to be dealt with (time, spatial coordinates and velocity components). (ii) The collisional operator in the Boltzmann equation is complex in nature. Due to these difficulties, only low-dimensional problems, for instance those having one dimension of coordinates and one dimension of velocity components, were tried in practical calculations.

In some of our works\[4][5\], it was argued that more fundamental difficulties existed with the standard kinetic theory. One of them was that distribution functions of Boltzmann gases involved in discontinuity and quasi-discontinuity, thus the effectiveness of using a finite-difference scheme to solve the Boltzmann equation, as well as the validity of the Boltzmann equation itself, became questionable.

Putting aside whether the arguments presented by our previous works are sufficiently convincing or not, we will, in this paper, engage our primary attention with the following subject. Is there any alternative approach with the aid of that one can use today’s computational means to calculate at least some of full-dimensional practical gases? A positive answer to this question will apparently arouse widespread interest.

It turns out that if an average-type distribution function, called the solid-angle-average distribution function, is introduced and the path-information of molecules is adequately taken into account, then the objective mentioned above can be accomplished.

The structure of this paper is the following. In Sec. 2, the standard approach to the Boltzmann gas is employed to “derive” a lemma that the distribution function of a collisionless Boltzmann gas, if continuous at the beginning, will keep its value along a molecule’s path. In applying the lemma to various situations, we are led to an unexpected conclusion that strictly continuous and well-behaved distribution functions exist only on a theoretical assumption. In Sec 3, we examine two kinds of discontinuous distribution functions. The first kind is related to point-like molecular sources
and the second kind to surface-like molecular sources. It is shown that the solid-angle-average distribution function needs to be introduced in order to treat discontinuous distribution functions related to the molecular sources. Sec. 4 offers a comprehensive formulation in which both continuous and discontinuous distribution functions are formulated in terms of path-integrals defined by initial-state and boundary conditions. The final section, Sec. 5, gives a brief survey on essential features of the new formalism.

2 Evolution of continuous distribution function

We suppose in this section that the distribution function of interest is perfectly continuous, differentiable in a more exact language, in the position-velocity space ($\mu$-space).

Under this supposition, according to the standard kinetic theory, the collisionless Boltzmann equation holds and it reads

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0,$$

in which the collisional effects between molecules have been disregarded (as the title of this paper has suggested). If the initial state

$$f(t_0 + 0, \mathbf{r}, \mathbf{v}) = f(t_0, \mathbf{r}, \mathbf{v})$$

and the boundary condition

$$f(t, \mathbf{r}, \mathbf{v}) = \int K(\mathbf{v}, \mathbf{v}_1) f(t, \mathbf{r}, \mathbf{v}_1) d\mathbf{v}_1,$$

where the shape of $K$ represents the collisional effects between molecules and boundaries, are regarded as known ones, the solution of Eq. (1) can be constructed by means of a finite-difference scheme. In such a scheme, notably, the governing equation (1) and the initial and boundary conditions (2)-(3) constitute a complete equation set, and any additional information, such as the path-information of individual molecules, becomes theoretically dispensable. (In a sense, the whole idea behind introducing the conservation-type partial differential equations into kinetic theory is just to avoid knowing paths of individual molecules.)

Instead of making a detailed analysis of the standard formalism outlined above, which has been done elsewhere, we now use the formalism to “derive” a relatively well-known lemma in statistical mechanics. The point
here is that the lemma will automatically lead us to the very essence of gas dynamics.

By relating the vector variables $\mathbf{r}$ and $\mathbf{v}$ in \( (1) \) to a molecule’s path, the partial differential equation can be rewritten in the form of a simple ordinary differential equation

$$\frac{df}{dt}\bigg|_{r(t),v(t)} = 0. \quad (4)$$

Of course, $\mathbf{r}(t)$ and $\mathbf{v}(t)$ are associated with the equations of motion for a single molecule

$$\frac{d\mathbf{r}(t)}{dt} = \mathbf{v}, \quad \frac{d\mathbf{v}(t)}{dt} = \frac{\mathbf{F}}{m}, \quad (5)$$

where $\mathbf{F}$ stands for all forces acting upon the molecule. Equation (4) simply means

$$f(t, \mathbf{r}, \mathbf{v})|_{r(t),v(t)} = \text{Constant}. \quad (6)$$

That is to say, in the absence of collisions a continuous distribution function keeps invariant along a molecular path in $\mu$-space. [Since formula (6) is the integral of (4) along a path, we may regard the formula as a primitive prototype of path-integral approach.] If the time development operator $T$ is employed to represent the equations of motion (5), namely if we have

$$T(t_0, t)[\mathbf{r}(t_0), \mathbf{v}(t_0)] = [\mathbf{r}(t), \mathbf{v}(t)], \quad (7)$$

then we can equivalently express (6) as

$$f(t, \mathbf{r}, \mathbf{v}) = f(t_0, \mathbf{r}_0, \mathbf{v}_0) = f(t_0, T^{-1}\mathbf{r}, T^{-1}\mathbf{v}), \quad (8)$$

where $\mathbf{r}_0 = \mathbf{r}(t_0)$, $\mathbf{v}_0 = \mathbf{v}(t_0)$ and $T^{-1} = T(t,t_0)$. In view of (8) and (3), we will refer to $f(t_0)$ as the “source” function and refer to $f(t)$ as the “image” function. In a similar spirit, it will be said that $\mathbf{r}_0$ is a source point and $\mathbf{r}$ an image point.

Now, we use the path-invariance expressed by (3) to derive some dynamical features of the Boltzmann gas. These features, though quite interesting and very essential, received no enough attention before. For simplicity only situations in that no external force exists will be considered, though equations (3)-(8) are valid more generally.

Suppose, to begin with, that the initial distribution function $f(t_0, \mathbf{r}, \mathbf{v})$ is known (which is continuous) and we are concerned with the velocity distribution at a specific point $\mathbf{r}$, denoted by $f_r(t, \mathbf{v})$ hereafter. Equation (3) shows that

$$f_r(t, \mathbf{v}) = f(t_0, T^{-1}\mathbf{r}, \mathbf{v}). \quad (9)$$
For one fixed value of $v_i = |v_i|$, the source points $r_i = T^{-1}r$ simply form a spherical surface, labeled as $S_i = S(v_i)$ in Fig. 1. The radius of such a surface can be expressed by

$$|r_i - r| = v_i \cdot (t - t_0).$$

(10)

To determine the velocity distribution, we must let $v_i$ take values from very small to very large, and thus the radius $|r - r_i|$ varies from very small to very large. This implies that the velocity distribution $f_r(t, v)$ is a condensed image of the entire spatial space. If $f(t_0, r, v)$ is not spatially uniform, $f_r(t, v)$ will possess a complex structure, infinitely complex in general situations (which reminds us of the famous Cantor set and many other interesting structures in the fractal studies). To make the situation even more worrisome, the inference presented above also suggests that any discontinuous things, if exist in the spatial space, will constantly create discontinuous images on velocity distributions in the nearby and distant regions (virtually everywhere).

To see the point in another perspective, let’s assume that a numerical work is being carried out and the velocity space is being divided into many small but finite cells (for time being pay less attention to the spatial space), of which one takes the form $\Delta v = v_2 \Delta v \Delta \Omega$. It is then up to the investigator to determine the distribution function for each of the cells, denoted by

$$f_r(t, \Delta v, \Delta \Omega).$$

(11)

In other words, each of $f_r(t, \Delta v, \Delta \Omega)$ should be endowed with one definite value. The task, though seems quite straightforward, cannot be done conventionally. Look at Fig. 2, in which the spatial cone $-\Delta \Omega$ corresponding to the velocity cone $\Delta \Omega$, called the effective cone hereafter, and the two spherical surfaces $S_i = S(v_i)$ and $S_{i+1} = S(v_{i+1})$, where $v_{i+1} - v_i = \Delta v$, are plotted. It is easy to find that when $v$ varies within the range $v^2 \Delta v \Delta \Omega$, the source point $T^{-1}r$ runs over the shaded volume in the figure. Since the thickness of the shaded volume is proportional to $\Delta v$ solely (for the fixed $t - t_0$), if we let $\Delta v$ be smaller and smaller the value of

$$\lim_{\Delta v \to 0} f_r(t, \Delta v, \Delta \Omega)$$

(12)

tends to a limit in the usual sense. Whereas, the size of $\Delta S_i$, the area element on $S(v_i)$ enclosed by the effective cone, is proportional to $v_i^2$, and if we let $\Delta \Omega$ be smaller and smaller the value of

$$\lim_{\Delta \Omega \to 0} f_r(t, v, \Delta \Omega)$$

(13)
tends to a limit at a rate that strongly depends on the magnitude of \( v \). That is to say, the velocity distribution at \( r \) is not uniformly continuous. According to mathematics textbooks\(^7\)\(^8\), a function that is not uniformly continuous may involve some irregularities and has to be treated carefully. As far as our situation is concerned, there indeed exist difficult things. As one thing, when \( v_i \) is rather large, the area of \( \Delta S_i \) must be rather large. If the source function \( f(t_0) \) on this large area element varies significantly (quite possible in practical situations), giving a unique value to the image function \( f_i(t, \Delta v, \Delta \Omega) \) becomes a tricky business. This type of difficulty has been named as quasi-discontinuity in our previous works\(^4\)\(^5\).

We now study boundary effects. At first suppose, if the path-invariance expressed by (6) is combined with the boundary condition (3), the boundary effects can be regarded as being formulated completely. The investigation below, however, tells a different story. First of all, note that a realistic boundary cannot be considered as having a geometrically and physically uniform surface. This, according to the spirit of calculus, leaves us no choice but to divide the boundary into many area elements, infinitesimally small in the theoretical sense. We are then supposed to examine how each of them receive and emit incident molecules. If we assume that an area element \( dS \) in Fig. 3 uniformly reemit the incident molecules and the distribution function immediately above it is known as \( f(r_o, v) \), it follows from (6) that, assuming the gas to be relatively stationary,
\[
f(r_o, v) = f(r_{p1}, v) = f(r_{p2}, v). \tag{14}
\]
An interesting question must arise. What is the difference between the velocity distributions at \( p_1 \) and at \( p_2 \)? Fig. 3b offers manifestation that the velocity distribution at \( p_1 \) takes the value of \( f(r_o, v) \) within the solid-angle range \( d\Omega_1 \) while the velocity distribution at \( p_2 \) takes the same value within \( d\Omega_2 \). An essential fact is that the infinitesimally small \( d\Omega_1 \) is significantly larger than the infinitesimally small \( d\Omega_2 \). It is then rather obvious that equation (14) alone cannot be deemed as a satisfactory description of the process. (The next section shows that introducing \( \delta \)-functions into the scheme does not provide much help either.)

We have seen that the path-invariance lemma, though intended to describe the evolution of continuous distribution function, discloses many features that cannot be well treated in terms of continuous distribution functions.

Before finishing this section and turning our attention to the next subject, we wish to comment on the differences between the Boltzmann-equation
approach and the approach represented by formulas (4)-(8), though it seems that formula (4) or (8) is “derived from” and “completely equivalent to” the collisionless Boltzmann equation (1).

According to most textbooks, the derivation of the Boltzmann equation is closely related to the conservation law in the phase space $\mu$-space$^{[1]}$. Ref. 4 and Ref. 5, however, argue that such a conservation law is not truly sound. On one hand, defining fluxes through five-dimensional hypersurfaces (six of them can enclose a six-dimensional volume element) is an absolute must for the conservation law; on the other hand, such fluxes cannot be well defined in either physical or mathematical sense. For instance, in defining a flux through the ordinary surface $dydz$ we invoke that the velocity $\dot{x} = v_x$ is perpendicular to the surface; whereas in defining a flux through the hypersurface $dv_x dv_y dv_z dydz$ we cannot invoke that the velocity $\dot{x} = v_x$ is perpendicular to the hypersurface, because $v_x$ itself is among the five dimensions of the hypersurface.

Formula (4) can be derived independently through a Jacobian approach under two assumptions$^{[1][2]}$. One is that the distribution function is perfectly continuous at an initial time. The other is that forces acting on all molecules are free from dissipation (independent of speed) and free from fluctuation (smooth everywhere). After obtaining (4), equation (1) can be obtained by abandoning the path-information expressed by equation (5). Noting that the abandonment involves an information loss, we wish to say that the approach represented by (4)-(8), instead of the collisionless Boltzmann equation (1), should be regarded as a more basic and more complete formalism. The discussion of this section, in which expressions (4)-(8), instead of (1), reveal the essential features of continuous distribution function, also substantiates the statement presented above.

The standard kinetic theory gets heritages from the ordinary fluid mechanics. It assumes that a local value of distribution function is largely influenced by its immediate neighborhood and the influence is exerted through two-dimensional surfaces or five-dimensional hypersurfaces. By adopting this assumption, the theory unanimously employs a conservation-type partial differential equation to set up its framework. Formulas (4)-(8), however, suggest that events of gas dynamics develop along molecular paths, which are one-dimensional lines in $\mu$-space. The new picture, quite different from the standard one in the physical and mathematical senses, implies that even a gas that initially possesses a perfectly continuous distribution function will not behave itself like a continuous medium. We have manifestly seen this point in the discussion related to the quasi-discontinuity.
Finally, formulas (4)-(8) offer, in a primitive manner though, different concepts concerning the way we approach to gas dynamics. Instead of relying on comprehensive, but difficult and delicate, differential equations, one is virtually led to accepting a procedure-type approach. Such approach supposedly includes the following steps: (i) to determine paths of individual molecules; (ii) to formulate how a local distribution function gives a contribution to another local distribution function through a path; (iii) to integrate all contributions associated with all possible molecular paths. The last step is necessary since, according to the basic principles of statistical mechanics, molecular paths must involve a probabilistic nature due to the molecule-boundary and molecule-molecule interaction. (All points in this paper are given in terms of classical mechanics.) We will, by following Feynman[9], call an approach of this type the path-integral approach.

3 Evolution of discontinuous distribution function

The last section has shown that the Boltzmann gas should be regarded less as a perfectly continuous medium and more as a special collection of individual molecules. In this section we will formulate how discontinuous distribution functions, each of which describes a set of molecules, develop along molecular paths.

For simplicity only discontinuous distribution functions that are produced by point-like sources and surface-like sources are of our interest. It is also assumed that molecules of the interested gases are free from external forces. If needed, the approach here can, in a straightforward way, be adapted to more general situations.

In Fig. 4, a point \( r_0 \) is plotted at which molecules are generated (for whatever reasons). To make the discussion applicable later, the molecular emission rate \( \rho \) is allowed to depend on the time, velocity magnitude and velocity direction. The number of molecular emission can thus be expressed by

\[
\rho(t_0, r_0, v, \Omega_0) dt_0 dv d\Omega_0,
\]

where \( \Omega_0 \) is defined in the frame whose origin is at \( r_0 \). Moving along a molecule’s path, it is found that at a later time \( t \) the emitted molecules spread over the volume

\[
|r - r_0|^2 v dt d\Omega_0
\]
where $r$ is the point in the spatial space such that

$$r - r_0 = v(t - t_0). \quad (17)$$

It follows from (15) and (16) that the density of molecules at $r$ is

$$n(r) = \frac{\rho dv dt_0 d\Omega_0}{|r - r_0|^2 v dt d\Omega_0} = \frac{\rho dv}{|r - r_0|^2 v}, \quad (18)$$

where $dt = dt_0$ has been understood. Since the distribution function $f$ at the point $r$ satisfies

$$\int_{\Omega} f v^2 dv d\Omega = n(r) = \frac{\rho dv}{|r - r_0|^2 v}, \quad (19)$$

the distribution function produced by the point-like source is

$$f(t, r, v, \Omega) = \rho(t_0, r_0, v, \Omega_0) \frac{\eta(\Omega)}{|r - r_0|^2 v^3} \delta(\Omega - \Omega_0). \quad (20)$$

Note that $\Omega_0$ in (20) takes the same direction as that of $(r - r_0)$. The form of (20) manifests that molecules produced by a point-like source are associated with a discontinuous distribution function. If one tries to apply the Boltzmann equation (1) to it, difficulties arise sharply with the differentiation operations.

Now, we consider a surface-like source of molecules. It seems that after the surface is divided into many small area elements and the formula Eq. (20) is applied to each of them, our task is virtually accomplished. However, the following discussion shows that if we stick to what the standard kinetic theory implies, more troublesome things will emerge and no progress can be made.

Let $\Delta S_{0i}$ denote one of area elements on the surface and $\eta(t_0, r_0, v, \Omega_0)$ denote the molecular emission rate per unit area on $\Delta S_{0i}$. By identifying

$$\eta(t_0, r_0, v, \Omega_0) \Delta S_{0i} \quad (21)$$

with the molecular emission rate $\rho$ in (20), we find the entire distribution function produced by the surface-like source to be

$$f(t, r, v, \Omega) = \sum_i \frac{\eta \Delta S_{0i}}{|r - r_{0i}|^2 v^3} \delta(\Omega - \Omega_{0i}), \quad (22)$$
where $i$ runs over all the elements on the surface. If one rewrites (22) in the integral form

$$f(t, r, v, \Omega) = \int \frac{\eta dS_0}{|r - r_0|^2 v^3} \delta(\Omega - \Omega_0),$$  

the following question will be of the immediate concern. Does equation (23) define a normally behaved distribution function? Fig. 5 demonstrates that each of $\Omega_0$ points to a different direction while the distribution function on the left side of (23) involves only one direction defined by $\Omega$. That is to say, expression (23) cannot be integrated in the usual sense.

It is quite interesting to look at the peculiarities that we have just encountered. In dealing with our discontinuous distribution functions neither the usual differentiation nor the usual integration works smoothly.

In order to find a way out of the difficult situation, we propose to use the following solid-angle-average distribution function such that if the exact distribution function $f(t, r, v)$ is known, which exists only in a pure academic sense, then the average distribution function is

$$\bar{f}(t, r, v, \Delta\Omega) = \frac{1}{\Delta\Omega} \int_{\Delta\Omega} f(t, r, v) d\Omega,$$

where $\Delta\Omega$ is a solid-angle range in the velocity space set by the investigator.

In practical calculations, it is convenient to employ the spherical coordinate system of velocity, in which $\Omega$ is defined by the polar angle $\theta$ and the azimuthal angle $\phi$, and the solid angle range can be expressed by

$$\Delta\Omega \approx \sin \theta \Delta\theta \Delta\phi.$$

On this understanding, the entire solid-angle range of velocity associated with a spatial point $r$ is divided into a large number of small, but finite, ranges, which may or may not be equal to each other. Of course, if the distribution function is smooth enough and $\Delta\Omega$ is sufficiently small, we may simply assume

$$\bar{f}(t, r, v, \Delta\Omega) = f(t, r, v, \Omega).$$

In the rest of this paper, we will always omit the bar notation when referring to such distribution function.

In terms of practical calculations, the size of $\Delta\Omega$ should be chosen properly so that the computational work can be done efficiently and at the same time no significant macroscopic phenomena will be overlooked.

As we may notice, an investigator of numerical work can take a similar strategy to treat distribution functions in terms of $\Delta r$ and $\Delta v$. The
difference here lies in that our solid-angle-average distribution function is introduced in a theoretical (analytical) consideration: the discontinuity represented by (20) and the quasi-discontinuity represented by (13) should, and have to, be handled under the new definition.

It is rather important to emphasize that the distribution function introduced above seems to be an “approximate” one, but it actually represents an “accurate” approach in the following two senses. One is that by letting $\Delta \Omega$ be sufficiently small, we can describe a statistical process with any desirable accuracy. The other is that errors related to giving up the exact distribution function are largely inherent to nature not to the way we approach to it.

With help of the new average distribution function, the deterministic nature and the probabilistic nature of a statistical process can be kept in a balanced way. By using all kinds of mathematical operations, such as differentiation and integration, to formulate the distribution function, we preserve the macroscopic causality. By taking the solid-angle average, some of the microscopic information, in particular those related to discontinuity and quasi-discontinuity, are forsaken forever.

We are now equipped to formulate the discontinuous distribution function due to the existence of a surface-like source, as shown in Fig. 6. For a chosen solid-angle range $\Delta \Omega$ in the velocity space there is an effective cone $-\Delta \Omega$ in the spatial space. A surface-like molecular source enclosed by the effective cone, the shaded area $\Delta S$ in Fig. 6, gives contributions to $f(t, r, v, \Delta \Omega)$.

Assuming the emission rate on the surface to be known and allowing expression (23), not normally behaved though, to represent the emitted molecules, we obtain from (24)

$$f = \frac{1}{\Delta \Omega} \int \int_{\Delta S} \frac{\eta dS_0}{|\mathbf{r} - \mathbf{r}_0|^2 v^3} \delta(\Omega - \Omega_0) d\Omega.$$  \hfill (27)

By exchanging the order of the integration, we finally arrive at

$$f(t, r, v, \Delta \Omega) = \frac{1}{\Delta \Omega} \int_{\Delta S} \frac{\eta(t_0, \mathbf{r}_0, v, \Omega_0) dS_0}{|\mathbf{r} - \mathbf{r}_0|^2 v^3}. \hfill (28)$$

In the integrand of (28) $\mathbf{r}_0$ is the position of $dS_0$, $t_0$ is equal to $t - |\mathbf{r} - \mathbf{r}_0|/v$ and $\Omega_0$ points to the direction of $(\mathbf{r} - \mathbf{r}_0)$.

It is easy to see that the distribution function expressed by (28) is finite and well behaved.
4 The complete path-integral formulation and its application

The discussion in the last two sections has shown that the distribution function at any specific point consists of two parts. The first part is a continuous one produced by the continuous distribution function existing previously; the second part is a discontinuous one produced by surface-like molecular sources. Here, we summarize the last two sections and give a comprehensive formulation for the dynamics of collisionless Boltzmann gas.

In Fig. 7 we assume that the complete solid-angle-average distribution function \( f(t, r, v, \Delta \Omega) \) is affected by a continuous distribution function and a surface-like source. Both the “sources” exist within the effective cone and constantly “emit” molecules into the region around the point \( r \). The complete distribution function can formally be expressed as

\[
\begin{align*}
  f(t, r, v, \Delta \Omega) &= f_{(i)} + f_{(ii)},
\end{align*}
\]

where \( f_{(i)} \) and \( f_{(ii)} \) are produced by the aforementioned two sources respectively.

First, we wish to determine \( f_{(i)} \) in terms of certain specifications of initial state. Providing the initial state of the continuous distribution function, denoted by \( f_{ct} \), is given only at one specific moment \( t_0 \), we have no other choices but to take the following approach. All relevant source points, according to Sec. 2, can be determined by the mapping \( T^{-1}r \) and by the effective cone \(-\Delta \Omega \). Namely, they distribute on an area element of the spherical surface \( |r_0 - r| = v(t - t_0) \), denoted by \( \Delta S_1 \) in Fig. 7. We will refer to such area element as a virtual effective surface in view of that similar surface-like sources (boundaries) are physical ones. From (6) and (24), the continuous part of the distribution function can be written as an integral

\[
\begin{align*}
  f_{(i)}(t, r, v, \Delta \Omega) &= \frac{1}{\Delta \Omega} \int_{\Delta \Omega} f_{ct}(t, r, v, \Omega) d\Omega \\
  &= \frac{1}{|r - r_0|^2 \Delta \Omega} \int_{\Delta S_1} f_{ct}(t_0, r_0, v, \Omega_0) U_{r_0 r} dS_0
\end{align*}
\]

where \( r_0 \) is the position of \( dS_0 \), \( \Omega_0 \) is in the direction \( (r - r_0) \), and \( U_{r_0 r} \) is a specially defined path-clearness function such that

\[
U_{r_0 r} = \begin{cases} 
1 & \text{no block along the path from } r_0 \text{ to } r \\
0 & \text{otherwise.}
\end{cases}
\]
Note that the difficulty of quasi-discontinuity discussed in Sec. 2 is no longer an issue: \( f_{(i)} \) is uniquely defined and makes appropriate physical sense no matter how dynamically the source function \( f^{cl}(t_0) \) varies on the virtual effective surface \( \Delta S_1 \).

If the distribution function is known within a period of time (before \( t_0 \)), we have freedom to choose the virtual effective surface. For instance, by choosing the surface \( \Delta S'_1 \) in Fig. 7, we have, as an alternative of (30),

\[
(f_{(i)}) = \frac{1}{\Delta \Omega} \int_{\Delta S'_1} f^{cl}(t_0, r_0, v, \Omega_0) \frac{|r - r_0|^2}{U |r - r_0|} \cos \alpha |dS_0, \tag{32}
\]

where \( \alpha \) is the angle between the direction \( (r - r_0) \) and the normal of the area element \( dS_0 \), and the time \( t_0 \) now depends on the position of \( dS_0 \), namely \( t_0 = t - |r - r_0|/v \).

Then, we wish to formulate the discontinuous part of the distribution function. As suggested in the last two sections, boundary surfaces in a gas can be treated as surface-like molecular sources, since they constantly reemit incident molecules. In Fig. 7, the boundary surface \( \Delta S_2 \) within the effective cone, called the physical effective surface, is singled out as a surface-like source that can affect \( f(t, r, v, \Delta \Omega) \).

The focus is naturally on the local emission rate \( \eta(t_0, r_0, v, \Omega_0) \) defined by (21). To determine it, we first consider the falling rate of incident molecules expressed by

\[
\xi(t_0, r_0, v_i, \Omega_i) = f(t_0, r_0, v_i, \Omega_i) \cos \theta_i U(\cos \theta_i), \tag{33}
\]

where \( \theta_i \) is the angle between the inward normal of the local surface and the incident direction of the molecules and \( U \) is a step function whose value is equal to unity if \( \cos \theta_i > 0 \) and equal to zero otherwise.

As well known, the functional relation between \( \eta \) and \( \xi \) has to be ultimately measured in experiments[6], though some kinds of theoretical models may be of use at some stages. To see how this relation can be formulated empirically, consider a molecule that moves with the velocity \( (v_i, \Omega_i) \), strikes an area element and leaves the area element with a velocity within the range \( dv \) \( d\Omega_0 \), with respect to the surface element, in a certain probability. If the probability is denoted by

\[
P(v_i, \Omega_i, v, \Omega_0) dv d\Omega_0 \tag{34}
\]

and its normalization takes the form

\[
\int P(v_i, \Omega_i, v, \Omega_0) dv d\Omega_0 = 1, \tag{35}
\]
then the emission rate of the area element, for rarefied gases, will satisfy

$$\eta(t_0, r_0, v, \Omega_0) = \int P(v_i, \Omega_i, v, \Omega_0) \xi v_i^2 dv_i d\Omega_i. \quad (36)$$

To verify the correctness of (36), one may integrate (36) and obtain, with the help of (35),

$$dt_0 d\Omega_0 \int \eta(t_0, r_0, v, \Omega_0) dv d\Omega_0 = dt_0 d\Omega_0 \int \xi(t_0, r_0, v_i, \Omega_i) v_i^2 dv_i d\Omega_i, \quad (37)$$

which is nothing but the conservation law of the molecular number on the surface element. It is now clear that the purpose of such experiment should be to determine the functional form of $P(v_i, \Omega_i, v, \Omega_0)$.

Under the assumption that the molecular emission rate $\eta$ of the involved boundary surface has been determined (by whatever means), the interested discontinuous part can, by virtue of Eq. (28), be written as

$$f_{(ii)} = \frac{1}{\Delta \Omega} \int_{\Delta S_2} \eta(t_0, r_0, v, \Omega_0) |r - r_0|^2 \xi v^3 U_{r_0 r} dS_0 \quad (38)$$

where the path-clearness function $U_{r_0 r}$ has been defined by (31).

The final result is then

$$f(t, r, v, \Delta \Omega) = \frac{1}{\Delta \Omega} \int_{\Delta S_1} \frac{f^{ct}(t_0, r_0, v, \Omega_0) \cos \alpha}{|r - r_0|^2} U_{r_0 r} dS_0$$

$$+ \frac{1}{\Delta \Omega} \int_{\Delta S_2} \frac{\eta(t_0, r_0, v, \Omega_0)}{|r - r_0|^2} U_{r_0 r} dS_0, \quad (39)$$

where the first term of the right side can be replaced by (30). If macroscopic quantities are of interest, the distribution function expressed by (39) can be used as a conventional one.

At this point, it is interesting to comment on the time-irreversibility of the formalism given above. It is kind of well-known that the time-reversibility dilemma related to a dynamical process can be eliminated if a proper statistical average is taken. With the statistical average, two issues get involved. (i) Some pieces of microscopic information are forsaken. (ii) Conservative basic forces are converted into fluctuating and dissipative (speed-dependent) forces. Notably, the second issue mentioned above is directly responsible for the time-irreversibility of the interested process. In this approach, it appears that the time-irreversibility has nicely been embedded. Though the pure evolution of continuous distribution function expressed by
is time-reversible, other treatments, including the definition of the solid-angle-average distribution function and the formulation of boundary effects, are manifestly time irreversibil. In particular, by allowing the molecule-boundary interaction to be determined by empirical laws (or other adequate statistical laws), the formulation in this paper is fully in harmony with the Langevin theory\[10\], in which fluctuating and dissipative forces naturally arise from the interaction between a moving body and its surrounding molecules.

At the end of this section, we give a brief look at what will happen if a calculation suggested by this paper is practically performed. Fig. 8 offers schematic of a gas leaking out of a large container through a small hole. (Ref. 4 shows that the standard theory encounters many difficulties in treating the case.) Since the container is rather large one may assume that the distribution function on a surface, labeled as $S$ in the figure, constantly takes the value

$$f = n_0 \left( \frac{m}{2\pi\kappa T} \right)^{3/2} \exp \left( -\frac{mv^2}{2\kappa T} \right),$$

(40)

provided that the surface $S$ is not very close to the hole. It is obvious that the values of distribution function at the starting points of paths 1, 2 and 3 are all equal to the value of (40). If contributions from complex paths, such as path 3, are neglected, we can directly use an ordinary PC-type computer to calculate (39) on the understanding that the molecular emission rate $\eta$ in the formulation has been determined empirically.

5 Conclusion

We have set up a new formalism that exhibits many features strongly different from those related to the standard theory. They can briefly be listed as the following.

1. Instead of pursuing the exact distribution function, a special type of distribution function, called the solid-angle-average distribution function, is introduced. The new-type distribution function can describe statistical phenomena with any desirable accuracy.

2. Instead of relying on a partial differential equation, which is difficult and delicate, the new approach gives a set of tamable integral formulas. As well known, for a law of nature the integral formulation often enjoys advantages.
3. Instead of disregarding the path-information, the new approach bases its formulation on the path-information of molecules. With the path-information included, many sophisticated and important features of kinetic systems become explicable and treatable.

4. Instead of treating the collisionless Boltzmann gas as a completely continuous medium, the new approach treats the discontinuity and quasi-discontinuity at the very beginning. No singularity of any type exists with the final result of the formalism.

5. Instead of falling into the time-reversibility paradox, the new approach admits its inability to formulate all microscopic details. In treating boundary effects, the time irreversibility has explicitly been embedded in the formalism.

The complete dynamics of the Boltzmann gas, including collisional effects, will be formulated in different works. Helpful discussion with Prof. Keying Guan is greatly appreciated. This work is partly supported by the fund provided by Education Ministry, PRC.

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[10] See for instance R.K. Pathria, *Statistical Mechanics*, (Pergamon Press, 1972) in which a body immersed in a gas is investigated in terms of Brownian motion of molecules.

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Figure captions

1. Local distribution as an image of the entire space.

2. Source points affecting the local distribution within $v^2 \Delta \Omega \Delta v$.

3. Local distributions near an area element.

4. A point-like molecular source.

5. Schematic of discontinuous distribution produced by a surface-like source.

6. A surface-like molecular source within an effective cone.

7. One physical surface and two virtual surfaces within an effective cone.

8. Molecules leaking out of a large container.
