Physical principles of the generalized Boltzmann kinetic theory of gases

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<u>Abstract.</u> This paper addresses the fundamental principles of generalized Boltzmann physical kinetics, which introduces terms accounting for the variation of the distribution function over times of the order of the collision time into the Boltzmann equation. The paper is primarily aimed at clarifying the qualitative aspects of the theory whose mathematical formalism was developed in the author's earlier work. There is a detailed discussion of how the generalized Boltzmann equation obtained by the multiscale method relates to other alternative approaches used in the development of kinetic equations. The application of the generalized Boltzmann equation to certain classical transport processes is discussed.

1. Introduction

In 1872 L Boltzmann, then a mere 28 years old, published his famous kinetic equation for the one-particle distribution function $f(\mathbf{r}, \mathbf{v}, t)$ [1]. He expressed the equation in the form

$$\frac{\mathrm{D}f}{\mathrm{D}t} = J^{\mathrm{st}}(f)\,,\tag{1.1}$$

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Received 8 December 1999, revised 21 March 2000 Uspekhi Fizicheskikh Nauk **170** (6) 649–679 (2000) Translated by E G Strel'chenko; edited by A Radzig where J^{st} is the collision ('stoß') integral, and

$$\frac{\mathbf{D}}{\mathbf{D}t} = \frac{\partial}{\partial t} + \mathbf{v} \cdot \frac{\partial}{\partial \mathbf{r}} + \mathbf{F} \cdot \frac{\partial}{\partial \mathbf{v}}$$
(1.2)

is the substantial (particle) derivative, \mathbf{v} and \mathbf{r} being the velocity and radius vector of the particle, respectively.

Equation (1.1) governs the transport processes in a onecomponent gas which is sufficiently rarefied that only binary collisions between particles are of importance. While we are not concerned here with the explicit form of the collision integral (which determines the change of the distribution function f in binary collisions), note that it should satisfy conservation laws. For the simplest case of elastic collisions in a one-component gas we have

$$\int J^{st} \psi_i \, \mathrm{d}\mathbf{v} = 0 \qquad (i = 1, 2, 3) \,, \qquad \mathrm{d}\mathbf{v} \equiv \mathrm{d}v_x \, \mathrm{d}v_y \, \mathrm{d}v_z \,, \quad (1.3)$$

where ψ_i are the collisional invariants ($\psi_1 = m$, $\psi_2 = m\mathbf{v}$, $\psi_3 = mv^2/2$, *m* is the mass of the particle) related to the laws of conservation of mass, momentum, and energy.

Integrals of the distribution function (i.e. its moments) determine the macroscopic hydrodynamic characteristics of the system, in particular the number density of particles

$$n = \int f \,\mathrm{d}\mathbf{v} \tag{1.4}$$

and the temperature *T*:

$$\frac{3}{2}kT = \frac{1}{2}m\int f(\mathbf{v} - \mathbf{v}_0)^2 \,\mathrm{d}\mathbf{v}\,.$$
 (1.5)

Here k is the Boltzmann constant, and \mathbf{v}_0 the hydrodynamical flow velocity.

It follows then that multiplying the Boltzmann integrodifferential equation term by term by collisional invariants ψ_i , integrating over all particle velocities, and using the conservaThe Boltzmann equation is not of course as simple as its symbolic form above might suggest, and it is in only a few special cases that it is amenable to a solution. One example is that of a Maxwellian distribution in a locally, thermodynamically equilibrium gas in the event when no external forces are present. In this case the equality

$$J^{\rm st} = 0 \tag{1.6}$$

is met, giving the Maxwellian distribution function

$$f^{(0)} = n \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left(-\frac{mV^2}{2kT}\right), \qquad (1.7)$$

where $\mathbf{V} = \mathbf{v} - \mathbf{v}_0$ is the thermal velocity.

It was much later, years after Boltzmann's death in 1906, that an analytic method for solving the Boltzmann equation was developed for the purpose of calculating transport coefficients. This method, developed in 1916-1917 by Chapman and Enskog [2-5], led to explicit expressions for the coefficients of viscosity, thermal conductivity, diffusion, and later thermal diffusion in a system with a small parameter (which for Chapman and Enskog's particular problem of a nonreacting gas was the Knudsen number, the ratio of the particle's mean free path to a characteristic hydrodynamic dimension).

However, even in Boltzmann's days there was a complete awareness that his equation acquires a fundamental importance for physics and that its range of validity stretches from transport processes and hydrodynamics all the way to cosmology — thus fully justifying the keen attention it attracted and debates it provoked.

Of the many results L Boltzmann derived from his kinetic equation, one of the most impressive is the molecular-kinetic interpretation of the second principle of thermodynamics and in particular of the statistical meaning of the concept of entropy. It turned out that it is possible to define the function

$$H = \int f \ln f \,\mathrm{d}\mathbf{v} \,, \tag{1.8}$$

(*H* being for heat) which behaves monotonically in a closed system.

If the relation between *S*, the entropy per unit volume of an ideal gas, and the *H*-function is written in the form

$$S = -kH + \text{const}, \qquad (1.9)$$

then one can prove the inequality

$$\frac{\partial S}{\partial t} \ge 0. \tag{1.10}$$

The laconic formula

$$S = k \ln W \tag{1.11}$$

connecting the entropy S and the thermodynamic probability W is inscribed on Boltzmann's tombstone.

Ever since their creation, Boltzmann's physical kinetics and the Boltzmann equation have received severe criticism, much of which remains of interest even today. Let us elaborate on this. To begin with, Boltzmann's contemporaries were very much in the dark regarding the relation between the Boltzmann equation and classical mechanics — in particular, with the Newton equation. The Boltzmann equation was obtained in a phenomenological manner based on convincing physical arguments and reflects the fact that the distribution function does not change along the particle's trajectory between collisions but rather changes as a result of an 'instantaneous' interaction between colliding particles.

J Loschmidt noted in 1876 that the Boltzmann equation underlying the *H*-theorem includes only the first time derivative whereas the Newton equation contains the second ('square of time') and hence the equations of motion are reversible in time. This means that if a system of hard-sphere particles starts a 'backward' motion due to the particles reversing their direction of motion at some instant of time, it passes through all its preceding states up to the initial one, and this will increase the *H*-function whose variation is originally governed by reversible equations of motion. The essential point to be made here is that the observer cannot prefer one of the situations under study, the 'forward' motion of the system in time, in favor of the second situation, its 'backward' motion. In other words, the problem of the reversibility of time arises here.

Although somewhat differently formulated, essentially the same objection was made in 1896 by Planck's student E Zermelo, who noted that the *H*-theorem is inconsistent with Poincaré's 'recurrence' theorem proved in 1890 and stated that any physical system, even with irreversible thermodynamic processes operating in it, has a nonzero probability of returning to its original state. Boltzmann, himself fully aware of this possibility, wrote in the second part of his *Lectures on the Theory of Gases* (see Ref. [6], p. 251): "As a result of the motion of gas molecules, the *H*function always decreases. The unidirectional nature of this process does not follow from the equations of motion which the molecules obey. Indeed, these equations do not change if time changes sign."

There is a well-known example from probability theory which Boltzmann employed as an argument in his discussions — sometimes very heated ones — with Zermelo, Planck and Ostwald. If a six-sided die is thrown 6000 times, one expects each side to turn up about 1000 times. The probability of, say, a six turning up 6000 times in a succession has a vanishingly small value of $(1/6)^{6000}$. This example does not clear up the matter, however. Nor do the two papers which Boltzmann's student P Ehrenfest wrote in co-authorship with T Afanas'eva-Ehrenfest after the death of the great Austrian physicist.

Their first model, reported by Afanas'eva-Ehrenfest at the February 12, 1908 meeting of the Russian Physico-Chemical Society, involved the application of the *H*-theorem to the 'plane' motion of a gas [7]. Suppose *P*-molecules, non-transparent to one another, start moving normally to axis *y* and travel with the same velocity in the direction of axis *x*. Suppose further that in doing so they undergo elastic collisions with *Q*-particles, squares with sides at an angle of 45° to axis *y*, which are nontransparent to the molecules and are all at rest.

It is readily shown that shortly after, all the molecules will divide themselves into four groups, and it is a simple matter to write down the change in the number of molecules P in each group in a certain time Δt and then to define a 'planar-gas'

H-function

$$H = \sum_{i=1}^{4} f_i \ln f_i, \qquad (1.12)$$

where f_i is the number of molecules of the *i*th kind, i.e. of those moving in one of the four possible directions. If all the velocities reverse their direction, the *H*-function starts to increase and reverts to the value it had when the *P*-molecules started their motion from the *y* axis. While this simple model confirms the Poincaré–Zermelo theorem, it does not at all guarantee that the *H*-function will decrease when the far more complicated Boltzmann model is used.

P and T Ehrenfest's second model [8], known as the 'lottery' model, features two boxes, A and B, and N numbered balls to which there correspond 'lottery tickets' placed in a certain box and which are all in box A initially. The balls are then taken one by one from A and transferred to B according to the number of a lottery ticket, drawn randomly. Importantly, the ticket is not eliminated after that but rather is returned to the box. In the event that the newly drawn ticket corresponds to a ball contained in B, the ball is returned to A. As a result, there will be approximately N/2 balls in either box.

Now suppose one of the boxes contains *n* balls — and the other accordingly N - n balls — at a certain step *s* in the drawing process. We can then define Δ , a function which determines the difference in the number of balls between the two boxes: $\Delta = n - (N - n) = 2n - N$. In 'statistical' equilibrium, $\Delta = 0$ and n = N/2. The dependence $\Delta(s)$ will imitate the behavior of the *H*-function in a Boltzmann gas.

This example is also not convincing enough because this 'lottery' game will necessarily lead to a fluctuation in the Δ function, whereas Boltzmann kinetic theory excludes completely fluctuations in the *H*-function. By the end of his life Boltzmann went over to fluctuation theory, in which the decrease of the *H*-function in time is only treated as the process the system is most likely to follow. This interpretation, however, is not substantiated by his kinetic theory since the origin of the primary fluctuation remains unclear (the galactic scale of such fluctuation included).

One of the first physicists to see that Boltzmann equations must be modified in order to remove the existing contradictions was J Maxwell. Maxwell thought highly of the results of Boltzmann, who in his turn did much to promote Maxwell electrodynamics and its experimental verification.

We may summarize Maxwell's ideas as follows. The equations of fluid dynamics are a consequence of the Boltzmann equation. From the energy equation, limiting ourselves to one dimension for the sake of simplicity and neglecting some energy transfer mechanisms (in particular, convective heat transfer), we obtain the well-known heat conduction equation

$$\frac{\partial T}{\partial t} = a^2 \frac{\partial^2 T}{\partial x^2} \,. \tag{1.13}$$

The fundamental solution of Eqn (1.13) up to the dimensional constant is

$$T(x,t) = \frac{1}{2\sqrt{\pi a^2 t}} \exp\left(-\frac{x^2}{4a^2 t}\right)$$
(1.14)

and represents the temperature at point x at instant t provided at time t = 0 an amount of heat $c\rho$, with ρ the density and a the thermal diffusivity of the medium, is evolved at the origin of coordinates. Defining an argument of a function T as $\theta = a^2 t$ with the dimension of a coordinate squared we obtain

$$T = \frac{1}{2\sqrt{\pi\theta}} \exp\left(-\frac{x^2}{4\theta}\right). \tag{1.15}$$

The temperature distribution given by this equation is unsatisfactory physically. For small values of θ , the temperature at the heat evolution point x = 0 is indefinitely large. On the other hand, at any arbitrarily distant point x the temperature produced by an instantaneous heat source will be different from zero for arbitrarily small times. While this difference may be small, it is a point of principal importance that it has a finite value.

As Landau and Lifshitz noted in their classical *Course of Theoretical Physics* ([9], p. 283), "The heat conduction process described by the equations obtained here has the property that any thermal perturbation becomes instantaneously felt over all space". This implies an infinitely fast propagation of heat, which is absurd from the point of view of molecular-kinetic theory. In the courses of mathematical physics this result is usually attributed to the fact that the heat conduction equation is derived phenomenologically, neglecting the molecular-kinetic mechanism of heat propagation. However, as has been already noted, the parabolic equation (1.13) follows from the Boltzmann equation. Some of Maxwell's ideas, phenomenological in nature and aimed at the generalization of the Boltzmann equation, are discussed in Woods' monograph [10].

Although the examples above are purely illustrative and the exhaustive list of difficulties faced by Boltzmann kinetic theory would of course be much longer, it should be recognized that after the intense debates of the early 20th century, the search for an alternative kinetic equation for a one-particle distribution function has gradually levelled off or, perhaps more precisely, has become of marginal physical importance. Both sides of the dispute have exhausted their arguments. On the other hand, the Boltzmann equation has proven to be successful in solving a variety of problems, particularly in the calculation of kinetic coefficients. Thus, the development of Boltzmann kinetic theory has turned out to be typical for any revolutionary physical theory — from rejection to recognition and further to a kind of 'canonization'.

Work on the hyperbolic equation of heat conduction was no longer related directly to the Boltzmann equation but rather was of a phenomenological nature. Without expanding the details of this approach, we only point out that the idea of the improvement of Eqn (1.13) was to introduce the second derivative with respect to time thus turning Eqn (1.13) into the hyperbolic form [11]

$$\tau_{\rm rel} \, \frac{\partial^2 T}{\partial t^2} + \frac{\partial T}{\partial t} = a^2 \, \frac{\partial^2 T}{\partial x^2} \,, \tag{1.16}$$

where τ_{rel} is treated as a certain relaxation kinetic parameter with the dimensions of time. The wave equation (1.16) leads to final propagation velocities for a thermal perturbation although it should be remarked parenthetically that the quasilinear parabolic equations may also produce wave solutions.

Following its introduction, stable and high-precision computational schemes were developed for the hyperbolic equation of heat conduction [12], whose applications included, for example, two-temperature nonlocal heat conduction models and the study of the telegraph equation as a paradigm for possible generalized hydrodynamics [13, 14]. The fundamental shortcoming shared by all these studies is that they are phenomenological and intuitive and fully alien to Boltzmann classical kinetic theory. However, the major conclusion to which we are inevitably led is that any attempt at 'improving' the heat conduction equation will lead to a new hydrodynamic theory which in turn must follow from a kinetic equation other than Boltzmann's.

A breakthrough period in the history of kinetic theory occurred in the late 1930s and early 1940s, when it was shown through efforts of many scientists — of which Bogolyubov certainly tops the list — how, based on the Liouville equation for the multiparticle distribution function f_N of a system of N interacting particles, one can obtain a one-particle representation by introducing a small parameter $\varepsilon = nv_B$, where n is the number of particles per unit volume and v_B is the interaction volume [15–19]. This hierarchy of equations is usually referred to as the Bogolyubov or BBGKY (Bogolyubov–Born–Green–Kirkwood–Yvon) chain.

We do not present the technical details but refer the reader to the classical works cited above or, for example, to Ref. [20]. Some fundamental points of the problem are worth mentioning here, however.

(1) Integrating the Liouville equation

$$\frac{\partial f_N}{\partial t} + \sum_{i=1}^N \mathbf{v}_i \cdot \frac{\partial f_N}{\partial \mathbf{r}_i} + \sum_{i=1}^N \mathbf{F}_i \cdot \frac{\partial f_N}{\partial \mathbf{v}_i} = 0$$
(1.17)

subsequently over phase volumes $d\Omega_{s+1}, \ldots, d\Omega_N$ $(d\Omega_j \equiv d\mathbf{r}_j d\mathbf{v}_j)$, one obtains a kinetic equation for the *s*-particle distribution function, with the distribution function f_{s+1} in the integral part of the corresponding equation.

In other words, the set of integro-differential equations turns out to be a linked one, so that in the lowest-order approximation the distribution function f_1 depends on f_2 . This means formally that, strictly speaking, the solution procedure for such a set should be as follows. First find the distribution function f_N and then solve the set of BBGKY equations subsequently for decreasingly lower-order distributions. But if we know the function f_N , there is no need at all to solve the equations for f_s and it actually suffices to employ the definition of the function

$$f_s = \int f_N(t, \Omega_1, \dots, \Omega_N) \,\mathrm{d}\Omega_{s+1} \dots \,\mathrm{d}\Omega_N \,. \tag{1.18}$$

We thus conclude that the rigorous solution to the set of BBGKY equations is again equivalent to solving Liouville equations. On the other hand, the seemingly illogical solution procedure involving a search for the distribution function f_1 is of great significance in kinetic theory and in nonequilibrium statistical mechanics. This approach involves breaking the BBGKY chain by introducing certain additional assumptions (which have a clear physical meaning, though). These assumptions are discussed in detail below.

(2) For a nonreacting gas, the Boltzmann equation is valid for two time scales of distribution functions: one of the order of the mean free time of the particles, and the other the hydrodynamic flow time. The Boltzmann equation is invalid for time lengths of the order of the collision times. Notice that a change from the time scale to the length scale can of course be made if desired.

(3) After the BBGKY chain is broken and f_2 represented as a product of one-particle distribution functions (which is

quite reasonable for a rarefied gas), the Boltzmann equation cannot be written in a classical form with only one small parameter ε and it reduces instead to the Vlasov equation in a self-consistent field.

(4) Because the Boltzmann equation does not work at distances of the order of the particle interaction radius (or at the $r_{\rm B}$ scale), Boltzmann particles are pointlike and structureless, and it is one of the inconsistencies of the Boltzmann theory that the resulting collision cross sections of the particles enter the theory by the collision integral.

(5) Usually the one-particle distribution function is normalized to the number of particles per unit volume. For Boltzmann particles the distribution function is 'automatically' normalized to an *integer* because a pointlike particle may only be either inside or outside a trial contour in a gas unlike finite-diameter particles which of course may overlap the boundary of the contour at some instant of time. Vlasov [21] attempted to eliminate the inconsistencies of the Boltzmann theory through the inclusion of additional dynamical variables in the one-particle distribution function $f(\mathbf{r}, \mathbf{v}, \dot{\mathbf{v}}, \ddot{\mathbf{v}}, \dots, t)$.

Another noteworthy point is that the mean free path in Boltzmann kinetic theory is only meaningful for particles modelled by hard elastic spheres. Other models face difficulties related, though, to the level of one-particle description employed. The requirement for the transition to a oneparticle model is that molecular chaos should exist prior to a particle collision.

The advent of the BBGKY chain led to the recognition that whatever generalization of Boltzmann kinetic theory is to be made, the logic to be followed should involve all the elements of the chain, i.e. the Liouville equation, the kinetic equations for *s*-particle distribution functions f_s , and the hydrodynamical equations. This logical construction was not generally adhered to.

In 1951, N Slezkin published two papers [22, 23] on the derivation of alternative equations for describing the motion of gas. The idea was to employ Meshcherskii's variable-mass point dynamics theory [24], well known for its jet propulsion applications.

The assumption of a variable-mass particle implies that at each point a liquid particle, close to this point and moving with a velocity \mathbf{v} , adds or loses a certain mass, whose absolute velocity vector \mathbf{U} differs, as Slezkin puts it, by a certain appreciable amount from the velocity vector \mathbf{v} of the particle itself. Since there are different directions for this mass to come or go off, the associated mass flux density vector \mathbf{Q} is introduced.

By applying the laws of conservation of mass, momentum, and energy in the usual way, Slezkin then proceeds to formulate a set of hydrodynamical equations, of which we will here rewrite the continuity equation for a one-component nonreacting gas:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\rho \mathbf{v} + \mathbf{Q}\right) = 0.$$
(1.19)

The mass flux density \mathbf{Q} is written phenomenologically in terms of the density and temperature gradients.

Thus, the continuity equation is intuitively modified to incorporate a source term giving

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{v} = \frac{\partial}{\partial \mathbf{r}} \cdot \left(D \, \frac{\partial \rho}{\partial \mathbf{r}} + \beta \, \frac{\partial T}{\partial \mathbf{r}} \right), \tag{1.20}$$

where the coefficient D is that of self-diffusion, and β is related to thermal diffusion. Thus, we now have fluctuation terms on the right-hand side of Eqn (1.20), which are generally proportional to the mean free time τ and, hence, after Eqn (1.20) is made dimensionless, to the Knudsen number which is small in the hydrodynamic limit.

At very nearly the time of the publication of Slezkin's first paper [23], Vallander [25] argued that the standard equations of motion are ill grounded physically and should therefore be replaced by other equations based on the introduction of additional mass Q_i and energy t_i fluxes (i = 1, 2, 3):

$$Q_i = D_1 \frac{\partial \rho}{\partial r_i} + D_2 \frac{\partial T}{\partial r_i}, \quad t_i = k_1 \frac{\partial \rho}{\partial r_i} + k_2 \frac{\partial T}{\partial r_i}.$$

where, to quote, "*D* is the density self-diffusion coefficient, D_2 is the thermal self-diffusion coefficient, k_1 is the density heat conductivity, and k_2 , the temperature heat conductivity".

Heuristic and inconsistent with Boltzmann's theory, the work of Slezkin and Vallander came under sufficiently severe criticism. Shaposhnikov [26] noted that in these papers, "which are almost identical in content ... the essential point is that instead of the conventional expression ρv_0 , additional effects — 'concentration self-diffusion' and 'thermal self-diffusion' — are introduced into the mass flux density which, in addition to the macroscopic mass transfer, cause a molecular mass transfer, much as the macroscopic energy and momentum transfer in a moving fluid goes in parallel with analogous molecular transport (heat conduction and viscosity)". Shaposhnikov then proceeds to derive the equation of continuity from the Boltzmann equation for a one-component gas and shows that the hydrodynamic equations of Slezkin and Vallander are in conflict with the Boltzmann kinetic theory.

Note that Slezkin and Vallander also modified the equations of motion and energy for a one-component gas in a similar way (by including self-diffusion effects). Possible consequences of additional mass transfer mechanisms for the Boltzmann kinetic theory were not analyzed by these authors.

Boltzmann's 'fluctuation hypothesis' was repeatedly addressed by Ya Terletskiĭ (see, for instance, Refs [27, 28]) whose idea was to estimate fluctuations by using the expression the general theorems of Gibbs (see, for example, Ref. [29], pp. 85-88) yield for the mean-square deviation of an arbitrary generalized coordinate. To secure that fluctuations in statistical equilibrium be noticeable, Terletskiĭ modifies the equation of perfect gas state by introducing a gravitational term, which immediately extends his analysis beyond the Boltzmann kinetic theory leaving the question about the irreversible change of the Boltzmann *H*-function unanswered.

In recent years, possible generalizations of the Boltzmann equation have been discussed widely in the scientific literature. Since the term 'generalized Boltzmann equation' has usually been given to any new modification published, we will only apply this term to the particular kinetic equation derived in Refs [30-32] to avoid confusion.

L Woods (see, e.g., Ref. [33]), following ideas dating back to Maxwell, introduces in his theory a phenomenological correction to the substantial first derivative on the left-hand side of the Boltzmann equation to take account of the further influence of pressure on transport processes. It is argued that the equation of motion of a liquid particle may be written as where **P** is a certain additional force proportional to the pressure gradient: $\mathbf{P} = -\rho^{-1} \partial p / \partial \mathbf{r}$, with the result that the left-hand side of the Boltzmann equation becomes

$$\frac{\mathbf{D}f}{\mathbf{D}t} \equiv \frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{r}} + \left(\mathbf{F} - \frac{1}{\rho} \frac{\partial p}{\partial \mathbf{r}}\right) \cdot \frac{\partial f}{\partial \mathbf{v}}, \qquad (1.21)$$

whereas the collisional term remains unchanged. The phenomenological equation (1.21) has no solid foundation and does not fall into the hierarchy of Bogolyubov kinetic equations.

Other suggestions on possible generalizations of the Boltzmann equation are best described by leaning upon the basic principles of the generalized Boltzmann physical kinetics developed by the present author. We now proceed to discuss these principles.

2. Generalized Boltzmann equation

Of the numerous scales involved in reacting gas problems, three major groups of scales pertaining to length, time, and velocity deserve special consideration. In this case the particle interaction scale $r_{\rm B}$ presents only one of the scales (and the shortest) in the scale hierarchy in molecular systems, where the λ scale related to the particle mean free path and the hydrodynamic *L* scale, for example, the length or diameter of the flow channel, the characteristic size of the streamline body, etc., always exist. In gas dynamics, the conditions

$$r_{\rm B} \ll \lambda \ll L \tag{2.1}$$

are usually satisfied. If desired, inequalities (2.1) can be rewritten in terms of such parameters as the characteristic collision time, mean free time, and hydrodynamic flow time. Because the Boltzmann equation is valid only on the λ and *L* scales, the fundamental problem arises here of how to adequately describe kinetic processes at all the three scales of a system's evolution.

The corresponding generalized Boltzmann equation was derived by the present author in 1987 and was presented in his lectures on physical kinetics given at Sofia University, Bulgaria, in the same year. Later, the equation and its derivation procedure were published in the abstracts of the papers presented at the 7th Meeting on the Mechanics of Reacting Media in Krasnoyarsk, Russia, 1988. The equation reads

$$\frac{\mathrm{D}f}{\mathrm{D}t} - \frac{\mathrm{D}}{\mathrm{D}t} \left(\tau \, \frac{\mathrm{D}f}{\mathrm{D}t}\right) = J^{\mathrm{st}} \,. \tag{2.2}$$

Here τ is the mean free time, J^{st} is the Boltzmann collision integral, and D/D*t* is the operator defined by Eqn (1.2).

For a multicomponent reacting gas, the generalized Boltzmann equation can be rewritten as

$$\frac{\mathbf{D}f_{\alpha}}{\mathbf{D}t} - \frac{\mathbf{D}}{\mathbf{D}t} \left(\tau_{\alpha} \; \frac{\mathbf{D}f_{\alpha}}{\mathbf{D}t} \right) = J_{\alpha}^{\mathrm{st,el}} + J_{\alpha}^{\mathrm{st,r}} \,, \tag{2.3}$$

where f_{α} is the distribution function for a particle of the α th kind, τ_{α} is the mean free time for a particle of the α th kind, and $J_{\alpha}^{\text{st,el}}$ and $J_{\alpha}^{\text{st,r}}$ are the Boltzmann collision integrals for elastic and inelastic collisions, respectively.

Since both the derivation of the generalized Boltzmann equation and some of its applications have subsequently been

 $\dot{\mathbf{v}} = \mathbf{F} + \mathbf{P} \,,$

published repeatedly both in Russia and abroad (see, e.g., Refs [30-32, 34-38]), and since, further, some of these derivations are too cumbersome to reproduce, we confine our attention here to the fundamental physical aspects of this equation and to some subtleties of its derivation. Our starting point is the classical Liouville equation (1.17), which describes the evolution, in 6*N*-dimensional space, of the *N*-particle distribution function f_N for a system of N particles whose motion is completely determined by specifying their positions \mathbf{r}_i at a certain instant of time and momenta \mathbf{p}_i .

We now proceed by applying Bogolyubov's procedure and writing down the dimensionless equation for the oneparticle distribution function. In doing so, we follow the multiscale method [39] and introduce three groups of scales:

at the $r_{\rm B}$ level — the particle interaction radius $r_{\rm B}$, characteristic collision velocity $v_{\rm B0}$, and the characteristic collision time $r_{\rm B}/v_{\rm B0}$;

at the λ level — the mean free path λ , the mean free-flight velocity $v_{\lambda 0}$, and the characteristic time scale $\lambda/v_{\lambda 0}$, and

at the L level — the characteristic hydrodynamic dimension L, the hydrodynamic velocity v_{L0} , and the hydrodynamic time L/v_{L0} .

We shall assume that the arguments of the *s*-particle function \hat{f}_s are the above three groups of scaled variables and a small parameter $\varepsilon = nv_{\rm B} = nr_{\rm B}^3$. A hat over a symbol means that the quantity so labelled is made dimensionless. The normalization of the distribution functions is given by

$$\hat{f}_s = f_s \, \frac{v_{\rm B0}^{3s}}{n} \,. \tag{2.4}$$

We now write down an asymptotic series for the function \hat{f}_s :

$$\hat{f}_s = \sum_{v=0}^{\infty} \hat{f}_s^{v}(\hat{t}_{\mathbf{B}}, \hat{\mathbf{r}}_{i\mathbf{B}}, \hat{\mathbf{v}}_{i\mathbf{B}}; \hat{t}_{\lambda}, \hat{\mathbf{r}}_{i\lambda}, \hat{\mathbf{v}}_{i\lambda}; \hat{t}_L, \hat{\mathbf{r}}_{iL}, \hat{\mathbf{v}}_{iL}) \varepsilon^v, \qquad (2.5)$$

and take the derivatives on the left-hand side of the *s*th BBGKY equation

$$\frac{\partial \hat{f}_s}{\partial \hat{t}} + \sum_{i=1}^s \hat{\mathbf{v}}_{i\mathbf{B}} \cdot \frac{\partial \hat{f}_s}{\partial \hat{\mathbf{r}}_{i\mathbf{B}}} + \sum_{i=1}^s \hat{\mathbf{F}}_{ij} \cdot \frac{\partial \hat{f}_s}{\partial \hat{\mathbf{v}}_{i\mathbf{B}}} + \alpha \sum_{i=1}^s \hat{\mathbf{F}}_{i\mathbf{B}} \cdot \frac{\partial \hat{f}_s}{\partial \hat{\mathbf{v}}_{i\mathbf{B}}}$$
$$= -\varepsilon \frac{1}{N} \sum_{i=1}^s \sum_{j=s+1}^N \int \hat{\mathbf{F}}_{ij} \cdot \frac{\partial}{\partial \hat{\mathbf{v}}_{i\mathbf{B}}} \hat{f}_{s+1}(\hat{t}, \hat{\Omega}_1, \dots, \hat{\Omega}_s, \hat{\Omega}_j) \, \mathrm{d}\hat{\Omega}_j \,,$$
(2.6)

according to the rules intended for taking the derivatives of the composite functions. Equating the coefficients of ε^0 and ε^1 now yields

$$\begin{aligned} \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{t}_{B}} + \hat{\mathbf{v}}_{1B} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{r}}_{1B}} + \alpha \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{v}}_{1B}} &= 0, \qquad (2.7) \\ \frac{\partial \hat{f}_{1}^{1}}{\partial \hat{t}_{B}} + \hat{\mathbf{v}}_{1B} \cdot \frac{\partial \hat{f}_{1}^{1}}{\partial \hat{\mathbf{r}}_{1B}} + \alpha \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{v}}_{1B}} \\ &+ \varepsilon_{2} \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{t}_{\lambda}} + \hat{\mathbf{v}}_{1B} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{r}}_{1\lambda}} + \varepsilon_{2} \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{v}}_{1\lambda}} \\ &+ \varepsilon_{1} \varepsilon_{2} \varepsilon_{3} \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{t}_{L}} + \varepsilon_{1} \hat{\mathbf{v}}_{1B} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{r}}_{1L}} + \frac{\varepsilon_{2}}{\varepsilon_{3}} \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{v}}_{1L}} \\ &= -\sum_{\delta=1}^{\mu} \frac{N_{\delta}}{N} \int \hat{\mathbf{F}}_{1,j \in N_{\delta}} \cdot \frac{\partial}{\partial \hat{\mathbf{v}}_{1B}} \hat{f}_{2,j \in N_{\delta}}^{0} \, d\Omega_{j \in N_{\delta}} \,. \qquad (2.8) \end{aligned}$$

Here $\varepsilon_1 = \lambda/L$ denotes the Knudsen number, $\varepsilon_2 = v_{\lambda 0}/v_{B0}$, $\varepsilon_3 = v_{L0}/v_{\lambda 0}$, $\alpha = F_{\lambda 0}/F_0$; as a scale of the internal forces F_0 , the quantity v_{B0}^2/r_B was used. Equation (2.8) is written down for a multicomponent gaseous mixture, and the index *j* determines the particle attachment to a group N_{δ} ($\delta = 1, ..., \mu$) in the μ -component gaseous mixture.

By manipulating Eqn (2.8) we obtain

$$\frac{D_1 \hat{f}_1^1}{D \hat{t}_B} + \frac{d_1 \hat{f}_1^0}{d \hat{t}_{\lambda,L}} = \hat{J}^{\text{st},0}, \qquad (2.9)$$

where we have introduced the notation

$$\frac{\mathbf{D}_{1}f_{1}^{1}}{\mathbf{D}\hat{t}_{B}} = \frac{\partial f_{1}^{1}}{\partial \hat{t}_{B}} + \hat{\mathbf{v}}_{1B} \cdot \frac{\partial f_{1}^{1}}{\partial \hat{\mathbf{r}}_{1B}} + \alpha \hat{\mathbf{F}}_{1} \cdot \frac{\partial f_{1}^{1}}{\partial \hat{\mathbf{v}}_{1B}} ,$$

$$\frac{\mathbf{d}_{1}\hat{f}_{1}^{0}}{\mathbf{d}\hat{t}_{\lambda,L}} = \varepsilon_{2} \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{t}_{\lambda}} + \hat{\mathbf{v}}_{1B} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{r}}_{1\lambda}} + \varepsilon_{2} \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{v}}_{1\lambda}} + \varepsilon_{1} \varepsilon_{2} \varepsilon_{3} \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{r}}_{1\lambda}} + \varepsilon_{1} \hat{\mathbf{v}}_{1B} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{r}}_{1\lambda}} + \varepsilon_{2} \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{v}}_{1\lambda}} + \varepsilon_{1} \varepsilon_{2} \varepsilon_{3} \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{1}^{0}}{\partial \hat{\mathbf{v}}_{1L}} .$$
(2.10)

The following remarks are of fundamental importance in connection with the theory being developed.

(1) No restrictions are placed on the values of ε_1 , ε_2 , ε_3 , including the Knudsen number ε_1 .

(2) The dimensionless distribution functions \hat{f} have two indices, of which the upper denotes the order of approximation in the small- ε expansion. The lower index denotes the number of the equation and the number of particles, both of which should be accounted for simultaneously when constructing the proper distribution function.

(3) Equation (2.9) contains linking not only with respect to the lower but also with respect to the upper index, implying that in order to employ the kinetic equation, additional assumptions should be made to reduce the equation to one dependent variable.

(4) The collision integral $\hat{J}^{\rm st,0}$ transforms to the Boltzmann collision integral if the pair correlation functions in the zero-order ε -expansion vanish and if one can ignore, at the $r_{\rm B}$ scale, the explicit effect, on a given trial particle, of the self-consistent force of internal origin. We shall address this point in more detail below, when discussing the relationship between the generalized Boltzmann equations and alternative derivations of kinetic equations. The zero-order two-particle distribution function entering the Boltzmann collision integral is calculated at the λ scale and is presented, as usual, as a product of zero-order one-particle functions; this means that interacting particles are not correlated prior to a collision.

(5) The use of this representation makes it possible to express the collision integral $\hat{J}^{\text{st},0}$ in the Boltzmannian form. The presence of superscript '0' in $\hat{J}^{\text{st},0}$ is physically meant that even though the variation of the distribution function on the r_{B} scale is taken into account [the first term on the right-hand side of Eqn (2.9)], the form of the Boltzmann collision integral containing the function f_1^0 remains unchanged.

(6) It is crucial that the term $D_1 \hat{f}_1^1 / D\hat{f}_B$ in Eqn (2.9), accounting for the variation of the distribution function on the r_B scale, is of the same order of magnitude as the λ - and Lscale terms. This has nothing to do with whatever approximations for $D_1 \hat{f}_1^1 / D\hat{f}_B$ may later be made to break the Bogolyubov chain. The (unjustified) formal neglect of the term $D_1 \hat{f}_1^1 / D\hat{t}_B$ reduces Eqn (2.9) to the Boltzmann equation. This means, in turn, that the r_B -scale distribution function is left out of consideration in the Boltzmann kinetic theory; particles featuring in the Boltzmann kinetic theory are pointlike and structureless. The system can be described in terms of the independent variables \mathbf{r} , \mathbf{p} , t, and the change in the distribution function due to collisions is instantaneous and is accounted for by the source term $\hat{J}^{\text{st},0}$.

We now proceed to break the Bogolyubov chain at the r_B scale with respect to the superscript in $D_1 \hat{f}_1^1 / D\hat{t}_B$. This term allows the exact representation

$$\frac{\mathbf{D}_1 \hat{f}_1^1}{\mathbf{D}\hat{t}_{\mathbf{B}}} = \frac{\mathbf{D}_1}{\mathbf{D}\hat{t}_{\mathbf{B}}} \left(\frac{\partial \hat{f}_1}{\partial \varepsilon}\right)_{\varepsilon=0}$$
(2.11)

using the series (2.5). Note, however, that in the 'field' description the distribution function f_1 at the interaction (r_B) scale depends on ε through the dynamical variables **r**, **v**, *t* interrelated by the laws of classical mechanics. We can therefore use the approximation

$$\begin{split} \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left[\left(\frac{\partial \hat{f}_{1}}{\partial \varepsilon} \right)_{\varepsilon=0} \right] &= \frac{\mathbf{D}_{1}}{\mathbf{D}(-\hat{t}_{B})} \left[\frac{\partial \hat{f}_{1}}{\partial (-\hat{t}_{B})} \left(\frac{\partial (-\hat{t}_{B})}{\partial \varepsilon} \right)_{\varepsilon=0} \right] \\ &+ \frac{\partial \hat{f}_{1}}{\partial \hat{\mathbf{r}}_{B}} \cdot \frac{\partial \hat{\mathbf{r}}_{B}}{\partial (-\hat{t}_{B})} \left(\frac{\partial (-\hat{t}_{B})}{\partial \varepsilon} \right)_{\varepsilon=0} + \frac{\partial \hat{f}_{1}}{\partial \hat{\mathbf{v}}_{B}} \cdot \frac{\partial \hat{\mathbf{v}}_{B}}{\partial (-\hat{t}_{B})} \left(\frac{\partial (-\hat{t}_{B})}{\partial \varepsilon} \right)_{\varepsilon=0} \right] \\ &= -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left[\left(\frac{\partial \hat{t}_{B}}{\partial \varepsilon} \right)_{\varepsilon=0} \frac{\mathbf{D}_{1}\hat{f}_{1}}{\mathbf{D}\hat{t}_{B}} \right] \\ &= -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left[\left(\frac{\partial \hat{t}_{B}}{\partial \varepsilon} \right)_{\varepsilon=0} \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}} \right] = -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}} \right). \quad (2.12) \end{split}$$

The approximation introduced here proceeds against the course of time and corresponds to the condition that there be no correlations as $t_0 \rightarrow -\infty$, where t_0 is some instant of time on the r_B scale at which the particles start to interact with each other. In the Boltzmann kinetic theory, the condition of correlation weakening has the form

$$\lim_{t_0 \to -\infty} W_2 \big[\mathbf{r}_1 - \mathbf{v}_1(t - t_0), \mathbf{v}_1; \, \mathbf{r}_2 - \mathbf{v}_2(t - t_0), \mathbf{v}_2; \, t_0 \big] = 0 \,,$$
(2.13)

where W_2 is the pair correlation function. For $t_0 \rightarrow -\infty$ (but not for $t_0 \rightarrow +\infty$!), the condition (2.13) of correlation weakening, together with the approximation (2.12), single out a time direction and lead to the time irreversibility in real physical processes [15]. The next section of this paper discusses this point in detail in connection with the proof of the generalized *H*-theorem.

Reverting now to the dimensional form of the equation, normalizing the distribution function to the number density of the particles, and using Eqn (2.12), Eqn (2.9) becomes

$$\frac{\mathbf{D}f_{\alpha}}{\mathbf{D}t} - \frac{\mathbf{D}}{\mathbf{D}t} \left(\tau_{\alpha} \, \frac{\mathbf{D}f_{\alpha}}{\mathbf{D}t} \right) = \sum_{\beta=1}^{\mu} \int \left[f_{\alpha}' f_{\beta}' - f_{\alpha} f_{\beta} \right] g_{\alpha\beta} b \, \mathrm{d}b \, \mathrm{d}\varphi \, \mathrm{d}v_{\beta} \,.$$
(2.14)

Here $g_{\alpha\beta}$ is the relative velocity of the colliding particles α and β , *b* is the impact parameter, and φ the azimuth angle.

Several comments on the generalized Boltzmann equation (2.14) are in order.

(1) The particle numbered 1 in the multicomponent system belongs to the α th component of the gas mixture, which is indicated by the subscript α on the distribution

function symbol. Note the absence of the superscript '0' on f — it does not make sense to carry it along since the generalized Boltzmann equation contains only functions of zero order in the expansion in terms of the density parameter ε .

(2) The physical meaning of the parameter τ_{α} can be understood by considering the relation

$$\frac{1}{\tau_{\alpha}} = \left(\frac{\partial \varepsilon}{\partial t}\right)_{\varepsilon=0}.$$
(2.15)

Here ε is the number of particles of all kinds which happen to be within the interaction volume of an α particle by the instant of time *t*. The right-hand side of Eqn (2.15) is interpreted as indicating the number of particles within the interaction volume of a certain particle of sort α per unit time (to calculate the required derivative, the additional condition $\varepsilon = 0$ is imposed). Clearly, their number is equal to the number of collisions which the α particle experiences with the remaining particles in a unit time.

Thus, the parameter τ_{α} is the mean time between the successive collisions of the α particle with particles of all kinds, defined by

$$\tau_{\alpha} = \frac{n_{\alpha}}{\sum_{\beta=1}^{\mu} N_{\alpha\beta}} .$$
(2.16)

The number $N_{\alpha\beta}$ of collisions between particles of α and β sorts per unit volume in a unit time is calculated using the functions f_{α} and f_{β} . For the Maxwellian distribution functions [40]

$$N_{\alpha\beta} = 2n_{\alpha}n_{\beta}\,\sigma_{\alpha\beta}^2 \left(\frac{2\pi kT}{m_{\alpha\beta}}\right)^{1/2},\tag{2.17}$$

where σ_{α} is the diameter of the particle α , and $m_{\alpha\beta}$ the reduced mass.

(3) In the hydrodynamic limit and within the hard-sphere model, the first (Maxwellian) approximation yields

$$\tau^{(0)}p = 0.8\mu\,,\tag{2.18}$$

where p is the static pressure, and μ denotes the dynamic viscosity.

(4) The generalized Boltzmann equation contains not only second derivatives with respect to time but also mixed (time-velocity and time-coordinate) partial derivatives. Introducing the 'averaged' distribution function

$$f^{a} = f - \tau \frac{\mathrm{D}f}{\mathrm{D}t}, \qquad (2.19)$$

it assumes the form

$$\frac{\mathrm{D}f^{\,\mathrm{a}}}{\mathrm{D}t} = J^{\mathrm{st}}(f) \tag{2.20}$$

similar to the Boltzmann equation (1.1). Now it becomes clear that the Boltzmann equation, which does not contain fluctuation terms, is not a closed one, and there is no rigorous solution (to put it mildly) to the closure problem for the system of moment equations in the theory of turbulence based on hydrodynamical equations derived from the Boltzmann equations. (5) The parameter τ in the generalized Boltzmann equation can be assigned a clear physical meaning and, unlike the so-called kinetically consistent difference schemes [41], to be discussed later, does not lead to secular terms.

(6) The generalized Boltzmann equation in the dimensionless form is written as [2]

$$\frac{\mathbf{D}\hat{f}_{\alpha}}{\mathbf{D}\hat{t}} - \frac{\mathbf{D}}{\mathbf{D}\hat{t}} \left(\mathbf{K}\mathbf{n}\,\hat{\tau}_{\alpha}\,\frac{\mathbf{D}\hat{f}_{\alpha}}{\mathbf{D}\hat{t}} \right) = \frac{1}{\mathbf{K}\mathbf{n}}\,\hat{J}^{\mathrm{st}}\,,\qquad\mathbf{K}\mathbf{n}=\varepsilon_{1}\,.\qquad(2.21)$$

From this it follows that the second term is of the order of the Knudsen number (Kn) and turns out to dominate the lefthand side of this equation as the Knudsen number increases. Needless to say, this is not going beyond the free-molecular limit of the equation because

$$\frac{D}{Dt}\frac{Df_{\alpha}}{D\hat{t}} = 0 \quad \text{for} \quad Kn \to \infty.$$
(2.22)

The solution of Eqn (2.22) is the equation of Knudsen flow

$$\frac{\mathbf{D}\hat{f}_{\alpha}}{\mathbf{D}t} = 0, \qquad (2.23)$$

i.e. the analogue of the Liouville equation for a one-particle distribution function. Note, however, that the second term in Eqn (2.21) cannot be ignored even for small Knudsen numbers because in that case Kn acts as a small coefficient of higher derivatives, with an unavoidable consequence that the effect of this term will be strong in some regions. The neglect of formally small terms is equivalent, in particular, to dropping the (small-scale) Kolmogorov turbulence from consideration.

In closing this section we want to emphasize the fundamental point that the introduction of the third scale, which describes the distribution function variations on a time scale of the order of the collision time, leads to the single-order terms in the Boltzmann equation prior to Bogolyubov-chaindecoupling approximations, and to terms proportional to the mean time between collisions after these approximations. It follows that the Boltzmann equation requires a radical modification — which, in our opinion, is exactly what the generalized Boltzmann equation provides.

3. Generalized *H*-theorem and the time irreversibility

A centerpiece of the kinetic theory, the Boltzmann *H*-theorem provides in fact the kinetic justification for the notion of entropy. The generalized *H*-theorem was proved in 1992 (see, e.g., Ref. [37]). We now sketch the proof and discuss it from the viewpoint of time irreversibility.

Let us first consider a simple gas of spherical molecules, assumed to be uniform and free of external forces. The generalized Boltzmann equation then takes the form

$$\frac{\partial f}{\partial t} - \frac{\partial}{\partial t} \left(\tau \, \frac{\partial f}{\partial t} \right) = J^{\text{st}} \,. \tag{3.1}$$

Let us introduce the Boltzmann H-function

$$H = \int f \ln f \,\mathrm{d}\mathbf{v} \,. \tag{3.2}$$

Multiplying both sides of Eqn (3.1) by $\ln f$ and performing some manipulations we obtain

$$\frac{\partial}{\partial t}(f\ln f) - \tau \frac{\partial^2}{\partial t^2}(f\ln f) + \tau \frac{1}{f} \left(\frac{\partial f}{\partial t}\right)^2 - \frac{\partial \tau}{\partial t} \frac{\partial}{\partial t}(f\ln f) = (1 + \ln f)J^{\text{st}}, \qquad (3.3)$$

which when integrated term by term over all particle velocities yields

$$\frac{\mathrm{d}H}{\mathrm{d}t} - \frac{\mathrm{d}}{\mathrm{d}t} \left(\tau \,\frac{\mathrm{d}H}{\mathrm{d}t}\right) = -\tau \int \frac{1}{f} \left(\frac{\partial f}{\partial t}\right)^2 \mathrm{d}\mathbf{v} + \int (1 + \ln f) J^{\mathrm{st}} \,\mathrm{d}\mathbf{v} \,, \tag{3.4}$$

where the definition of the *H*-function has been used. Now because the inequality

$$-\tau \int \frac{1}{f} \left(\frac{\partial f}{\partial t}\right)^2 d\mathbf{v} + \int (1 + \ln f) J^{\text{st}} d\mathbf{v} \leqslant 0$$
(3.5)

is satisfied it turns out that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(H-\tau\,\frac{\mathrm{d}H}{\mathrm{d}t}\right)\leqslant0\,.\tag{3.6}$$

We now define the H^{a} -function such that

$$H^{a} = H - \tau \, \frac{\mathrm{d}H}{\mathrm{d}t} \,. \tag{3.7}$$

Then the following inequality holds

$$\frac{\mathrm{d}H^{\mathrm{a}}}{\mathrm{d}t} \leqslant 0\,,\tag{3.8}$$

which expresses the conclusion of a generalized *H*-theorem.

The lower bound on the generalized H^{a} -function is determined by the same factors determining the lower bound for the *H*-function. The following two statements can be proved [32]:

(1) if

$$\frac{\mathrm{d}H}{\mathrm{d}t} \leqslant 0$$
, then also $\frac{\mathrm{d}H^{\mathrm{a}}}{\mathrm{d}t} \leqslant 0$; (3.9)

(2) if at a certain stage of the system's evolution 1

$$\frac{\mathrm{d}H}{\mathrm{d}t} \ge 0$$
, then also $\frac{\mathrm{d}H^{\mathrm{a}}}{\mathrm{d}t} \ge 0$, (3.10)

which is forbidden by inequality (3.8).

For a multicomponent gas, the analogue of Eqn (3.1) has the form

$$\frac{\partial f_{\alpha}}{\partial t} - \frac{\partial}{\partial t} \left(\tau_{\alpha} \frac{\partial f_{\alpha}}{\partial t} \right) = J_{\alpha}^{\text{st}}, \qquad (3.11)$$

and as a result the *H*-function for a component α ($\alpha = 1, ..., \mu$) of the mixture can be written as

$$H_{\alpha} = \int f_{\alpha} \ln f_{\alpha} \, \mathrm{d} \mathbf{v}_{\alpha} \,. \tag{3.12}$$

¹ The possibility of there being a fluctuation of *H* growing exponentially with time in the equilibrium state (for $H^{a} = 0$) is ruled out by setting the constant of integration equal to zero, because a spatially uniform model of a physical system is incorrect in this case (see p. 619).

The remaining arguments go through exactly as before, and inequality (3.8) becomes

$$\frac{\mathrm{d}H^{\mathrm{a}}_{\alpha}}{\mathrm{d}t} \leqslant 0. \tag{3.13}$$

Summation over all components now yields the *H*-function for the multicomponent gas mixture:

$$H = \sum_{\alpha} f_{\alpha} \ln f_{\alpha} \,\mathrm{d}\mathbf{v}_{\alpha}\,, \qquad (3.14)$$

with

$$H^{a} = H - \sum_{\alpha=1}^{\mu} \tau_{\alpha} \frac{\mathrm{d}H_{\alpha}}{\mathrm{d}t}, \qquad (3.15)$$

and the inequality

$$\frac{\mathrm{d}H^{\mathrm{a}}}{\mathrm{d}t} \leqslant 0\,,\tag{3.16}$$

the latter following from Eqn (3.13).

If bimolecular chemical reactions

 $A_{\alpha} + A_{\beta} \leftrightarrow A_{\gamma} + A_{\delta}$ $(\alpha, \beta, \gamma, \delta = 1, \dots, \mu)$

proceed in the multicomponent gas mixture, then applying the principle of microscopic reciprocity we again find the *H*theorem to be formulated in terms of Eqn (3.16).

If we now turn to the entropy description then, within an insignificant constant S_0 specified only by the entropy reference adopted, we arrive at the classical relation

 $S = -kH + S_0 \,,$

leading to the thermodynamic inequality

$$\frac{\mathrm{d}S}{\mathrm{d}t} \ge 0. \tag{3.17}$$

Let us now examine the latter inequality from the causeand-effect as well as the time irreversibility points of view. The first question to be answered is how exactly the generalized Boltzmann physical kinetics gave rise to inequality (3.16) leading to the entropy increase (3.17) and to the existence of irreversible processes. This effect is a direct consequence of approximation (2.12), which involves motion against the flying direction of an 'arrow of time' with the result that the state of a system at a given instant is predetermined by collisions that occurred in the past.

We introduce the physical causality principle as an operator which of all the events that may occur at a given time 'cuts out' only that — certain — event, whose causes lie in the past and which translates the certain event under study at the moment to the class of causal relations for some potential event in the future. It is in this way that the time irreversibility enters the theory. In other words, the causality principle cannot be ascribed any meaning unless the notion of time irreversibility is used.

What will happen if we abandon the causality principle formally in this particular case? If one removes the additional assertion that cause precedes effect, then one may replace τ by $-\tau$ formally in Eqn (3.4), to obtain

$$\frac{\mathrm{d}H^{\mathrm{a}'}}{\mathrm{d}t} - \tau \int \frac{1}{f} \left(\frac{\partial f}{\partial t}\right)^2 \mathrm{d}\mathbf{v}$$
$$= \frac{1}{4} \int \ln \frac{ff_1}{f'f_1'} (f'f_1' - ff_1)gb \,\mathrm{d}b \,\mathrm{d}\varphi \,\mathrm{d}\mathbf{v}_1 \,, \qquad (3.18)$$

where

$$H^{\mathrm{a}\prime} = H + \tau \, \frac{\mathrm{d}H}{\mathrm{d}t} \,,$$

or in a different way

$$\frac{\mathrm{d}H^{\mathrm{a}\prime}}{\mathrm{d}t} - \tau \int \frac{1}{f} \left(\frac{\partial f}{\partial t}\right)^2 \mathrm{d}\mathbf{v} \leqslant 0.$$
(3.19)

This says nothing about the sign of the derivative $dH^{a'}/dt$.

Inequality (3.19) may also retain its truth in the case where $dH^{a'}$

 $\frac{\mathrm{d}H^{\mathrm{a}\prime}}{\mathrm{d}t} > 0\,,$

because this quantity is decreased by subtracting the non-negative integral

$$\tau \int \frac{1}{f} \left(\frac{\partial f}{\partial t} \right)^2 \mathrm{d} \mathbf{v} \,,$$

which does not change when t is replaced by -t.

Thus, the principle of increase of entropy is a direct consequence of the principle of time irreversibility.

We now proceed to examine the relation between the generalized Boltzmann equation obtained by the multiscale method and alternative approaches to the derivation of kinetic equations.

4. Generalized Boltzmann equation and the 'physical' derivation of the Boltzmann equation

Let us consider the relationship between the generalized Boltzmann equation and the so-called 'physical' derivation of the Boltzmann equation. Of course, the discussion below will no longer be rigorous, but it will nevertheless be useful for understanding the situation. For this purpose consider the change in the number of particles of the sort α which at instant of time *t* fill a volume d**r**^{*t*} d**v**^{*t*}_{α} in phase space. In the absence of collisions, after a time interval d*t* these particle will occupy the volume d**r**^{*t*+dt} d**v**^{*t*+dt}_{α}, and the difference

$$f_{\alpha} \left[\mathbf{r}(t+\mathrm{d}t), \mathbf{v}_{\alpha}(t+\mathrm{d}t), t+\mathrm{d}t \right] \mathrm{d}\mathbf{r}^{t+\mathrm{d}t} \mathrm{d}\mathbf{v}_{\alpha}^{t+\mathrm{d}t} - f_{\alpha}(\mathbf{r}, \mathbf{v}_{\alpha}, t) \mathrm{d}\mathbf{r}^{t} \mathrm{d}\mathbf{v}_{\alpha}^{t}$$

will be zero.

In the presence of external forces \mathbf{F}_{α} , for example, Lorentz forces, there is generally no reason to consider that elementary phase volume does not change with time, and the Boltzmann equation is therefore written as

$$f_{\alpha}\left[\mathbf{r} + \mathbf{v}_{a} \,\mathrm{d}t + \frac{1}{2} \,\mathbf{F}_{\alpha}(\mathrm{d}t)^{2}, \mathbf{v}_{\alpha} + \mathbf{F}_{\alpha} \,\mathrm{d}t + \frac{1}{2} \,\frac{\partial \mathbf{F}_{\alpha}}{\partial t}(\mathrm{d}t)^{2}, t + \mathrm{d}t\right] \\ \times \frac{\mathrm{d}\left[\mathbf{r}^{t+\mathrm{d}t}, \mathbf{v}_{\alpha}^{t+\mathrm{d}t}\right]}{\mathrm{d}\left[\mathbf{r}^{t}, \mathbf{v}_{\alpha}^{t}\right]} - f_{\alpha}(\mathbf{r}, \mathbf{v}_{\alpha}, t) = J_{\alpha}^{\mathrm{st}} \,\mathrm{d}t \,.$$
(4.1)

This equation retains the terms of order big $O[(dt)^2]$, and the calculation of the Jacobian gives

$$\frac{\mathbf{d}\left[\mathbf{r}^{t+\mathrm{d}t},\mathbf{v}_{\alpha}^{t+\mathrm{d}t}\right]}{\mathbf{d}\left[\mathbf{r}^{t},\mathbf{v}_{\alpha}^{t}\right]} = 1 + \left[\left(\frac{q_{\alpha}}{m_{\alpha}}\right)^{2}B^{2} - \frac{1}{2}\frac{\partial}{\partial\mathbf{r}}\cdot\mathbf{F}_{\alpha}\right].$$
(4.2)

Here q_{α} is the charge of α particle, *B* is the magnetic induction, and F_{α} , the external force acting on the unit mass of α particles.

Expanding the distribution function in a series and keeping the terms of order big $O[(dt)^2]$, we obtain the following integro-differential difference equation

$$\frac{\partial f_{\alpha}}{\partial t} + \mathbf{v}_{\alpha} \cdot \frac{\partial f_{\alpha}}{\partial \mathbf{r}} + \mathbf{F}_{\alpha} \cdot \frac{\partial f_{\alpha}}{\partial \mathbf{v}_{\alpha}} + \tau \left[\mathbf{F}_{\alpha} \cdot \frac{\partial f_{\alpha}}{\partial \mathbf{r}} + \frac{\partial \mathbf{F}_{\alpha}}{\partial t} \cdot \frac{\partial f_{\alpha}}{\partial \mathbf{v}_{\alpha}} + 2 \left(\frac{q_{\alpha}}{m_{\alpha}} \right)^2 B^2 f_{\alpha} - f_{\alpha} \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{F}_{\alpha} + \frac{\partial f_{\alpha}}{\partial \mathbf{v}_{\alpha}} \mathbf{F}_{\alpha} : \frac{\partial}{\partial \mathbf{v}_{\alpha}} \mathbf{F}_{\alpha} \\ + \frac{\partial f_{\alpha}}{\partial \mathbf{v}_{\alpha}} \mathbf{v}_{\alpha} : \frac{\partial}{\partial \mathbf{r}} \mathbf{F}_{\alpha} + \frac{\partial^2 f_{\alpha}}{\partial \mathbf{v}_{\alpha} \partial \mathbf{v}_{\alpha}} : \mathbf{F}_{\alpha} \mathbf{F}_{\alpha} + 2 \frac{\partial^2 f_{\alpha}}{\partial \mathbf{v}_{\alpha} \partial \mathbf{r}} : \mathbf{v}_{\alpha} \mathbf{F}_{\alpha} \\ + 2 \frac{\partial^2 f_{\alpha}}{\partial \mathbf{v}_{\alpha} \partial t} \cdot \mathbf{F}_{\alpha} + \frac{\partial^2 f_{\alpha}}{\partial t^2} + 2 \frac{\partial^2 f_{\alpha}}{\partial \mathbf{r} \partial t} \cdot \mathbf{v}_{\alpha} + \frac{\partial^2 f_{\alpha}}{\partial \mathbf{r} \partial \mathbf{r}} : \mathbf{v}_{\alpha} \mathbf{v}_{\alpha} \right] = J_{\alpha}^{\text{st}} ,$$

$$(4.3)$$

where $\tau = \Delta t/2$ is the difference interval.

Equation (4.3) should be treated as a source of differential-difference approximations for the left-hand side of the Boltzmann equation (4.1). Of course, the differential-difference operator in Eqn (4.3) is not identical to the differential operator in the generalized Boltzmann equation (2.14) — the parameter τ is just the time difference interval, and formally increasing it gives rise to secular terms on the left-hand side of Eqn (4.3). The τ -parametrized differential operator in Eqn (4.3) is formally identical to the corresponding operator of the generalized Boltzmann equation provided $\tau = \text{const}$, the magnetic induction B = 0, and the external forces acting on the system are independent of **r**.

If we put the external forces F_{α} to be zero, Eqn (4.3) takes the form

$$\frac{Df_{\alpha}}{Dt} + \tau \frac{D}{Dt} \frac{Df_{\alpha}}{Dt} = J_{\alpha}^{\text{st}}, \qquad (4.4)$$

where

$$\frac{\mathbf{D}}{\mathbf{D}t} = \frac{\partial}{\partial t} + \mathbf{v}_{\alpha} \cdot \frac{\partial}{\partial \mathbf{r}} \,. \tag{4.5}$$

The question which remains to be answered regarding the formal 'physical' derivation of the Boltzmann equation is how to achieve a highly accurate approximation for J_{α}^{st} . The parameter τ in Eqn (4.4) is a constant which has the opposite sign as compared to its counterpart in Eqn (2.14).

Is it possible to obtain a differential-difference approximation with a minus sign for the second substantial derivative? The answer is a definite yes: the approximation of the form

$$f_{\alpha}(t, \mathbf{r}, \mathbf{v}_{\alpha}) - f_{\alpha}(t - \Delta t, \mathbf{r} - \Delta \mathbf{r}, \mathbf{v}_{\alpha} - \Delta \mathbf{v}_{\alpha})$$

$$= \left[\frac{Df_{\alpha}}{Dt}\right]_{t} \Delta t - \frac{(\Delta t)^{2}}{2} \left[\frac{D}{Dt}\frac{Df_{\alpha}}{Dt}\right]_{t} + \dots$$
(4.6)

directed 'backward' in time leads to the balance equation

$$\frac{Df_{\alpha}}{Dt} - \tau \frac{D}{Dt} \frac{Df_{\alpha}}{Dt} = J_{\alpha}^{\text{st}}, \quad \tau = \frac{\Delta t}{2}.$$
(4.7)

Mathematically, both differential-difference approximations are entirely equivalent, and it is only for reasons of stability that one may be preferred over the other. The assumptions mentioned above result in the differentialdifference approximation being identical to the generalized Boltzmann equation — provided, of course, that the time interval $\Delta t = \text{const}$ of the difference scheme is used formally as two times the mean free time in the generalized Boltzmann kinetic theory.

Thus, two mathematically equivalent difference approximations (4.4) and (4.7) have various physical meaning [cf. Eqn (2.12)]: while one involves the notion of the 'predicted future', the other relates to the 'predetermined past' corresponding to the principle of time irreversibility. The important point to make is that as far as the 'physical' derivation of the Boltzmann equation is concerned, this fact is of no significance because the evolution of the distribution function on the $r_{\rm B}$ scale is not considered at all and, as a consequence, both these approximations lead to the same result.

Thus, Boltzmann's result $dH/dt \le 0$, a consequence of the phenomenological derivation of the Boltzmann equation, may be obtained without explicitly introducing the hypothesis of time irreversibility, whereas its analogue in the generalized theory requires that the time irreversibility assumption (alias, the causality principle) be explicitly used.

We turn next to consider the theory of kinetically consistent difference schemes (see, for example, Refs [41– 43]). The basic ideas of the theory can be traced back to Reitz's (see, e.g., Ref. [44]) method of splitting physical processes into a kinetic and a hydrodynamic stage when addressing transport problems. Unlike paper [44], the theory of kinetically consistent difference schemes uses the expansion of the distribution function as a Taylor series in powers of $v\tau$ (τ being a certain arbitrary parameter determined by the ratio of the mesh width h in space to the characteristic hydrodynamical velocity v_h) correct to third order:

$$f^{j+1}(\mathbf{r}, \mathbf{v}, t^{j+1}) = f_0^j - \tau \sum_{\alpha=1}^3 \frac{\partial f_0^j}{\partial r_\alpha} + \frac{\tau^2}{2} \sum_{\alpha, \beta=1}^3 \frac{\partial^2 f_0^j}{\partial r_\alpha \, \partial r_\beta} \, v_\alpha v_\beta + \dots,$$
(4.8)

where f_0 is the Maxwellian distribution function, and *j* refers to the step number in time.

Work [41] dealing with the theory of kinetically consistent difference schemes introduces three parameters

$$\tau^{x} = \frac{h^{x}}{2v_{\rm h}}, \quad \tau^{y} = \frac{h^{y}}{2v_{\rm h}}, \quad \tau^{z} = \frac{h^{z}}{2v_{\rm h}},$$
(4.9)

which are determined by the space step along the coordinates x, y, z. To find the values of the gas-dynamic parameters at the next time layer $t = t^{j+1}$, the expansion above is multiplied by the mechanical balance invariants and integrated over the molecular velocities of a one-component gas. This yields a system of differential-difference equations whose right-hand sides, unlike those of classical hydrodynamics, contain additional terms which are a combination of second spatial derivatives multiplied by the particular time step employed.

The approach of Ref. [43] does not lead to any new hydrodynamic picture. Furthermore, the derivation of Eqn (4.3) suggests that in the general case this approach does not even provide a second-order approximation either to the Boltzmann equation or to the generalized hydrodynamical equations, the latter being in fact a direct consequence of the generalized Boltzmann equations (see also Refs [35, 36]). Attempts to justify the theory of kinetically consistent difference schemes by using a modified Boltzmann equation with an additional relaxation term break down because the Boltzmann equation works through the times of the order of the relaxation time. In particular, this approximation unlike the generalized hydrodynamical equation and the generalized Boltzmann equation — does not contain any mixed partial time - space derivatives, nor second partial time derivatives. As a consequence, the theory of kinetically consistent difference schemes is of no value when dealing with such problems as (a) the adequate modelling of turbulent flows, (b) the construction of a generalized Navier-Stokes approximation, (c) the inclusion of external forces, (d) the clarification of the physical meaning of the parameter τ which gives rise to secular terms in equations, and (e) the assessment of the impact the unavoidable modification of the collisional integral has on the hydrodynamical equations. As pointed out by Klimontovich [45], "the common drawback of papers [41, 46] is, in particular, that the additional terms they introduce violate the invariance of the kinetic equation with respect to the Galilean transformation. Here too, no sufficient justification was given for introducing additional terms".

An analogy might be appropriate here. Suppose we wish to write the finite-difference approximation for the second Newton law, $\ddot{x} = F/m$. Depending on the accuracy of the scheme used, finite-difference increments of the second and higher orders may appear in the finite-difference approximation, but this does not mean that reverting to the differential formulation we shall obtain a new law of nature of the type $\ddot{x} + \tau \ddot{x} = F/m$. The reason is quite obvious: one cannot obtain a qualitatively new physical description just by using a formally higher-level difference approximation for a classical equation.

In his approach, instead of the usual Liouville equation, Klimontovich [45, 47] used a kinetic equation obtained from the Liouville equation by adding a source (or, to use the terminology of Ref. [45], p. 319, 'seeding') term which when written in the τ -form is

$$\frac{f_N(\mathbf{r},\mathbf{v},t) - \tilde{f}_N(\mathbf{r}',\mathbf{v}',t)}{\tau_{\rm ph}}$$

This term, according to Ref. [45], "describes the 'tuning' of the microscopic particle distribution to the corresponding smoothed distribution".

In the transition to a one-particle description later in the derivation, the parameter τ_{ph} is taken to be τ . The resulting equation then turns out to be a combination of the Boltzmann and Fokker – Planck descriptions (the differential part of the Boltzmann equation remaining unchanged), with the additional 'collision integral' (see Ref. [45], p. 251)

$$I_{(\mathbf{R})}(\mathbf{R}, v, t) = \frac{\partial}{\partial \mathbf{R}} \left[D \, \frac{\partial f}{\partial \mathbf{R}} - bF(\mathbf{R})f \right], \tag{4.10}$$

which accounts for the smoothing process with respect to the size of the 'point', where D is one of the three kinetic coefficients (kinematic viscosity, thermal diffusivity, or self-diffusion coefficient), and b is the mobility. It is assumed that the three kinetic coefficients are all the same and that the difference between them may be accounted for by using another, somewhat more complicated smoothing function.

An analogy can be drawn between the continuity equation due to Slezkin [22, 23] and that due to Klimontovich [45]. Other analogies of hydrodynamical equations are not worth discussing here in our view. As a matter of fact, a source term in the Liouville equation may result from an incomplete statistical description of a reacting system or may be due to the presence of radiation or nonholonomic constraints of some special types, and the size of Klimontovich's 'point' is determined by the $r_{\rm B}$ -scale left out of account earlier in the Boltzmann equations.

5. Generalized Boltzmann equation and iterative construction of higher-order equations in the Boltzmann kinetic theory

Let us consider the relation between the generalized Boltzmann equation and the iterative construction of higher-order equations in the Boltzmann kinetic theory. Neglecting external forces, the Boltzmann equation for a spatially homogeneous case, with the right-hand side taken in the Bhatnagar-Gross-Krook (BGK) form, is given by

$$\frac{\partial f_{\alpha}}{\partial t} = -\frac{f - f_0}{\tau_{\rm rel}} \,, \tag{5.1}$$

where τ_{rel} is the relaxation time, and f_0 the equilibrium distribution function. From Eqn (5.1) it follows that

$$f = f_0 - \tau_{\rm rel} \,\frac{\partial f}{\partial t} \cong f_0 - \tau_{\rm rel} \,\frac{\partial f_0}{\partial t} \,. \tag{5.2}$$

The second iteration is constructed in a similar fashion giving

$$f = f_0 - \tau_{\rm rel} \frac{\partial}{\partial t} \left(f_0 - \tau_{\rm rel} \frac{\partial f}{\partial t} \right) \cong f_0 - \tau_{\rm rel} \frac{\partial f_0}{\partial t} + \tau_{\rm rel}^2 \frac{\partial^2 f_0}{\partial t^2} .$$
(5.3)

Thus we obtain for the distribution function the series representation

$$f = \sum_{i=0}^{\infty} (-1)^i \frac{\partial^i f_0}{\partial t^i} \tau^i_{\text{rel}}, \qquad (5.4)$$

where the zero-order derivative operator corresponds to the distribution function f_0 .

From Eqn (5.3) there follows an analogue of the kinetic equation (5.1) for the second approximation:

$$-\tau_{\rm rel} \,\frac{\partial^2 f_0}{\partial t^2} + \frac{\partial f_0}{\partial t} = -\frac{f - f_0}{\tau_{\rm rel}} \,. \tag{5.5}$$

It is important to note that the second time derivative of the distribution function f_0 in Eqn (5.5) occurs with a minus sign. In the general case we have the expansion

$$\sum_{i=1}^{\infty} \tau_{\rm rel}^{i-1} (-1)^{i-1} \, \frac{\partial^i f_0}{\partial t^i} = -\frac{f - f_0}{\tau_{\rm rel}} \,. \tag{5.6}$$

We now proceed to show that the generalized Boltzmann equation permits an iterative procedure similar to that just described. To this end we can write the second approximation in the form

$$\frac{\mathbf{D}_{1}\hat{f}_{1}^{1}}{\mathbf{D}\hat{t}_{B}} = -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}}{\mathbf{D}\hat{t}_{B}}\right) \cong -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left[\tau \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} (\hat{f}_{1}^{0} + \hat{f}_{1}^{1})\right]
= -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}} + \tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{1}}{\mathbf{D}\hat{t}_{B}}\right)
= -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}}\right) + \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left[\tau \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}}\right)\right], \quad (5.7)$$

using approximation (2.12).

Higher approximations follow the same pattern. Thus one obtains

$$\frac{\mathbf{D}_{1}\hat{f}_{1}^{1}}{\mathbf{D}\hat{t}_{B}} = -\frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}} \right) + \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left[\tau \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}} \right) \right]
- \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left\{ \tau \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left[\tau \frac{\mathbf{D}_{1}}{\mathbf{D}\hat{t}_{B}} \left(\tau \frac{\mathbf{D}_{1}\hat{f}_{1}^{0}}{\mathbf{D}\hat{t}_{B}} \right) \right] \right\} + \dots \quad (5.8)$$

Assuming a spatially homogeneous system free of forces, we obtain

$$\frac{\partial f_1^1}{\partial t} = \sum_{i=2}^{\infty} \tau^{i-1} (-1)^{i-1} \frac{\partial^i f_1^0}{\partial t^i}$$
(5.9)

from Eqn (5.8) with $\tau = \text{const.}$ It follows that in this particular case the generalized Boltzmann equation takes the form

$$\sum_{i=2}^{\infty} \tau^{i-1} (-1)^{i-1} \frac{\partial^i f_1^0}{\partial t^i} + \frac{\partial f_1^0}{\partial t} = J^{\text{st},0}$$
(5.10)

or, collecting terms on the left, one finds

$$\sum_{i=1}^{\infty} \tau^{i-1} (-1)^{i-1} \frac{\partial^i f_1^0}{\partial t^i} = J^{\text{st},0} .$$
 (5.11)

The analogy between Eqns (5.6) and (5.11) is clearly seen.

In solid-state problems — concerning, for example, charge and energy transfer in nondegenerate semiconductors — one solves the Boltzmann equation iteratively for a spatially homogeneous system in the presence of an external electromagnetic field. For the BGK-approximated collision integral, the Boltzmann equation becomes

$$F\frac{\partial f}{\partial v_z} = -\frac{f - f_0}{\tau_{\rm rel}}$$
(5.12)

(for a z-directed external force F), and the distribution function is written as

$$f = f_0 - \tau_{\rm rel} F \frac{\partial f}{\partial v_z} \,. \tag{5.13}$$

In a first approximation, we obtain

$$f = f_0 - \tau_{\rm rel} F \frac{\partial f_0}{\partial v_z} \,. \tag{5.14}$$

Substituting Eqn (5.14) into the left-hand side of Eqn (5.12) yields the second-order approximation,

$$f = f_0 - \tau_{\rm rel} F \frac{\partial f_0}{\partial v_z} + \tau_{\rm rel}^2 F^2 \frac{\partial^2 f_0}{\partial v_z^2} + \dots, \qquad (5.15)$$

provided the external force F acting on the particle is velocityindependent. The dots in this equation indicate that the procedure of constructing the series may be continued by this algorithm. From Eqn (15), the second-order accurate equation is

$$F\frac{\partial f_0}{\partial v_z} - \tau_{\rm rel} F^2 \frac{\partial^2 f_0}{\partial v_z^2} = -\frac{f - f_0}{\tau_{\rm rel}} .$$
 (5.16)

This equation turns out to be a particular case of the generalized Boltzmann equation if the system under study is

stationary, spatially homogeneous, and if the applied field is sufficiently weak — giving hope for the convergence of the series (5.15), in which the corresponding derivatives are taken of the equilibrium distribution function. The representation of the distribution function in a series form, Eqns (5.15) or (5.4), is only possible when one uses the BGK model for the Boltzmann collision integral.

Thus, the generalized Boltzmann equation automatically captures the second iteration in the Boltzmann theory for $\tau = \tau_{rel}$, but it does not of course presuppose the fulfillment of all the conditions listed. Note also that the appearance of the minus sign in the right-hand sides of Eqns (5.1) and (5.12) in the BGK approximation has a deep physical meaning: this sign makes it possible to prove the *H*-theorem for the BGK-approximated Boltzmann equation and is related directly to the approximation proceeded against the course of time.

6. Generalized Boltzmann equation and the theory of kinetic equations with time delay

It is of interest to examine the relation between the Boltzmann equation and the theory of kinetic equations accounting for time delay effects. We resort to the Bogolyubov equation for determining the evolution of the *s*-particle distribution function in a one-component gas:

$$\frac{\partial f_s}{\partial t} + \sum_{i=1}^s \mathbf{v}_i \cdot \frac{\partial f_s}{\partial \mathbf{r}_i} + \sum_{i=1}^s \mathbf{F}_i \cdot \frac{\partial f_s}{\partial \mathbf{v}_i} + \sum_{ij=1}^s \mathbf{F}_{ij} \cdot \frac{\partial f_s}{\partial \mathbf{v}_i}$$
$$= -\frac{1}{N} \sum_{i=1}^s \sum_{j=s+1}^s \mathbf{F}_{ij} \cdot \frac{\partial f_s}{\partial \mathbf{v}_i} .$$
(6.1)

In writing Eqn (6.1) the normalization condition

$$\int f_s \,\mathrm{d}\Omega_1 \dots \,\mathrm{d}\Omega_s = N^s \tag{6.2}$$

was used and it was also assumed that the dynamic state of the system is fully described by the phase variables Ω_i .

Introducing the correlation functions W, the two-particle distribution function may be written as

$$f_2(\Omega_1, \Omega_2, t) = f_1(\Omega_1, t) f_1(\Omega_2, t) + W_2(\Omega_1, \Omega_2, t).$$
 (6.3)

At the $r_{\rm B}$ scale, variables Ω_1 and Ω_2 turn out to be correlated, but because of definition (6.3) this effect is accounted for by the function W_2 . Consequently, in this approach it is the integral term containing W_2 which must lead to the Boltzmann (or a more general) collision integral.

The BBGKY-1 equation has the form

$$\frac{\partial f_1}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1}{\partial \mathbf{r}_1} + \mathbf{F}_1 \cdot \frac{\partial f_1}{\partial \mathbf{v}_1} + \frac{1}{N} \sum_{j=2}^N \frac{\partial f_1}{\partial \mathbf{v}_1} \cdot \int \mathbf{F}_{ij} f_1(2) \, \mathrm{d}\Omega_2$$
$$= -\frac{1}{N} \sum_{i=2}^s \int \mathbf{F}_{ij} \cdot \frac{\partial W_2}{\partial \mathbf{v}_1} \, \mathrm{d}\Omega_2 \,. \tag{6.4}$$

The internal force $\mathbf{F}_1^{(in)}$ exerted on a given particle 1 from the side of particle 2 at its arbitrary location in phase space may be written as

$$\frac{1}{N} \sum_{j=2}^{N} \int \mathbf{F}_{1j} f_1(2) \, \mathrm{d}\Omega_2 = \mathbf{F}_1^{(\mathrm{in})} \,. \tag{6.5}$$

Here, as usual, the symbol '2', the argument of the oneparticle distribution function $f_1(2)$, denotes the phase variables of the particle 2. For identical particles, one finds

$$\mathbf{F}_{1}^{(\text{in})} = \frac{N-1}{N} \int \mathbf{F}_{12} f_{1}(2) \, \mathrm{d}\Omega_{2} \cong \int \mathbf{F}_{12} f_{1}(2) \, \mathrm{d}\Omega_{2}$$
$$= \int \mathbf{F}_{1j} f_{1}(j) \, \mathrm{d}\Omega_{j} \quad (j = 2, 3, \ldots) \,.$$
(6.6)

If the self-consistent force acting on a probe particle in the one-particle picture is introduced as the sum

$$\mathbf{F}_{1}^{(\mathrm{sc},1)} = \mathbf{F}_{1} + \mathbf{F}_{1}^{(\mathrm{in})} \tag{6.7}$$

of the external force \mathbf{F}_1 and the internal force $\mathbf{F}_1^{(in)}$ defined by Eqn (6.5), then we arrive at the equation

$$\frac{\partial f_1}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1}{\partial \mathbf{r}_1} + \mathbf{F}_1^{(\text{sc},1)} \cdot \frac{\partial f_1}{\partial \mathbf{v}_1} = -\frac{1}{N} \sum_{j=2}^N \mathbf{F}_{1j} \cdot \frac{\partial W_2}{\partial \mathbf{v}_1} \, \mathrm{d}\Omega_2 \,. \quad (6.8)$$

The BBGKY-2 equation has the form

$$\frac{\partial f_2}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_2}{\partial \mathbf{r}_1} + \mathbf{v}_2 \cdot \frac{\partial f_2}{\partial \mathbf{r}_2} + \mathbf{F}_1 \cdot \frac{\partial f_2}{\partial \mathbf{v}_1} + \mathbf{F}_2 \cdot \frac{\partial f_2}{\partial \mathbf{v}_2} + \mathbf{F}_{12} \cdot \frac{\partial f_2}{\partial \mathbf{v}_1} + \mathbf{F}_{21} \cdot \frac{\partial f_2}{\partial \mathbf{v}_2} = -\frac{1}{N} \sum_{j=3}^N \int \left[\mathbf{F}_{1j} \cdot \frac{\partial f_3}{\partial \mathbf{v}_1} + \mathbf{F}_{2j} \cdot \frac{\partial f_3}{\partial \mathbf{v}_2} \right] d\Omega_3.$$
(6.9)

We next express the distribution function f_3 in terms of the correlation functions as

$$f_{3}(\Omega_{1}, \Omega_{2}, \Omega_{3}, t) = f_{1}(\Omega_{1}, t) f_{1}(\Omega_{2}, t) f_{1}(\Omega_{3}, t) + f_{1}(\Omega_{1}, t) W_{2}(\Omega_{2}, \Omega_{3}, t) + f_{1}(\Omega_{2}, t) W_{2}(\Omega_{1}, \Omega_{3}, t) + f_{1}(\Omega_{3}, t) W_{2}(\Omega_{1}, \Omega_{2}, t) + W_{3}(\Omega_{1}, \Omega_{2}, \Omega_{3}, t)$$
(6.10)

and apply the theory of correlation functions to obtain an approximation for collision integrals.

Assumption 1. The correlation function W_3 may be neglected.

Using Eqn (6.2), Eqn. (6.10) can be put into the form

$$f_3(1,2,3) = f_1(3) f_2(1,2) + f_1(2) W_2(1,3) + f_1(1) W_2(2,3).$$
(6.11)

Substituting Eqn (6.11) into Eqn (6.9) and introducing selfconsistent forces in the framework of a two-particle description (j = 3, 4, 5, ...), viz.

$$\mathbf{F}_{1}^{(\text{sc},2)} = \mathbf{F}_{1} + \mathbf{F}_{12} + \int \mathbf{F}_{1j} f_{1}(j) \,\mathrm{d}\Omega_{j},$$

$$\mathbf{F}_{2}^{(\text{sc},2)} = \mathbf{F}_{2} + \mathbf{F}_{21} + \int \mathbf{F}_{2j} f_{1}(j) \,\mathrm{d}\Omega_{j},$$
 (6.12)

we arrive at the equation for $f_2(1,2)$:

$$\frac{\partial f_2}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_2}{\partial \mathbf{r}_1} + \mathbf{v}_2 \cdot \frac{\partial f_2}{\partial \mathbf{r}_2} + \mathbf{F}_1^{(\mathrm{sc},2)} \cdot \frac{\partial f_2}{\partial \mathbf{v}_1} + \mathbf{F}_2^{(\mathrm{sc},2)} \cdot \frac{\partial f_2}{\partial \mathbf{v}_2}$$
$$= f_1(2) \left[\frac{\partial f_1(1)}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1(1)}{\partial \mathbf{r}_1} + \mathbf{F}_1^{(\mathrm{sc},1)} \cdot \frac{\partial f_1(1)}{\partial \mathbf{v}_1} \right]$$
$$+ f_1(1) \left[\frac{\partial f_1(2)}{\partial t} + \mathbf{v}_2 \cdot \frac{\partial f_1(2)}{\partial \mathbf{r}_2} + \mathbf{F}_2^{(\mathrm{sc},1)} \cdot \frac{\partial f_1(2)}{\partial \mathbf{v}_2} \right], \quad (6.13)$$

making use of the results

$$\frac{\partial f_1(1)}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1(1)}{\partial \mathbf{r}_1} + \mathbf{F}_1^{(\mathrm{sc},1)} \cdot \frac{\partial f_1(1)}{\partial \mathbf{v}_1} = -\int \mathbf{F}_{13} \cdot \frac{\partial W_2(1,3)}{\partial \mathbf{v}_1} \, \mathrm{d}\Omega_3 \,, \qquad (6.14)$$

$$\frac{\partial f_1(2)}{\partial t} + \mathbf{v}_2 \cdot \frac{\partial f_1(2)}{\partial \mathbf{r}_2} + \mathbf{F}_2^{(\mathrm{sc},1)} \cdot \frac{\partial f_1(2)}{\partial \mathbf{v}_2}$$
$$= -\int \mathbf{F}_{23} \cdot \frac{\partial W_2(2,3)}{\partial \mathbf{v}_2} \, \mathrm{d}\Omega_3 \,. \tag{6.15}$$

In writing Eqn (6.13) we have used the following assumption. Assumption 2. The polarization effects leading to the integrals

$$-\frac{1}{N}\sum_{j=3}^{N}\int \mathbf{F}_{1j} \cdot \frac{\partial}{\partial \mathbf{v}_{1}} \left(f_{1}(1) W_{2}(2,3)\right) \mathrm{d}\Omega_{3},$$

$$-\frac{1}{N}\sum_{j=3}^{N}\int \mathbf{F}_{2j} \cdot \frac{\partial}{\partial \mathbf{v}_{2}} \left(f_{1}(2) W_{2}(1,3)\right) \mathrm{d}\Omega_{3},$$

may be ignored.

We next introduce the substantial derivatives

$$\frac{\mathbf{D}f_2(1,2)}{\mathbf{D}t} = \frac{\partial f_2}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_2}{\partial \mathbf{r}_1} + \mathbf{v}_2 \cdot \frac{\partial f_2}{\partial \mathbf{r}_2} + \mathbf{F}_1^{(\mathrm{sc},2)} \cdot \frac{\partial f_2}{\partial \mathbf{v}_1} + \mathbf{F}_2^{(\mathrm{sc},2)} \cdot \frac{\partial f_2}{\partial \mathbf{v}_2}, \qquad (6.16)$$

$$\frac{\mathbf{D}_1 f_1(1)}{\mathbf{D}t} = \frac{\partial f_1}{\partial t} + \mathbf{v}_1 \cdot \frac{\partial f_1}{\partial \mathbf{r}_1} + \mathbf{F}_1^{(\mathrm{sc},\,1)} \cdot \frac{\partial f_1}{\partial \mathbf{v}_1} , \qquad (6.17)$$

$$\frac{\mathbf{D}_2 f_1(2)}{\mathbf{D}t} = \frac{\partial f_1}{\partial t} + \mathbf{v}_2 \cdot \frac{\partial f_1}{\partial \mathbf{r}_2} + \mathbf{F}_2^{(\mathrm{sc},1)} \cdot \frac{\partial f_1}{\partial \mathbf{v}_2}, \qquad (6.18)$$

which when substituted into Eqn (6.13) yield

$$\frac{\mathbf{D}f_2(1,2)}{\mathbf{D}t} = f_1(2) \frac{\mathbf{D}_1 f_1(1)}{\mathbf{D}t} + f_1(1) \frac{\mathbf{D}_2 f_1(2)}{\mathbf{D}t} \,. \tag{6.19}$$

Let us now integrate with respect to time along the phase trajectory in a six-dimensional space:

$$f_{2}(1,2) = f_{2,0}(1,2) + \int_{t_{0}}^{t_{0}+\tau} f_{1}(2) \frac{\mathbf{D}_{1}f_{1}(1)}{\mathbf{D}t} dt + \int_{t_{0}}^{t_{0}+\tau} f_{1}(1) \frac{\mathbf{D}_{2}f_{1}(2)}{\mathbf{D}t} dt, \qquad (6.20)$$

where $f_{2,0}(1,2)$ denotes the initial value of the two-particle distribution function.

Assumption 3. We resort to the Bogolyubov condition of the weakening of initial correlations corresponding to a certain initial instant of time t_0 [see Eqn (2.13)]:

$$\lim_{t_0 \to -\infty} W_2 \big[\mathbf{r}_1(t_0 - t), \mathbf{v}_1(t_0 - t); \, \mathbf{r}_2(t_0 - t), \mathbf{v}_2(t_0 - t); \, t_0 - t \big] = 0 \,.$$
(6.21)

This condition implies that (a) we are dealing with infinite motion in a two-body problem, (b) we may speak of the condition of molecular chaos being fulfilled prior to the collision of the particles 1 and 2, which corresponds to the approximation in Eqn (2.12) proceeded against the course of time, and (c) Eqn (6.21) is written at the $r_{\rm B}$ scale even though no scale is introduced explicitly.

Because of assumption 3, Eqn (6.20) may be represented in the form

$$f_{2}(1,2) = f_{1}(\mathbf{r}_{1}(t_{0}), \mathbf{v}_{1}(t_{0}), t_{0}) f_{1}(\mathbf{r}_{2}(t_{0}), \mathbf{v}_{2}(t_{0}), t_{0}) + \int_{t_{0}}^{t_{0}+\tau} f_{1}(2) \frac{\mathbf{D}_{1}f_{1}(1)}{\mathbf{D}t} dt + \int_{t_{0}}^{t_{0}+\tau} f_{1}(1) \frac{\mathbf{D}_{2}f_{1}(2)}{\mathbf{D}t} dt.$$
(6.22)

Assumption 4. The collision of the probe particles, 1 and 2, is dominated by the forces of their internal interaction, so that [see Eqns (6.7) and (6.12)] one obtains

$$\mathbf{F}_{1}^{(\mathrm{sc},2)} = \mathbf{F}_{1}^{(\mathrm{sc},1)}, \quad \mathbf{F}_{2}^{(\mathrm{sc},2)} = \mathbf{F}_{2}^{(\mathrm{sc},1)}.$$
 (6.23)

Equation (6.22) then becomes

$$f_{2}(1,2) = f_{1}(\mathbf{r}_{1}(t_{0}), \mathbf{v}_{1}(t_{0}), t_{0}) f_{2}(\mathbf{r}_{2}(t_{0}), \mathbf{v}_{2}(t_{0}), t_{0}) + \int_{t_{0}}^{t_{0}+\tau} \frac{\mathbf{D}_{12}}{\mathbf{D}t} [f_{1}(\mathbf{r}_{1}, \mathbf{v}_{1}, t) f_{2}(\mathbf{r}_{2}, \mathbf{v}_{2}, t)] dt. \quad (6.24)$$

Integrating by parts we find

$$f_{2}(1,2) = f_{1}(\mathbf{r}_{1},\mathbf{v}_{1},t) f_{2}(\mathbf{r}_{2},\mathbf{v}_{2},t) + \tau \left\{ \frac{\mathbf{D}_{12}}{\mathbf{D}t} \left[f_{1}(\mathbf{r}_{1}(t),\mathbf{v}_{1}(t),t_{0}) f_{1}(\mathbf{r}_{2}(t),\mathbf{v}_{2}(t),t_{0}) \right] \right\}_{t=t_{0}} - \int_{t_{0}}^{t_{0}+\tau} t \frac{\mathbf{D}_{12}}{\mathbf{D}t} \frac{\mathbf{D}_{12}}{\mathbf{D}t} \left[f_{1}(1)f_{1}(2) \right] \mathrm{d}t .$$
(6.25)

Assumption 5. Delay is sufficiently small that linearization in delay time can be used.

The sum of the first two terms in Eqn (6.25) determines the product $f_1(1) f_1(2)$ at the instant of time t in the linear approximation in τ , the velocities of particles 1 and 2 corresponding to their initial values at time t_0 (taken to be $t_0 = -\infty$ on the $r_{\rm B}$ scale).

If we now substitute $f_2(1,2)$ from Eqn (6.25) into the BBGKY-1 equation, we obtain

$$\frac{\partial f_{1}(1)}{\partial t} + \mathbf{v}_{1} \cdot \frac{\partial f_{1}(1)}{\partial \mathbf{r}_{1}} + \mathbf{F}_{1} \cdot \frac{\partial f_{1}(1)}{\partial \mathbf{v}_{1}} = -\int \mathbf{F}_{12} \cdot \frac{\partial}{\partial \mathbf{v}_{1}} \left[f_{1}(\mathbf{r}_{1}, \mathbf{v}_{1}(-\infty), t) f_{1}(\mathbf{r}_{2}, \mathbf{v}_{2}(-\infty), t) \right] d\Omega_{2} + \int \mathbf{F}_{12} \cdot \frac{\partial}{\partial \mathbf{v}_{1}} \left\{ \int_{t_{0}}^{t_{0}+\tau} t \frac{\mathbf{D}_{12}}{\mathbf{D}t} \frac{\mathbf{D}_{12}}{\mathbf{D}t} \left[f_{1}(1) f_{1}(2) \right] dt \right\} d\Omega_{2} . \quad (6.26)$$

The first integral on the right corresponds to the classical form of the Bogolyubov collision integral and can be transformed in the usual manner to the Boltzmann collision integral [15]. The second collision integral accounts for the time delay effect and is amenable to a differential approximation analogous to Eqn (2.12). To obtain this approximation, the following assumption is made.

Assumption 6. For an arbitrary location of particle 2 in the phase space of interacting particles 1 and 2, the dependence on the integrand inside the braces in the time delay integral

$$J_{2}^{\text{st}} = \int \mathbf{F}_{12} \cdot \frac{\partial}{\partial \mathbf{v}_{1}} \left\{ \int_{t_{0}}^{t_{0}+\tau} t \, \frac{\mathbf{D}_{12}}{\mathbf{D}t} \frac{\mathbf{D}_{12}}{\mathbf{D}t} \left[f_{1}(1) \, f_{1}(2) \right] \mathrm{d}t \right\} \, \mathrm{d}\Omega_{2}$$
(6.27)

is determined by the acting internal force F_{12} via the change in the particle velocities ².

From Eqn (6.27) we have [cf. Eqn (4.7)]

$$J_{2}^{\mathrm{st}} = \int \mathbf{F}_{12} \cdot \frac{\partial}{\partial \mathbf{v}_{1}} \left\{ \int_{t_{0}}^{t} t' \frac{\mathbf{D}_{12}}{\mathbf{D}t'} \frac{\mathbf{D}_{12}}{\mathbf{D}t'} [f_{1}(1) f_{1}(2)] \, \mathrm{d}t' \right\} \mathrm{d}\Omega_{2}$$

$$= \int \left(\mathbf{F}_{12} \cdot \frac{\partial}{\partial \mathbf{v}_{1}} + \mathbf{F}_{21} \cdot \frac{\partial}{\partial \mathbf{v}_{2}} \right)$$

$$\times \left\{ \int_{t_{0}}^{t} t' \frac{\mathbf{D}_{12}}{\mathbf{D}t'} \frac{\mathbf{D}_{12}}{\mathbf{D}t'} [f_{1}(1) f_{1}(2)] \, \mathrm{d}t' \right\} \mathrm{d}\Omega_{2}$$

$$\cong \tau_{\mathrm{r}} \int \frac{\mathbf{D}_{12}}{\mathbf{D}t} \frac{\mathbf{D}_{12}}{\mathbf{D}t} [f_{1}(1) f_{1}(2)] \, \mathrm{d}\Omega_{2} = \tau_{\mathrm{r}} \frac{\mathbf{D}_{1}}{\mathbf{D}t} \frac{\mathbf{D}_{1}f_{1}(1)}{\mathbf{D}t}, \qquad (6.28)$$

where the assumption 5 has been used again and an effective delay time τ_r introduced.

Generally speaking, integration with respect to time in Eqn (6.28) is 'eliminated' by the substantial derivative, which also contains spatial differentiation. However, to the linear approximation in the delay time this contribution is negligible. This can be seen by writing

$$\begin{split} J_{2}^{\text{st}} &= \int \left\{ \left[\mathbf{F}_{12} \cdot \frac{\partial}{\partial \mathbf{v}_{1}} + \mathbf{F}_{21} \cdot \frac{\partial}{\partial \mathbf{v}_{2}} + (\mathbf{v}_{2} - \mathbf{v}_{1}) \cdot \frac{\partial}{\partial \mathbf{x}_{21}} \right] \right. \\ &\times \int_{t_{0}}^{t} t' \frac{\mathbf{D}_{12}}{\mathbf{D}t'} \frac{\mathbf{D}_{12}}{\mathbf{D}t'} \left[f_{1}(1) f_{1}(2) \right] dt' \right\} d\Omega_{2} \\ &- \int \left\{ (\mathbf{v}_{2} - \mathbf{v}_{1}) \cdot \frac{\partial}{\partial \mathbf{x}_{21}} \int_{t_{0}}^{t} t' \frac{\mathbf{D}_{12}}{\mathbf{D}t} \frac{\mathbf{D}_{12}}{\mathbf{D}t'} \left[f_{1}(1) f_{1}(2) \right] dt' \right\} d\Omega_{2} \\ &= \tau_{r} \frac{\mathbf{D}_{1}}{\mathbf{D}t} \frac{\mathbf{D}_{1} f_{1}(1)}{\mathbf{D}t} \\ &- \int \left\{ (\mathbf{v}_{2} - \mathbf{v}_{1}) \cdot \frac{\partial}{\partial \mathbf{x}_{21}} \int_{t_{0}}^{t} t' \frac{\mathbf{D}_{12}}{\mathbf{D}t'} \frac{\mathbf{D}_{12}}{\mathbf{D}t'} \left[f_{1}(1) f_{1}(2) \right] dt' \right\} d\Omega_{2} \\ &= \tau_{r} \frac{\mathbf{D}_{1}}{\mathbf{D}t} \frac{\mathbf{D}_{1} f(1)}{\mathbf{D}t} \\ &+ \int \left\{ (\mathbf{v}_{2} - \mathbf{v}_{1}) \cdot \frac{\partial}{\partial \mathbf{x}_{21}} \left[f_{1}(1) f_{1}(2) \right] - \left[f_{1}(1) f_{1}(2) \right]_{t_{0}} \\ &- \tau_{r} \frac{\mathbf{D}_{1}}{\mathbf{D}t} \left[f_{1}(1) f_{1}(2) \right]_{t_{0}} \right] \right\} d\Omega_{2} \cong \tau_{r} \frac{\mathbf{D}_{1}}{\mathbf{D}t} \frac{\mathbf{D}_{1} f_{1}(1)}{\mathbf{D}t} , \quad (6.29) \end{split}$$

where $\mathbf{x}_{21} = \mathbf{r}_2 - \mathbf{r}_1$.

Thus, the appearance of the second substantial derivative with respect to time in the generalized Boltzmann equation may be considered as a differential approximation to the time delay integral that emerges in the theory of correlation functions for kinetic equations.

It would appear that the above theory does not require at all that we apply the multiscale method and expand the distribution function in a power series of a small parameter $\varepsilon = nr_{\rm B}^3$. However, such is not the case. As we have seen above, the integration at the $r_{\rm B}$ scale must be employed anyway, and giving up the ε -expansion of the distribution function, on the other hand, makes it impossible to estimate the value of $\tau_{\rm r}$. Each of the approaches outlined above actually complement one another and are interrelated with one another. The generalized Boltzmann equation can be treated both from the point of view of a higher-order Boltzmann theory and as a result of differential approximations to the collision integral accounting for time delay effects.

² This assumption was used by Bogolyubov (see Ref. [48], p.203).

There is another point to be made. From Eqn (2.6), the equation for the distribution function f_2^{0} accurate to the zeroth order in ε is

$$\frac{\partial \hat{f}_{2}^{0}}{\partial \hat{t}_{B}} + \mathbf{v}_{1B} \cdot \frac{\partial \hat{f}_{2}^{0}}{\partial \mathbf{r}_{1B}} + \mathbf{v}_{j \in N_{\delta}} \cdot \frac{\partial \hat{f}_{2}^{0}}{\partial \mathbf{r}_{j \in N_{\delta}, B}} + \hat{\mathbf{F}}_{1, j \in \delta} \cdot \frac{\partial \hat{f}_{2}^{0}}{\partial \mathbf{v}_{1B}} + \hat{\mathbf{F}}_{j \in N_{\delta}, 1} \cdot \frac{\partial \hat{f}_{2}^{0}}{\partial \mathbf{v}_{j \in N_{\delta}, B}} + \alpha \hat{\mathbf{F}}_{1} \cdot \frac{\partial \hat{f}_{2}^{0}}{\partial \mathbf{v}_{1B}} + \alpha \hat{\mathbf{F}}_{j \in N_{\delta}} \cdot \frac{\partial \hat{f}_{2}^{0}}{\partial \mathbf{v}_{j \in N_{\delta}, B}} = 0$$

$$(6.30)$$

Comparing this with Eqns (6.9) and (6.10) shows that the correlation functions accurate to zeroth order in ε are zero and that forces exerted on the colliding particles 1 and 2 from the side of other particles are not considered in the zero-order approximation at the $r_{\rm B}$ scale. This result is used for transforming the collision integral $\hat{J}^{\rm st,0}$ to the Boltzmann form in the multiscale method.

We may summarize then by saying that the derivation of the kinetic equation in the context of the theory of correlation functions for one-particle distribution functions leads to a kinetic equation of the form

$$\frac{\mathrm{D}f}{\mathrm{D}t} = J^{\mathrm{B}} + J^{\mathrm{td}} \,, \tag{6.31}$$

where J^{B} and J^{td} are the Boltzmann collision integral and the collision integral accounting for time delay effects, respectively.

The popularity of the BGK approximation to the Boltzmann collision integral:

$$J^{\rm B} = \frac{f^{(0)} - f}{\tau} \tag{6.32}$$

is due to the drastic simplifications it affords. Essentially, the generalized Boltzmann physical kinetics offer a local approximation for the second collision integral

$$J^{\text{td}} = \frac{D}{Dt} \left(\tau \frac{Df}{Dt} \right). \tag{6.33}$$

Thus, Eqn (6.31) in its 'simplest' version takes the form

$$\frac{\mathrm{D}f}{\mathrm{D}t} = \frac{f^{(0)} - f}{\tau} + \frac{\mathrm{D}}{\mathrm{D}t} \left(\tau \frac{\mathrm{D}f}{\mathrm{D}t}\right). \tag{6.34}$$

Since the ratio of the second to the first term on the right of this equation is $J^{\rm td}/J^{\rm B} \approx O({\rm Kn}^2)$, Kn being the Knudsen number, it would seem that the second term can be neglected for hydrodynamically small Knudsen numbers. However, in the transition to the hydrodynamic limit (after multiplying the kinetic equation by the collision invariants and subsequently integrating over velocities), the Boltzmann integral term vanishes, while the second term on the right-hand side of Eqn (6.34) gives a single-order contribution in the generalized Navier – Stokes description (let alone the effect of the small parameter of the higher derivative).

A well-known example of a local approximation to a nonlocal integral term in kinetic theory is the Enskog theory of transport processes in a dense gas composed of hard spheres. To obtain a local version of the theory, Enskog used the expansion in terms of the small parameter σ/λ , where σ is the molecular diameter, and λ the mean free path (see Ref.

[49]). For example, for hydrogen at normal pressures and temperatures $\sigma \approx 3 \times 10^{-8}$ cm and $\lambda \approx 1.1 \times 10^{-5}$ cm, and the resulting $\sigma/\lambda = 2.7 \times 10^{-3}$ corresponds to the typical hydrodynamically-valid range of the Knudsen number variation. In the case of the expansion in terms of Kn, σ/λ would imply $L \approx 0.4 \times 10^{-2}$ cm as the characteristic hydrodynamic size whereat the smoothing is proceeding.

7. Generalized hydrodynamical equations and the theory of turbulent flows

The generalized Boltzmann equation necessarily leads to a new formulation of the hydrodynamical equations, yielding what we will call the generalized hydrodynamical equations. The classical Enskog, Euler, and Navier–Stokes equations of fluid dynamics are special cases of these new equations. The derivation of the generalized hydrodynamical equations is given in Refs [31, 38] and because it is too cumbersome to be reproduced here, we will only consider the fundamental points of this derivation, taking as an example the generalized Euler equations as used in the theory of turbulent flows.

The turbulent fluid motion has been the subject of intense research for over a hundred years because it has numerous applications in aerodynamics, hydraulics, combustion and explosion processes, and hence is of direct relevance to processes occurring in turbines, engines, compressors, and other modern-day machines. The scientific literature on this subject is enormous, and a detailed analysis of all the existing models is beyond the scope of this paper. Here the object is to discuss the currently available turbulence concept in the context of generalized equations of fluid dynamics. In what follows we will discuss 'classical' turbulence, usually treated starting from the Navier-Stokes equations, moment methods, and similarity theory. We will also see how this picture corresponds to the generalized Boltzmann kinetics and will try to find out which of the known approaches may be used and which should be abandoned.

It is commonly held that a fully developed turbulence may be characterized by the irregular variation of velocity with time at each point in the flow and that hydrodynamic quantities undergo fluctuations (turbulent ones or pulsations), whose scale varies over the wide range from the external (using the terminology of Ref. [9]) scale comparable to the characteristic flow size, to a small scale on which the dynamic fluid viscosity begins to dominate.

Because of the major role of the Reynolds criterion in the theory of turbulence, the study of fluid motion on various typical scales crucially depends on the construction of the Reynolds number

$$\operatorname{Re} = \frac{v_l l}{v}$$

Here, l is the fluctuation scale, v_l the characteristic velocity, and v the kinematic viscosity. If $l \sim L$, with L being the typical hydrodynamic size, then the Reynolds number Re is large and the effect of molecular viscosity small — so that one may neglect it altogether and apply the similarity theory (the Kolmogorov–Obukhov law) to get some idea of the fluctuations.

From the large-scale fluctuations, the energy goes (practically undissipated) to the small-scale ones, where viscous dissipation takes place (Richardson model of 1922). And even though the dissipation of mechanical energy ε

(falling at the unit mass per unit time) occurs on the least possible scale $l_{\rm K}$ (referred to below as the Kolmogorov turbulence scale), it is believed that the quantity ε also determines the properties of turbulent motion on larger scales. Between the Kolmogorov (or, using the terminology of Ref. [9], internal) scale $l_{\rm K}$ and the external scale $l_L \sim L$ there is an inertial interval where the typical size *l* satisfies the inequality

$$l_{\mathrm{K}} \ll l \leqslant l_{L}$$

For want of a better model, it is assumed that turbulent motion is described by the same equations of fluid mechanics (Navier–Stokes equations) used for laminar flows, with a consequence that turbulence emerges as a flow instability or, in this particular case, as an instability in the Navier–Stokes flow model. This gives rise to many inconsistencies, however. It is known, for example, that "although no comprehensive theoretical study has thus far been made for flows through a circular pipe, there is compelling evidence that this motion is stable with respect to infinitesimal perturbations (in an absolute as well as a convective sense) for any Reynolds numbers" [9]. This contradicts experimental data.

In 1924, W Heisenberg published a study on the instability of laminar flows [50]. A year later, E Noether "published another paper" — we are quoting Heisenberg [51] — "in which she proved with all mathematical rigour that the problem admits of no unstable solutions at all and that a flow must be everywhere stable ... What about the rigorous mathematics then? I think that even now nobody knows what is wrong with Noether's work". It would appear that rather than Noether's mistake, the drawbacks of the Navier–Stokes flow model are to blame.

The notions of averaged and fluctuating motions prompted Reynolds [52] to explicitly isolate the fluctuation terms in the Navier–Stokes equations and to subsequently average them over a certain time interval. But neither this approach nor the later technique of averaging over the masses of liquid volumes (sometimes called Favre averaging [53]) provide close solutions, and indeed neither of them are adequate when it comes to physics because, as we will see below, the Navier–Stokes equations are not written for true physical quantities.

One further approach to the problem involves the evaluation of velocity correlation functions with the aim of establishing the relation between the velocities at two neighboring flowfield points within the theory of local turbulence. For example, the simplest correlation function is the second-rank tensor

$$B_{ik} = \left\langle (v_{2i} - v_{1i})(v_{2k} - v_{1k}) \right\rangle,\,$$

where \mathbf{v}_1 and \mathbf{v}_2 are the fluid velocities at two neighboring points, and the angle brackets denote time averaging. A question remains, however, what exactly 'neighboring points' means and how the time averaging procedure is to be carried out. The theory of correlation functions attracted a great deal of attention after L Keller and A Fridman first introduced them into the hydrodynamics of turbulent motions back in 1924.

In 1944, L Landau gave a comprehensive assessment of this line of research. To quote him from Ref. [9], p. 200, "One would imagine that in principle it is possible to derive a universal formula, applicable to any turbulent motion, for determining B_{rr} , B_{tt} for all distances r small compared to l_L . In reality, however, such a formula cannot exist at all as the following argument shows. The instantaneous value of the quantity $(v_{2i} - v_{1i})(v_{2k} - v_{1k})$ could in principle be expressed in terms of the energy dissipation ε at the same instant of time t. However, the averaging of these expressions depends significantly on how ε varies in time throughout periods of large-scale (of order l_L) motions. But this variation is different for various specific cases of motion, so the result of such averaging cannot be universal''.

One can but agree with this view. To put it another way, if the Kolmogorov scale admits an explicit universal formulation for turbulent fluctuations (as we will show later on), then large-scale fluctuations are determined by solving a specific boundary-value problem.

A Kolmogorov advanced the hypothesis that the statistical regime of the small-scale components is universal and is determined by only two dimensional parameters, the average rate of energy dissipation ε and the kinematic viscosity v. From dimensional considerations it follows that the Kolmogorov fluctuation scale $l_{\rm K}$ is of the order of $v^{3/4}\varepsilon^{-1/4}$ and corresponds to the particle mean free path in a gas.

We now apply the generalized hydrodynamical equations to the theory of turbulence and demonstrate that they enable one to write explicitly the fluctuations of all hydrodynamic quantities on the Kolmogorov turbulence scale $l_{\rm K}$. Importantly, these turbulent fluctuations can be tabulated for any type of flow and in this sense can serve as 'universal formulas,' to use the terminology of monograph [9]. We start by writing down the generalized hydrodynamical equations and, for the sake of simplicity, employ the generalized Euler equations for the special case of a one-component gas flow in a gravitational field. To this end we multiply the generalized Boltzmann equations by the particles' elastic collision invariants ($m, mv, mv^2/2$) and integrate the resulting equations term by term with respect to velocity.

The calculation of the moments using the Maxwellian distribution function yields the system of generalized Euler equations which includes:

the continuity equation

$$\frac{\partial}{\partial t} \left\{ \rho - \Pi \frac{\mu}{p} \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0) \right] \right\} + \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \rho \mathbf{v}_0 - \Pi \frac{\mu}{p} \left[\frac{\partial}{\partial t} (\rho \mathbf{v}_0) + \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{v}_0 \mathbf{v}_0 + \mathbf{\vec{I}} \cdot \frac{\partial p}{\partial \mathbf{r}} - \rho \mathbf{g} \right] \right\} = 0,$$
(7.1)

the equation of motion

$$\frac{\partial}{\partial t} \left\{ \rho \mathbf{v}_{0} - \Pi \frac{\mu}{p} \left[\frac{\partial}{\partial t} (\rho \mathbf{v}_{0}) + \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{v}_{0} \mathbf{v}_{0} + \frac{\partial p}{\partial \mathbf{r}} - \rho \mathbf{g} \right] \right\}$$

$$- \mathbf{g} \left[\rho - \Pi \frac{\mu}{p} \left(\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_{0}) \right) \right]$$

$$+ \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \rho \mathbf{v}_{0} \mathbf{v}_{0} + p \overrightarrow{\mathbf{I}} - \Pi \frac{\mu}{p} \left[\frac{\partial}{\partial t} (\rho \mathbf{v}_{0} \mathbf{v}_{0} + p \overrightarrow{\mathbf{I}}) + \frac{\partial}{\partial \mathbf{r}} \cdot \rho (\mathbf{v}_{0} \mathbf{v}_{0}) \mathbf{v}_{0} + 2 \overrightarrow{\mathbf{I}} \left(\frac{\partial}{\partial \mathbf{r}} \cdot (p \mathbf{v}_{0}) \right)$$

$$+ \frac{\partial}{\partial \mathbf{r}} \cdot (\overrightarrow{\mathbf{I}} p \mathbf{v}_{0}) - \rho \mathbf{g} \mathbf{v}_{0} - \rho \mathbf{v}_{0} \mathbf{g} \right] \right\} = 0, \qquad (7.2)$$

and the equation of energy

$$\begin{aligned} \frac{\partial}{\partial t} \left\{ \frac{\rho v_0^2}{2} + \frac{3}{2} p - \Pi \frac{\mu}{p} \left[\frac{\partial}{\partial t} \left(\frac{\rho v_0^2}{2} + \frac{3}{2} p \right) \right. \\ \left. + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\frac{1}{2} \rho v_0^2 \mathbf{v}_0 + \frac{5}{2} p \mathbf{v}_0 \right) - \mathbf{g} \rho \mathbf{v}_0 \right] \right\} \\ \left. + \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \frac{1}{2} \rho v_0^2 \mathbf{v}_0 + \frac{5}{2} p \mathbf{v}_0 - \Pi \frac{\mu}{p} \left[\frac{\partial}{\partial t} \left(\frac{1}{2} \rho v_0^2 \mathbf{v}_0 + \frac{5}{2} p \mathbf{v}_0 \right) \right. \\ \left. + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\frac{1}{2} \rho v_0^2 \mathbf{v}_0 \mathbf{v}_0 + \frac{7}{2} p \mathbf{v}_0 \mathbf{v}_0 + \frac{1}{2} p v_0^2 \vec{\mathbf{I}} + \frac{5}{2} \frac{p^2}{\rho} \vec{\mathbf{I}} \right) \right. \\ \left. - \rho \mathbf{g} \cdot \mathbf{v}_0 \mathbf{v}_0 - p \mathbf{g} \cdot \vec{\mathbf{I}} - \frac{1}{2} \rho v_0^2 \mathbf{g} - \frac{3}{2} \mathbf{g} p \right] \right\} \\ \left. - \left\{ \rho \mathbf{g} \cdot \mathbf{v}_0 - \Pi \frac{\mu}{p} \left[\mathbf{g} \cdot \left(\frac{\partial}{\partial t} (\rho \mathbf{v}_0) + \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{v}_0 \mathbf{v}_0 + \frac{\partial}{\partial \mathbf{r}} \cdot \rho \mathbf{v}_0 \mathbf{v}_0 \right) \right] \right\} = 0, \end{aligned}$$
(7.3)

where we have used the hydrodynamic approximation $\underline{\tau}_{i}^{(0)} = \Pi \mu / p$ (for the hard-sphere model, $\Pi = 0.8$) and where \underline{I} is the unit tensor.

We next introduce ρ_{∞} , v_{∞} , p_{∞} , and μ_{∞} as the density, velocity, pressure, and viscosity scales, respectively. We take the characteristic dimension to be *L*, and the time scale, L/v_{∞} . Then the dimensionless equation of continuity takes the form

$$\frac{\partial}{\partial \hat{t}} \left\{ \hat{\rho} - \Pi \, \frac{\hat{\mu}}{\hat{p}} \, \frac{\mu_{\infty} v_{\infty}}{p_{\infty} L} \left[\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left(\hat{\rho} \hat{\mathbf{v}}_{0} \right) \right] \right\} \\ + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left\{ \hat{\mathbf{p}} \hat{\mathbf{v}}_{0} - \Pi \, \frac{\hat{\mu}}{\hat{p}} \, \frac{\mu_{\infty}}{p_{\infty}} \frac{v_{\infty}}{L} \left[\frac{\partial}{\partial \hat{t}} (\hat{\rho} \hat{\mathbf{v}}_{0}) + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \hat{\rho} \hat{\mathbf{v}}_{0} \hat{\mathbf{v}}_{0} \right. \\ \left. + \frac{p_{\infty}}{\rho_{\infty} v_{\infty}^{2}} \, \overrightarrow{\mathbf{i}} \cdot \frac{\partial \hat{p}}{\partial \hat{\mathbf{r}}} - \frac{Lg}{v_{\infty}^{2}} \, \hat{\rho} \hat{g} \right] \right\} = 0 \,.$$
(7.4)

Dimensionless combinations of the scale quantities introduced above form the similarity criteria

$$\frac{\mu_{\infty}v_{\infty}}{p_{\infty}L} = \frac{\mu_{\infty}}{Lv_{\infty}\rho_{\infty}}\frac{\rho_{\infty}v_{\infty}^2}{p_{\infty}} = \operatorname{Re}^{-1}\operatorname{Eu}^{-1}, \quad \frac{v_{\infty}^2}{Lg} = \operatorname{Fr}.$$

Thus, the continuity equation (7.4) contains the Reynolds, Euler, and Frud similarity criteria and may be rewritten as

$$\frac{\partial}{\partial \hat{t}} \left\{ \hat{\rho} - \Pi \frac{\hat{\mu}}{\hat{p}} \frac{\mathrm{Eu}^{-1}}{\mathrm{Re}} \left[\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot (\hat{\rho} \hat{\mathbf{v}}_{0}) \right] \right\} + \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \hat{\rho} \hat{\mathbf{v}}_{0} - \Pi \frac{\hat{\mu}}{\hat{p}} \frac{\mathrm{Eu}^{-1}}{\mathrm{Re}} \left[\frac{\partial}{\partial \hat{t}} (\hat{\rho} \hat{\mathbf{v}}_{0}) + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \hat{\rho} \hat{\mathbf{v}}_{0} \hat{\mathbf{v}}_{0} \right] + \mathrm{Eu} \stackrel{\leftrightarrow}{\mathrm{I}} \cdot \frac{\partial \hat{p}}{\partial \hat{\mathbf{r}}} - \frac{1}{\mathrm{Fr}} \hat{\rho} \hat{\mathbf{g}} \right] \right\} = 0.$$
(7.5)

In a similar fashion we write the dimensionless equation of motion

$$\frac{\partial}{\partial \hat{t}} \left\{ \hat{p} \hat{\mathbf{v}}_{0} - \Pi \, \frac{\hat{\mu}}{\hat{p}} \frac{\mathrm{Eu}^{-1}}{\mathrm{Re}} \left[\frac{\partial}{\partial \hat{t}} (\hat{p} \hat{\mathbf{v}}_{0}) + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \hat{p} \hat{\mathbf{v}}_{0} \hat{\mathbf{v}}_{0} + \mathrm{Eu} \, \frac{\partial \hat{p}}{\partial \hat{\mathbf{r}}} \right. \\ \left. - \frac{1}{\mathrm{Fr}} \, \hat{p} \hat{\mathbf{g}} \right] \right\} - \frac{1}{\mathrm{Fr}} \, \hat{\mathbf{g}} \left[\hat{\rho} - \Pi \, \frac{\hat{\mu}}{\hat{p}} \frac{\mathrm{Eu}^{-1}}{\mathrm{Re}} \left(\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot (\hat{\rho} \hat{\mathbf{v}}_{0}) \right) \right]$$

$$+ \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left\{ \hat{\rho} \hat{\mathbf{v}}_{0} \hat{\mathbf{v}}_{0} + \operatorname{Eu} \hat{\rho} \overrightarrow{\mathbf{I}} - \Pi \frac{\hat{\mu}}{\hat{\rho}} \frac{\operatorname{Eu}^{-1}}{\operatorname{Re}} \left[\frac{\partial}{\partial \hat{t}} (\hat{\rho} \hat{\mathbf{v}}_{0} \hat{\mathbf{v}}_{0} + \operatorname{Eu} \hat{\rho} \overrightarrow{\mathbf{I}}) \right. \\ \left. + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \hat{\rho} (\hat{\mathbf{v}}_{0} \hat{\mathbf{v}}_{0}) \hat{\mathbf{v}}_{0} + 2 \operatorname{Eu} \overrightarrow{\mathbf{I}} \left(\frac{\partial}{\partial \hat{\mathbf{r}}} \cdot (\hat{\rho} \hat{\mathbf{v}}_{0}) \right) \right. \\ \left. + \operatorname{Eu} \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot (\overrightarrow{\mathbf{I}} \hat{\rho} \hat{\mathbf{v}}_{0}) - \frac{1}{\operatorname{Fr}} \hat{\rho} \hat{\mathbf{g}} \hat{\mathbf{v}}_{0} - \frac{1}{\operatorname{Fr}} \hat{\rho} \hat{\mathbf{v}}_{0} \hat{\mathbf{g}} \right] \right\} = 0, \quad (7.6)$$

and the dimensionless equation of energy

$$\begin{split} \frac{\partial}{\partial \hat{t}} &\left\{ \frac{\hat{\rho}\hat{v}_{0}^{2}}{2} + \frac{3}{2} \operatorname{Eu}\hat{p} - \Pi \frac{\hat{\mu}}{\hat{p}} \frac{\operatorname{Eu}^{-1}}{\operatorname{Re}} \left[\frac{\partial}{\partial \hat{t}} \left(\frac{\hat{\rho}\hat{v}_{0}^{2}}{2} + \frac{3}{2} \operatorname{Eu}\hat{p} \right) \right. \\ &\left. + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left(\frac{1}{2} \hat{\rho}\hat{v}_{0}^{2}\hat{\mathbf{v}}_{0} + \frac{5}{2} \operatorname{Eu}\hat{p}\hat{\mathbf{v}}_{0} \right) - \frac{1}{\operatorname{Fr}} \hat{\mathbf{g}}\hat{\rho}\hat{\mathbf{v}}_{0} \right] \right\} \\ &\left. + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left\{ \frac{1}{2} \hat{\rho}\hat{v}_{0}^{2}\hat{\mathbf{v}}_{0} + \frac{5}{2} \operatorname{Eu}\hat{p}\hat{\mathbf{v}}_{0} \right\} - \frac{1}{\operatorname{Fr}} \hat{\mathbf{g}}\hat{\rho}\hat{\mathbf{v}}_{0} \right] \right\} \\ &\left. + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left\{ \frac{1}{2} \hat{\rho}\hat{v}_{0}^{2}\hat{\mathbf{v}}_{0} + \frac{5}{2} \operatorname{Eu}\hat{p}\hat{\mathbf{v}}_{0} \right\} \\ &- \Pi \frac{\hat{\mu}}{\hat{p}} \frac{\operatorname{Eu}^{-1}}{\operatorname{Re}} \left[\frac{\partial}{\partial \hat{t}} \left(\frac{1}{2} \hat{\rho}\hat{v}_{0}^{2}\hat{\mathbf{v}}_{0} + \frac{5}{2} \operatorname{Eu}\hat{p}\hat{\mathbf{v}}_{0} \right) \\ &\left. + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left(\frac{1}{2} \hat{\rho}\hat{v}_{0}^{2}\hat{\mathbf{v}}_{0}\hat{\mathbf{v}}_{0} + \frac{7}{2} \operatorname{Eu}\hat{p}\hat{\mathbf{v}}_{0}\hat{\mathbf{v}}_{0} + \frac{1}{2} \operatorname{Eu}\hat{p}\hat{v}_{0}^{2}\hat{\mathbf{i}} \right] \\ &\left. + \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \left(\frac{1}{2} \hat{\rho}\hat{v}_{0}^{2}\hat{\mathbf{v}}_{0} - \frac{F}{2} \operatorname{Eu}\hat{p}\hat{\mathbf{v}}_{0}\hat{\mathbf{v}}_{0} + \frac{1}{2} \operatorname{Eu}\hat{p}\hat{v}_{0}^{2}\hat{\mathbf{j}} \right] \\ &- \frac{1}{\operatorname{Fr}} \hat{\rho}\hat{\mathbf{g}} \cdot \hat{\mathbf{v}}_{0}\hat{\mathbf{v}}_{0} - \frac{\operatorname{Eu}}{\operatorname{Fr}} \hat{p}\hat{\mathbf{g}} \cdot \hat{\mathbf{i}} - \frac{1}{2} \frac{1}{\operatorname{Fr}} \hat{\rho}\hat{v}_{0}^{2}\hat{\mathbf{g}} - \frac{3}{2} \frac{\operatorname{Eu}}{\operatorname{Fr}} \hat{\mathbf{g}}\hat{p} \right] \right\} \\ &- \left\{ \frac{1}{\operatorname{Fr}} \hat{\rho}\hat{\mathbf{g}} \cdot \hat{\mathbf{v}}_{0} - \Pi \frac{\hat{\mu}}{\hat{p}} \frac{\operatorname{Eu}^{-1}}{\operatorname{Re}} \left[\frac{1}{\operatorname{Fr}} \hat{\mathbf{g}} \cdot \left(\frac{\partial}{\partial \hat{t}} (\hat{\rho}\hat{\mathbf{v}}_{0} \right) \right) \\ &+ \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \hat{\rho}\hat{\mathbf{v}}_{0}\hat{\mathbf{v}}_{0} + \operatorname{Eu} \frac{\partial}{\partial \hat{\mathbf{r}}} \cdot \hat{\rho}\hat{\mathbf{i}} - \frac{1}{\operatorname{Fr}} \hat{p}\hat{\mathbf{g}} \right) \right] \right\} = 0 \,. \tag{7.7}$$

Equations (7.5)-(7.7) are notable for their structure. All the generalized equations of Euler fluid dynamics contain the Reynolds, Euler, and Frud numbers (similarity criteria). Naturally, the inclusion of forces of electromagnetic origin would lead to additional similarity criteria. For each hydrodynamical quantity — density, energy, and momentum as well as their fluxes — there is a corresponding temporally and spatially fluctuating term which is proportional to Re^{-1} and, hence, to the viscosity.

For small-scale fluctuations (i.e. smaller characteristic dimension l in the Reynolds number), viscosity increases in importance and starts to determine ε , the dissipation of the mechanical energy. The fluctuation terms thus determine turbulent Kolmogorov-scale fluctuations (small-scale fluctuations or, using the computational hydrodynamics term, submesh turbulence) which are of a universal nature and not problem specific.

To fully understand the situation, however, the following questions remain to be answered:

(1) Are there no contradictions in the system of fluctuations introduced in this way? In other words, is the set of fluctuations self-consistent?

(2) With a system of base (independent) fluctuations on hand, is it possible to derive explicit expressions for other hydrodynamical quantities and their moments?

(3) What do the generalized hydrodynamical equations for averaged quantities look like and how does the procedure for obtaining the averaged equations agree with the Reynolds procedure familiar from the theory of turbulence? In answering the above questions, the generalized Euler equations for a one-component gas will be employed for the sake of clarity. Implicit in the following analysis will be the fact, already noted above, that we are dealing with small-scale fluctuations.

The equations to be investigated are:

the continuity equation

$$\frac{\partial}{\partial t} \left\{ \rho - \tau \left(\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0) \right) \right\} + \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \rho \mathbf{v}_0 - \tau \left(\frac{\partial}{\partial t} (\rho \mathbf{v}_0) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0 \mathbf{v}_0) + \frac{\partial p}{\partial \mathbf{r}} - \rho \mathbf{g} \right) \right\} = 0;$$
(7.8)

the equation of motion

$$\frac{\partial}{\partial t} \left\{ \rho v_{0\beta} - \tau \left[\frac{\partial}{\partial t} (\rho v_{0\beta}) + \frac{\partial}{\partial r_{\alpha}} (p \delta_{\alpha\beta} + \rho v_{0\alpha}) - \rho g_{\beta} \right] \right\} - \left\{ \rho - \tau \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial r_{\alpha}} (\rho v_{0\alpha}) \right] \right\} g_{\beta} + \frac{\partial}{\partial r_{\alpha}} \left\{ p \delta_{\alpha\beta} + \rho v_{0\alpha} v_{0\beta} \right\} - \tau \left[\frac{\partial}{\partial t} (p \delta_{\alpha\beta} + \rho v_{0\alpha} v_{0\beta}) + \frac{\partial}{\partial r_{\gamma}} (p \delta_{\alpha\gamma} v_{0\beta} + p v_{0\alpha} \delta_{\beta\gamma} \right] + p v_{0\gamma} \delta_{\alpha\beta} + \rho v_{0\alpha} v_{0\beta} v_{0\gamma}) - g_{\alpha} \rho v_{0\beta} - g_{\beta} \rho v_{0\alpha} \right] \right\} = 0, \quad (7.9)$$

where we employ the Einstein summation rule for recurrent subscripts α , β , $\gamma = 1, 2, 3$ referring to components of vectors in the Cartesian coordinate system,

and the equation of energy

.

$$\frac{\partial}{\partial t} \left\{ 3p + \rho v_0^2 - \tau \left[\frac{\partial}{\partial t} (3p + \rho v_0^2) + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\mathbf{v}_0 (\rho v_0^2 + 5p) \right) \right. \\ \left. - 2\mathbf{g} \cdot \rho \mathbf{v}_0 \right] \right\} + \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \mathbf{v}_0 (\rho v_0^2 + 5p) - \tau \left[\frac{\partial}{\partial t} \left(\mathbf{v}_0 (\rho v_0^2 + 5p) \right) \right. \\ \left. + \frac{\partial}{\partial \mathbf{r}} \cdot \left[\vec{\mathbf{I}} p v_0^2 + \rho v_0^2 \mathbf{v}_0 \mathbf{v}_0 + 7p \mathbf{v}_0 \mathbf{v}_0 + 5 \vec{\mathbf{I}} \frac{p^2}{\rho} \right] \right. \\ \left. - 2\rho \mathbf{v}_0 \mathbf{v}_0 \cdot \mathbf{g} - 5p \vec{\mathbf{I}} \cdot \mathbf{g} - \rho v_0^2 \vec{\mathbf{I}} \cdot \mathbf{g} \right] \right\} \\ \left. - 2\mathbf{g} \cdot \left\{ \rho \mathbf{v}_0 - \tau \left[\frac{\partial}{\partial t} (\rho \mathbf{v}_0) + \frac{\partial p}{\partial \mathbf{r}} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0 \mathbf{v}_0) - \rho \mathbf{g} \right] \right\} = 0.$$

$$(7.10)$$

To calculate hydrodynamic fluctuations, the Reynolds procedure will be employed. Thus, for example, the product of the true density ρ and the true velocity \mathbf{v}_0 can be used to obtain the fluctuation quantity $\mathbf{v}_0^{\rm f}$. Indeed, we have

$$\rho \mathbf{v}_0 = (\rho^{\rm a} + \rho^{\rm f})(\mathbf{v}_0^{\rm a} + \mathbf{v}_0^{\rm f}), \qquad (7.11)$$

where the superscript 'a' denotes the average hydrodynamic quantities. Ignoring the fluctuation terms squared and keeping only first-order small quantities in relations of type (7.11) we find

$$(\rho \mathbf{v}_0)^{\rm f} = \rho \mathbf{v}_0 - \rho^{\rm a} \mathbf{v}_0^{\rm a} = \rho^{\rm a} \mathbf{v}_0^{\rm f} + \rho^{\rm f} \mathbf{v}_0^{\rm a} \,. \tag{7.12}$$

Thus one obtains

$$\mathbf{v}_{0}^{f} = \frac{(\rho \mathbf{v}_{0})^{f} - \rho^{f} \mathbf{v}_{0}^{a}}{\rho^{a}} .$$
(7.13)

From the continuity equation (7.8) we have

$$\rho^{\rm f} = \tau \left\{ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0) \right\},\tag{7.14}$$

$$(\rho \mathbf{v}_0)^{\mathrm{f}} = \tau \left\{ \frac{\partial}{\partial t} (\rho \mathbf{v}_0) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0 \mathbf{v}_0) + \frac{\partial p}{\partial \mathbf{r}} - \rho \mathbf{g} \right\}$$
(7.15)

and therefore from Eqn (7.13) it follows

$$\mathbf{v}_{0}^{\mathrm{f}} = \tau \left\{ \frac{\partial \mathbf{v}_{0}}{\partial t} + \left(\mathbf{v}_{0} \cdot \frac{\partial}{\partial \mathbf{r}} \right) \mathbf{v}_{0} + \frac{1}{\rho} \frac{\partial p}{\partial \mathbf{r}} - \mathbf{g} \right\}.$$
 (7.16)

Using Eqn (7.9), we find that the fluctuation of the combined hydrodynamical quantity $p\delta_{\alpha\beta} + \rho v_{0\alpha}v_{0\beta}$ is given by

$$(p\delta_{\alpha\beta} + \rho v_{0\alpha}v_{0\beta})^{f} = \tau \left[\frac{\partial}{\partial t}(p\delta_{\alpha\beta} + \rho v_{0\alpha}v_{0\beta}) + \frac{\partial}{\partial r_{\gamma}}(p\delta_{\alpha\gamma}v_{0\beta} + pv_{0\alpha}\delta_{\beta\gamma} + pv_{0\gamma}\delta_{\alpha\beta} + \rho v_{0\alpha}v_{0\beta}v_{0\gamma}) - g_{\alpha}\rho v_{0\beta} - g_{\beta}\rho v_{0\alpha}\right].$$
(7.17)

With the help of Eqn (7.17) we obtain

$$(3p + \rho v_0^2)^{\rm f} = \tau \left[\frac{\partial}{\partial t} (3p + \rho v_0^2) + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\mathbf{v}_0 (\rho v_0^2 + 5p) \right) - 2\mathbf{g} \cdot \rho \mathbf{v}_0 \right].$$
(7.18)

We now proceed to calculate $(\rho v_0^2)^{f}$:

$$(\rho v_0^2)^{\rm f} = \rho v_0^2 - \rho^{\rm a} v_0^{\rm a2} = (\rho^{\rm a} + \rho^{\rm f}) (\mathbf{v}_0^{\rm a} + \mathbf{v}_0^{\rm f})^2 - \rho^{\rm a} v_0^{\rm a2}$$

$$\cong (\rho^{\rm a} + \rho^{\rm f}) (v_0^{\rm a2} + 2\mathbf{v}_0^{\rm a} \cdot \mathbf{v}_0^{\rm f}) - \rho^{\rm a} v_0^{\rm a2}$$

$$\cong \rho^{\rm f} v_0^{\rm a2} + 2\rho^{\rm a} \mathbf{v}_0^{\rm a} \cdot \mathbf{v}_0^{\rm f}, \qquad (7.19)$$

which, when combined with Eqns (7.14) and (7.16), yields

$$(\rho v_0^2)^{\rm f} = \tau \left\{ v_0^{\rm a2} \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0) \right] + 2\rho^{\rm a} \mathbf{v}_0^{\rm a} \cdot \left[\frac{\partial \mathbf{v}_0}{\partial t} + \left(\mathbf{v}_0 \cdot \frac{\partial}{\partial \mathbf{r}} \right) \mathbf{v}_0 + \frac{1}{\rho} \frac{\partial \rho}{\partial \mathbf{r}} - \mathbf{g} \right\}.$$
(7.20)

The fluctuations of the remaining hydrodynamical quantities are obtained in a similar manner. The accompanying Table 1 lists the examples of Kolmogorov turbulent fluctuations for reference (the independent fluctuations are underlined).

That hydrodynamic fluctuations (proportional to the mean time τ between the collisions, and hence to viscosity) are bound to appear in the generalized hydrodynamical equations is easily understood from the molecular-kinetic point of view. Consider a gas of hard spheres contained in a cavity with a rigid wall (Fig. 1) and draw a reference contour at a distance of the order of the particle diameter from the wall. Turn now to the continuity equation as an example. The classical formulation of this equation, following from the

Num- ber	Hydrodynamical quantity A	Fluctuation <i>A</i> ^f
<u>1</u>	ρ	$\tau \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0) \right]$
<u>2</u>	$\rho \mathbf{v}_0$	$\tau \left[\frac{\partial}{\partial t} (\rho \mathbf{v}_0) + \frac{\partial}{\partial \mathbf{r}} \cdot (\rho \mathbf{v}_0 \mathbf{v}_0) + \frac{\partial p}{\partial \mathbf{r}} - \rho \mathbf{g} \right]$
3	\mathbf{v}_0	$\tau \left[\frac{\partial \mathbf{v}_0}{\partial t} + \left(\mathbf{v}_0 \cdot \frac{\partial}{\partial \mathbf{r}} \right) \mathbf{v}_0 + \frac{1}{\rho} \frac{\partial \rho}{\partial \mathbf{r}} - \mathbf{g} \right]$
<u>4</u>	$p\delta_{lphaeta}+ ho v_{0lpha}v_{0eta}$	$\tau \left[\frac{\partial}{\partial t} (p \delta_{\alpha\beta} + \rho v_{0\alpha} v_{0\beta}) + \frac{\partial}{\partial r_{\gamma}} (p v_{0\alpha} \delta_{\beta\gamma} + \rho v_{0\alpha} v_{0\beta}) \right]$
		$+pv_{0eta}\delta_{lpha\gamma}+pv_{0\gamma}\delta_{lphaeta}+ ho v_{0lpha}v_{0eta}v_{0\gamma}\Big)$
		$-g_{eta} ho v_{0lpha} - g_{lpha} ho v_{0eta} \bigg]$
5	$3p + \rho v_0^2$	$\tau \left\{ \frac{\partial}{\partial t} (3p + \rho v_0^2) \right\}$
		$+\frac{\partial}{\partial \mathbf{r}}\cdot\left[\mathbf{v}_{0}(\rho v_{0}^{2}+5p)\right]-2\mathbf{g}\cdot\rho\mathbf{v}_{0}\right\}$
6	р	$\tau \left[\frac{\partial p}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot (p \mathbf{v}_0) + \frac{2}{3} p \frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{v}_0 \right]$
<u>7</u>	$\mathbf{v}_0(\rho v_0^2 + 5p)$	$\tau \left\{ \frac{\partial}{\partial t} \left[\mathbf{v}_0(\rho v_0^2 + 5p) \right] \right\}$
		$+\frac{\partial}{\partial \mathbf{r}}\cdot\left(\rho v_0^2\mathbf{v}_0\mathbf{v}_0+\vec{\mathbf{i}}\rho v_0^2+7\rho\mathbf{v}_0\mathbf{v}_0+5\vec{\mathbf{i}}\frac{\rho^2}{\rho}\right)$
		$-2\rho\mathbf{v}_{0}\mathbf{v}_{0}\cdot\mathbf{g}-5\rho\vec{\mathbf{i}}\cdot\mathbf{g}-\rho v_{0}^{2}\vec{\mathbf{i}}\cdot\mathbf{g}$
		$-p\left[\frac{\partial}{\partial \mathbf{r}}\left(5\frac{p}{\rho}+v_0^2\right)+2\left(\mathbf{v}_0\cdot\frac{\partial}{\partial \mathbf{r}}\right)\mathbf{v}_0\right]$
		$-\frac{4}{3} \mathbf{v}_0 \left(\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{v}_0 \right) \Big] \bigg\}$

Table 1. Fluctuations of hydrodynamical quantities on the Kolmogorov scale in the framework of the generalized Euler equations.

Boltzmann equation or — in continuum mechanics — from balance equations, is valid only for pointlike structureless particles, which may be either inside or outside the reference contour.

A particle of finite diameter may be partly inside and partly outside the contour at some instant of time, which necessarily leads to fluctuation of the mass within the contour. Since the number of particles moving perpendicular to the wall has zero expectation, it follows that to a linear



Figure 1. Closed cavity and the reference contour containing particles of a finite diameter.

approximation the fluctuations are proportional to the mean free path (or the mean time τ between the collisions).

Let us define the Knudsen number Kn_l as the ratio of the mean free path λ to the distance l between the contour boundary and the wall. In the dimensionless Eqns (7.8)–(7.10), the Knudsen number Kn_l will appear as a coefficient of the fluctuation terms. If $l \rightarrow 0$, $\text{Kn}_l \rightarrow \infty$, and the reference contour coincides with the cavity wall, then there are no integral fluctuations within the volume — with the consequence that classical equations of continuity and motion should be obeyed at the wall. This is indeed the case: the fluctuation terms in the generalized continuity equation (7.8) contain the left-hand sides of the classical equations of continuity and motion terms at the wall provides additional boundary conditions necessary for the generalized hydrodynamical equations.

Notice also that the appearance of second time derivatives in the generalized Euler equations permits the use of the Cauchy-Kovalevskaya theorem in proving the existence and uniqueness of the solutions.

We next employ the generalized continuity equation to see how fluctuations are produced and smoothed out. We first note that the generalized Boltzmann equation is of parabolic type; for the one-dimensional unsteady case, using the BGK approximation with $\tau = \text{const}$, it may be written as

$$\frac{\partial f}{\partial t} + v \frac{\partial f}{\partial x} - \tau \left(\frac{\partial^2 f}{\partial t^2} + 2v \frac{\partial^2 f}{\partial x \partial t} + v^2 \frac{\partial^2 f}{\partial x^2} \right) = \frac{f^{(0)} - f}{k\tau} .$$
(7.21)

On changing to the characteristic variables $\zeta = x - vt$, $\xi = t$, this latter equation becomes

$$\tau \frac{\partial^2 f}{\partial \zeta^2} - \frac{\partial f}{\partial \zeta} = \frac{f - f^{(0)}}{k\tau}, \qquad (7.22)$$

which is integrated immediately to give

$$f = f_0 + C_1(\xi) \exp\left(-\frac{\sqrt{1+4k^{-1}}-1}{2\tau}t\right).$$
(7.23)

The second constant of integration C_2 , corresponding to the exponentially growing part of the general solution, is set equal to zero according to the physical meaning of the solution.

In the spatially homogeneous case under the same assumption (for example, for k = 5), we have the solutions

$$f^{\text{GBE}} = f_0 + C(v) \exp\left(-0.17 \frac{t}{\tau}\right), \qquad (7.24)$$

$$f^{\text{BE}} = f_0 + C(v) \exp\left(-0.2\frac{t}{\tau}\right) \tag{7.25}$$

for the generalized Boltzmann and Boltzmann descriptions, respectively. Note the similarity of these solutions.

Now what happens to the fluctuations that develop in the system? To see this, consider the generalized equation of continuity (7.8), which we write down here in the generalized Eulerian formulation under the assumption of no external forces for the one-dimensional unsteady case:

$$\frac{\partial}{\partial t} \left\{ \rho - \tau^{(0)} \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v_0) \right] \right\} + \frac{\partial}{\partial x} (\rho v_0)$$
$$= \frac{\partial}{\partial x} \left\{ \tau^{(0)} \left[\frac{\partial}{\partial t} (\rho v_0) + \frac{\partial}{\partial x} (p + \rho v_0^2) \right] \right\}, \tag{7.26}$$

where $\tau^{(0)}$ is the mean time between collisions calculated in the locally Maxwellian approximation: $\tau^{(0)}p = \Pi\mu$ (the factor Π being of order unity; for the hard-sphere model, $\Pi = 0.8$ to first-order approximation in Sonine polynomials [49]).

We shall assume that except for shock-wave-type regions (to be discussed below within the framework of the generalized Boltzmann equation) hydrodynamical quantities vary not too rapidly on the scale of the order of the mean time between collisions:

$$\frac{\rho}{\tau^{(0)}} \gg \frac{\partial \rho}{\partial t} , \qquad \frac{\rho}{\tau^{(0)}} \gg \frac{\partial}{\partial x} (\rho v_0) ,$$

the temperature variations are small, the convective transfer is negligible, and the chaotic motion is highly energetic as compared to the kinetic energy of the flow, i.e. $V^2/v_0^2 \ge 1$ (for example, for hydrogen at normal pressures and temperatures, we have $v_0 = 10$ cm s⁻¹, giving 3.4×10^8 for this ratio). Consequently, Eqn (7.26) becomes

$$\frac{\partial\rho}{\partial t} = \frac{\partial}{\partial x} \left(\frac{\tau^{(0)} p}{\rho} \frac{\partial\rho}{\partial x} \right)$$
(7.27)

or

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left(D \, \frac{\partial \rho}{\partial x} \right), \tag{7.28}$$

where $D = \Pi \mu / \rho$ is the self-diffusion coefficient (see Ref. [49], p. 134). Equation (7.28) is the diffusion equation, with the implication that (a) a locally increasing density fluctuation immediately activates the diffusion mechanism which smooths it out, and (b) the generalized Boltzmann *H*theorem proved above ensures that the smoothed fluctuations come to equilibrium.

A similar spatially inhomogeneous treatment may be performed for the generalized equation of balance of entropy.

We define the shear tensor \mathbf{S} such that its components are as follows

$$S_{ij} = \frac{1}{2} \left(\frac{\partial v_{0i}}{\partial r_j} + \frac{\partial v_{0j}}{\partial r_i} \right) - \frac{1}{3} \,\delta_{ij} \,\frac{\partial}{\partial \mathbf{r}} \cdot \mathbf{v}_0 \quad (i, j = 1, 2, 3) \quad (7.29)$$

and write the generalized Euler equation in terms of the average variables to obtain

$$\frac{\partial \rho^{a}}{\partial t} + \frac{\partial}{\partial \mathbf{r}} \cdot \left(\rho \mathbf{v}_{0}\right)^{a} = 0, \qquad (7.30)$$

$$\frac{\partial}{\partial t} (\rho \mathbf{v}_0)^a + \frac{\partial}{\partial \mathbf{r}} \cdot \left[p^a \stackrel{\leftrightarrow}{\mathbf{I}} + (\rho \mathbf{v}_0 \mathbf{v}_0)^a \right] = \rho^a \mathbf{g} \,, \tag{7.31}$$

$$\frac{\partial}{\partial t} (3p + \rho v_0^2)^{\mathbf{a}} + \frac{\partial}{\partial \mathbf{r}} \cdot \left[\mathbf{v}_0 (\rho v_0^2 + 5p) \right]^{\mathbf{a}} - 2\mathbf{g} \cdot (\rho \mathbf{v}_0)^{\mathbf{a}} = 2 \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \tau p \left[\frac{5}{2} \frac{\partial}{\partial \mathbf{r}} \left(\frac{p}{\rho} \right) + 2\mathbf{v}_0 \cdot \vec{\mathbf{S}} \right] \right\}.$$
(7.32)

From the system of generalized Euler equations (7.30) – (7.32) we conclude the following:

(1) The formulation of the hydrodynamical equations in terms of average quantities is the objective of 'classical' theory of turbulence. However, a rigorous approach based on the generalized Euler equations leads to a residual (with respect to true quantities) on the right of the equation of energy (7.32).

(2) The residual

$$\Pi^{e} = 2 \frac{\partial}{\partial \mathbf{r}} \cdot \left\{ \tau p \left[\frac{5}{2} \frac{\partial}{\partial \mathbf{r}} \left(\frac{p}{\rho} \right) + 2 \mathbf{v}_{0} \cdot \overrightarrow{\mathbf{S}} \right] \right\}$$
(7.33)

in Eqn (7.32) turns out to be proportional to τp and hence to the viscosity [cf. Eqn. (2.18)]. If one puts

$$\Pi^{e} = 0, \qquad (7.34)$$

then the set of equations (7.30)-(7.32) reduces formally to the Euler equations for averaged quantities. It follows that the residual Π^{e} , which is the variation in space of the thermal-energy and shear-energy dissipation, stimulates the development of turbulence in the physical system under study.

(3) The so-called 'soft' boundary conditions commonly imposed at the output of the computational flow region follow from condition (7.34):

$$\frac{\partial}{\partial r} \cdot \left\{ \mu \left[\frac{5}{2} \frac{\partial}{\partial \mathbf{r}} \left(\frac{p}{\rho} \right) + 2\mathbf{v}_0 \cdot \overrightarrow{\mathbf{S}} \right] \right\} = 0.$$
 (7.35)

(4) Equations (7.30) - (7.32) do not reduce exactly to the classical Euler equations even under condition (7.34) because the average of the product of hydrodynamical quantities is not equal to the product of their averages. Consequently, this system of equations contains more unknowns (namely, ρ^{a} , $(\rho v_{0})^{a}$, p^{a} , $(\rho v_{0}v_{0})^{a}$, and $[v_{0}(\rho v_{0}^{2} + 5p)]^{a})$ than equations, thus presenting the typical problem of the classical theory of turbulence, which consists in closing the moment equations.

The theory presented here overcomes this problem by simply reverting to the formulation of the hydrodynamical equations in terms of the true quantities. And it is only in the case when turbulent fluctuations are completely absent or, equivalently, when the average product of hydrodynamical quantities is equal to the product of their averages, that we arrive at the classical form of the Euler and, of course, Navier–Stokes equations. Thus, the classical Euler and Navier–Stokes equations are not written for true quantities, and it is physically meaningless to employ the formal Reynolds procedure to try to 'extract' small-scale fluctuations from these equations.

8. Numerical simulation of vortex gas flow using the generalized Euler equations

To demonstrate the research potential of numerical vortexflow simulation using the generalized hydrodynamical equations, we examine the two-dimensional unsteady flow of a compressible gas in a cavity [54–56]. The problem to be solved is the following. Consider a flow over a flat surface and suppose there suddenly appears — as a result of some mechanical action, for example — a certain cavity of square cross section, whose length is much longer than the side of the square (Fig. 2). It is assumed that at some instant of time gas suddenly starts to move along the segment *OL* of the axis x with the velocity V_s which is subsequently maintained constant.

The system of the generalized Euler equations for a twodimensional, unsteady and nonisothermic flow of compres-



Figure 2. Unsteady flow of compressible gas in a cavity.

sible gas is written in the following way:

$$\frac{\partial}{\partial t} \left\{ \rho - \tau \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho u) + \frac{\partial}{\partial y} (\rho v) \right] \right\} + \frac{\partial}{\partial x} \left\{ \rho u - \tau \left[\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2) + \frac{\partial}{\partial y} (\rho uv) + \frac{\partial p}{\partial x} \right] \right\} + \frac{\partial}{\partial y} \left\{ \rho v - \tau \left[\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{x} (\rho uv) + \frac{\partial}{\partial y} (\rho v^2) + \frac{\partial p}{\partial y} \right] \right\} = 0,$$
(8.1)

$$\frac{\partial}{\partial t} \left\{ \rho u - \tau \left[\frac{\partial}{\partial t} (\rho u) + \frac{\partial}{\partial x} (\rho u^2) + \frac{\partial}{\partial y} (\rho uv) + \frac{\partial p}{\partial x} \right] \right\} \\ + \frac{\partial}{\partial x} \left\{ p + \rho u^2 - \tau \left[\frac{\partial}{\partial t} (p + \rho u^2) + 3 \frac{\partial}{\partial x} (p u) + \frac{\partial}{\partial x} (\rho u^3) \right. \\ \left. + \frac{\partial}{\partial y} (\rho u^2 v) + 2 \frac{\partial}{\partial y} (p v) \right] \right\} + \frac{\partial}{\partial y} \left\{ \rho uv - \tau \left[\frac{\partial}{\partial t} (\rho uv) \right. \\ \left. + \frac{\partial}{\partial x} (\rho u^2 v) + \frac{\partial}{\partial y} (p u) + \frac{\partial}{\partial y} (\rho uv^2) \right] \right\} = 0, \qquad (8.2)$$

$$\begin{aligned} & \left\{ \begin{array}{c} \partial t \left[\left(-\frac{1}{2} \right) \left(\partial t \left(v \right) \right) + \frac{\partial}{\partial x} \left(\rho u v \right) + \frac{\partial}{\partial x} \left(\rho u^{2} v \right) \right) \right\} \\ & + \frac{\partial}{\partial y} \left(\rho u v^{2} \right) \right] \\ & + \frac{\partial}{\partial y} \left(\rho u v^{2} \right) \right] \\ & + \frac{\partial}{\partial y} \left(\rho u v^{2} \right) \right] \\ & + \frac{\partial}{\partial y} \left(\rho v^{3} \right) + \frac{\partial}{\partial x} \left(\rho u v^{2} \right) + 2 \frac{\partial}{\partial x} \left(\rho u \right) \right] \\ & = 0 , \end{aligned}$$

$$\begin{aligned} & \left\{ \begin{array}{c} \partial t \left(\rho u v^{2} \right) + \frac{\partial}{\partial y} \left(\rho u v^{2} \right) + 2 \frac{\partial}{\partial x} \left(\rho u v^{2} \right) \right\} \\ & = 0 , \end{aligned}$$

$$\end{aligned}$$

$$\end{aligned}$$

$$\frac{\partial}{\partial t} \left\{ \rho v_0^2 + 3p - \tau \left[\frac{\partial}{\partial t} (\rho v_0^2 + 3p) + \frac{\partial}{\partial x} (u (\rho v_0^2 + 5p)) \right] \right\} + \frac{\partial}{\partial t} \left\{ u(\rho v_0^2 + 5p) \right\} \\ + \frac{\partial}{\partial y} (v(\rho v_0^2 + 5p)) \left] \right\} + \frac{\partial}{\partial x} \left\{ u(\rho v_0^2 + 5p) \right\} \\ - \tau \left[\frac{\partial}{\partial t} (u(\rho v_0^2 + 5p)) + \frac{\partial}{\partial x} (u^2 \rho v_0^2 + p v_0^2 + 7p u^2 + 5 \frac{p^2}{\rho}) \right] \\ + \frac{\partial}{\partial y} (uv \rho v_0^2 + 7p uv) \right] \right\} + \frac{\partial}{\partial y} \left\{ v(\rho v_0^2 + 5p) \right\} \\ - \tau \left[\frac{\partial}{\partial t} (v(\rho v_0^2 + 5p)) + \frac{\partial}{\partial x} (\rho uv v_0^2 + 7p uv) \right] \\ + \frac{\partial}{\partial y} \left(v^2 \rho v_0^2 + p v_0^2 + 7p v^2 + 5 \frac{p^2}{\rho} \right) \right] \right\} = 0.$$
(8.4)

Here, $\tau = \Pi \mu / p$ and $v_0^2 = u^2 + v^2$, where \mathbf{v}_0 is the hydrodynamical flow velocity with components u and v.

The system of generalized equations (8.1)–(8.4) was made dimensionless by using the dimensionless variables $\hat{p} = p/p_{\infty}$, $\hat{\rho} = \rho/\rho_{\infty}$, $\hat{u} = u/V_s$, $\hat{v} = v/V_s$, and $\hat{t} = tV_s/L$.

The effect of the force of gravity is neglected, so that there are two similarity criteria in the picture: $\text{Eu} = p_{\infty}/(\rho_{\infty}V_s^2)$ and $\text{Re} = LV_s \rho_{\infty}/\mu_{\infty}$, where V_s is the velocity of the external flow. The parameter Π corresponds to the first-order approximation in the hard-sphere model: $\Pi = 0.8$.

The initial conditions (t = 0) are as follows

$$\begin{aligned} \rho &= \rho_{\infty} , \quad p = p_{\infty} , \quad v = 0 , \\ u &= V_{s} \text{ for } y = 0 , \quad u = 0 \text{ for } y > 0 , \\ \partial u &= \partial v \quad o \quad \partial \rho \quad o \quad \partial p \quad o \end{aligned}$$

$$\frac{\partial u}{\partial t} = 0$$
, $\frac{\partial v}{\partial t} = 0$, $\frac{\partial p}{\partial t} = 0$, $\frac{\partial p}{\partial t} = 0$

The boundary conditions to be satisfied are

$$\begin{split} & u(x,0) = V_{s}, \quad v(x,0) = 0, \\ & u(x,L) = 0, \quad v(x,L) = 0; \quad \text{for} \quad x \in [0,L], \\ & u(0,y) = 0, \quad v(0,y) = 0, \\ & u(L,y) = 0, \quad v(L,y) = 0 \quad \text{for} \quad y \in [0,L], \\ & \left[\frac{\partial \rho}{\partial x}\right]_{x=0} = 0, \quad \left[\frac{\partial \rho}{\partial y}\right]_{x=L} = 0 \quad \text{for} \quad y \in [0,L], \\ & \left[\frac{\partial \rho}{\partial x}\right]_{y=0} = 0, \quad \left[\frac{\partial \rho}{\partial y}\right]_{y=L} = 0 \quad \text{for} \quad x \in [0,L], \\ & \left[\frac{\partial p}{\partial y}\right]_{x=0} = 0, \quad \left[\frac{\partial p}{\partial x}\right]_{x=L} = 0 \quad \text{for} \quad y \in [0,L], \\ & \left[\frac{\partial p}{\partial y}\right]_{y=0} = 0, \quad \left[\frac{\partial p}{\partial y}\right]_{y=L} = 0 \quad \text{for} \quad x \in [0,L]. \end{split}$$

These boundary conditions imply that there is no slip, no leakage of compressible gas through the wall, and no heat transfer at the cavity wall — a good enough model to demonstrate the potential of the generalized hydrodynamical equations. The computations performed covered a wide Reynolds number range. Many calculated results, including those for other types of flow (along a heated cylinder and over a step) may be found elsewhere [54-56], and in what follows only some characteristic results will be given.

Along with the program described above, calculations using the generalized Euler equations and the Navier–Stokes equations were carried out simultaneously. While the cavity flowfield solutions obtained by the different approaches are qualitatively different for the drastically unsteady regime, they start getting closer for sufficiently large times. Increasing the Reynolds number increases the difference between the flowfield patterns obtained from the generalized Euler equations and the Navier–Stokes equations. Results for Re = 3200, Eu = 1.0, Kn = 0.0003915, and M = 0.775 at (dimensionless) instants of time $\hat{t} = 4.0$, 9.5, and 230.0 are shown in Figs 3 and 4 for the generalized Euler equations and the Navier–Stokes equations, respectively. Notice that the concept of a quasi-stationary regime becomes rather vague in this case.

Figure 5 shows the position of the center of the central vortex at large times. Points 1-11 were calculated from the generalized hydrodynamical equations for the dimensionless instants of time $\hat{t} = 201.0, 202.0, 203.5, 204.0, 205.0, 205.8$,



Figure 3. Gas flow in a cavity at times $\hat{t} = 4.0, 9.5, \text{ and } 230.0$. Calculations are done using the generalized Euler equations for Re = 3200, Eu = 1.



Figure 4. Gas flow in a cavity at times $\hat{t} = 4.0, 9.5, \text{ and } 230.0$. Calculations are done using the Navier–Stokes equations for Re = 3200, Eu = 1.



Figure 5. Position of the center of the central vortex (relative to the center of the cavity) for instants of time $\hat{t} = 201.0, 202.0, 203.5, 204.0, 205.0, 205.8, 207.0, 208.0, 209.0, 210.0, and 211.5 (points <math>I - II$, respectively). Calculations were done using the generalized hydrodynamical equations for Re = 3200, Eu = 1.

207.0, 208.0, 209,0, 210.0, and 211.5. It turns out that the vortex center performs a rotational motion. It is a well-known

fact that two-dimensional Navier – Stokes calculations for an incompressible isothermal fluid (water) for the central cross section of a cavity correlate very poorly with experimental data [57-59] even if the length of the cavity is much larger than its width. Nor do three-dimensional Navier – Stokes calculations improve the picture [60, 61]. It has been found that three-dimensional Navier – Stokes calculated results obtained on coarser meshes may agree better with experimental data than do formally more accurate solutions [60].

Unfortunately, we have no experimental results on the situation we are considering — i.e. gas flow in a cavity — and as to the comparison of experimental and theoretical flow data for a gas and a liquid (even at the same Re), this requires great caution. Nevertheless, the calculated Re dependence of the ratio of the size of the bottom near-wall vortex D_3 to the cavity width L (see Fig. 6) is in general agreement with experiment [57–59]. Interestingly, because of the growing oscillations of hydrodynamical quantities, it is found that even in the quasi-stationary regime fluctuations in the position of the vortex, D_3/L , increase in magnitude. As seen in Fig. 6, the region of fluctuations is represented by an expanding band which shows a transition to fully developed turbulence.

Figure 7 demonstrates oscillations in the absolute magnitude of the dimensionless velocity \hat{v}_0 at the point ($\hat{x} = 0.13$, $\hat{y} = 0.87$) over a dimensionless time period $\hat{t} = 0.6$ for Re = 3200. Note the irregular nature of the oscillations.



Figure 6. Relative size D_3/L of the bottom vortex plotted versus Reynolds number Re for Eu = 1. Solid lines represent theoretical results.



Figure 7. Oscillations of the absolute value of velocity \hat{v}_0 at the point $(\hat{x} = 0.13, \hat{y} = 0.87)$ over a period of $\hat{t} = 0.6$ in the near-'quasi-stationary' flow regime for Re = 3200, Eu = 1. Zero time $\hat{t}_0 = 185.0$.

Thus, already at Re = 3200 the flow starts to exhibit typical features of a turbulent regime.

Note that the use of the generalized hydrodynamical equations with viscous terms makes it possible to construct the extremely effective difference schemes, thus making these equations even more attractive.

9. Sound propagation studied with the generalized equations of fluid dynamics

The propagation of sound is a classical problem in kinetic and hydrodynamic theories. Let an infinite plate oscillate in a gas with the frequency ω in the direction of its normal. Put $a = \omega \tau$, where τ is the mean time between collisions. For a Boltzmann gas of hard spheres [49] one has

$$p\tau = \Pi \mu \,. \tag{9.1}$$

In addition to the static pressure p and dynamic viscosity μ , the hydrodynamic relation (9.1) contains the parameter Π , which is 0.786 if the distribution function is expanded in terms of Sonine polynomials, and 0.8 in the first-order (Maxwell) approximation.

The parameter a may be linked to the Reynolds number analogue

$$r = \frac{\Pi}{a} = \frac{p}{\omega\mu} \,. \tag{9.2}$$

For large enough values of *r*, classical hydrodynamics works quite satisfactorily. In linear acoustics, the attenuation of sound tends to zero as $r \to \infty$, and the velocity of sound is given by

$$c_0^2 = \gamma \, \frac{p_0}{\rho_0} \,, \tag{9.3}$$

where ρ_0 is the density of the unperturbed gas and

$$\gamma = \chi^{-1} = \frac{C_p}{C_V} \tag{9.4}$$

is the ratio of the heat capacity at constant pressure to that at constant volume.

Complications arise when $r \sim 1$ and especially in the limit as $r \rightarrow 0$. The Euler equations do not 'feel' that the situation has changed and yield a constant velocity of sound and zero attenuation over the entire range of r. The Navier–Stokes equation leads to an entirely unreasonable prediction that the attenuation tends to zero after having reached a maximum at $r \sim 1$, and that the speed of sound tends to infinity as $r \rightarrow 0$. Therefore, the problem of sound propagation at small rnumbers requires a kinetic theory treatment. Without entering into a detailed discussion of the methods mentioned (see, e.g., Ref. [62]), it should be admitted that the situation as a whole is unsatisfactory in this field.

In particular, the increased number of moments employed when solving the Boltzmann equation by moment methods gives a poorer agreement with experimental data. One commonly speaks of the 'critical Reynolds number' r_{cr} , below which it is impossible to obtain a plane-wave solution. For each particular type of model or moment equations there exists a unique number r_{cr} , thus revealing the purely mathematical — rather than physical — nature of the effect observed.

Let us apply the generalized equations of fluid dynamics to the propagation of sound waves in a monatomic gas. In linear acoustics, density and temperature perturbations are written as

ŀ

$$\rho = \rho_0 (1+s) \,, \tag{9.5}$$

$$T = T_0(1+\eta), (9.6)$$

respectively, and the solution of the generalized hydrodynamical equations is taken in the form

$$s = \bar{s} \exp(i\omega t - k'x), \qquad (9.7)$$

$$\eta = \bar{\eta} \exp(i\omega t - k'x), \qquad (9.8)$$

$$v = \bar{v} \exp(i\omega t - k'x), \qquad (9.9)$$

with v the hydrodynamical velocity, and k' the complex wave number.

We now write down the system of nonstationary generalized Euler equations in a one-dimension case [cf. Eqns (7.8) - (7.10)]:

$$\frac{\partial}{\partial t} \left\{ \rho - \tau \left[\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial t} (\rho v) \right] \right\} + \frac{\partial}{\partial x} \left\{ \rho v - \tau \left[\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (\rho v^2) + \frac{\partial \rho}{\partial x} \right] \right\} = 0, \quad (9.10)$$

$$\frac{\partial}{\partial t} \left\{ \rho v - \tau \left[\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (\rho v^2) + \frac{\partial p}{\partial x} \right] \right\} + \frac{\partial}{\partial x} \left\{ \rho v^2 + p - \tau \left[\frac{\partial}{\partial t} (\rho v^2 + p) + \frac{\partial}{\partial x} (\rho v^3 + 3pv) \right] \right\} = 0, \qquad (9.11)$$

$$\frac{\partial}{\partial t} \left\{ \rho v^{2} + 3p - \tau \left[\frac{\partial}{\partial t} (\rho v^{2} + 3p) + \frac{\partial}{\partial x} (\rho v^{3} + 5pv) \right] \right\}$$
$$+ \frac{\partial}{\partial x} \left\{ \rho v^{3} + 5pv - \tau \left[\frac{\partial}{\partial t} (\rho v^{3} + 5pv) + \frac{\partial}{\partial x} \left(\rho v^{4} + 8pv^{2} + 5\frac{p^{2}}{\rho} \right) \right] \right\} = 0.$$
(9.12)

From the equation of state

$$p = \rho RT, \tag{9.13}$$

in which R is the universal gas constant and which is valid for the Maxwellian distribution function, it follows that

$$p = p_0(1 + s + \eta). \tag{9.14}$$

On carrying out the linearization, Eqns (9.10)-(9.12) reduce to

$$\begin{aligned} \frac{\partial s}{\partial t} &+ \frac{\partial v}{\partial x} - \tau \left[\frac{\partial^2 s}{\partial t^2} + \frac{p_0}{\rho_0} \frac{\partial^2}{\partial x^2} (s+\eta) + 2 \frac{\partial^2 v}{\partial t \partial x} \right] = 0, \quad (9.15) \\ \frac{\partial v}{\partial t} &+ \frac{p_0}{\rho_0} \frac{\partial}{\partial x} (s+\eta) \\ &- \tau \left[\frac{\partial^2 v}{\partial t^2} + 2 \frac{p_0}{\rho_0} \frac{\partial^2}{\partial t \partial x} (s+\eta) + 3 \frac{p_0}{\rho_0} \frac{\partial^2 v}{\partial x^2} \right] = 0, \quad (9.16) \\ 3 \frac{\partial}{\partial t} (s+\eta) + 5 \frac{\partial v}{\partial x} - \tau \left[3 \frac{\partial^2}{\partial t^2} (s+\eta) \right] \\ &+ 5 \frac{p_0}{\rho_0} \frac{\partial^2}{\partial x^2} (s+2\eta) + 10 \frac{\partial^2 v}{\partial t \partial x} \right] = 0. \quad (9.17) \end{aligned}$$

To consider in somewhat more detail the linearization process, we use the continuity equation (9.10) as an example. Let us rewrite it as

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) - \tau \left[\frac{\partial^2 \rho}{\partial t^2} + \frac{\partial^2}{\partial x^2} (p + \rho v^2) \right] \\ + 2 \frac{\partial^2}{\partial t \partial x} (\rho v) - \left(\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x} (\rho v) \right) \frac{\partial \ln \tau}{\partial t} \\ - \left(\frac{\partial}{\partial t} (\rho v) + \frac{\partial}{\partial x} (p + \rho v_0^2) \right) \frac{\partial \ln \tau}{\partial x} \right] = 0.$$
(9.18)

Because for the one-component ('simple') gas of hard spheres

$$\tau = \frac{1}{2\sqrt{2}\pi\sigma^2} \sqrt{\frac{\pi m}{2kT}} = \frac{\text{const}}{n\sqrt{T}} , \qquad (9.19)$$

we have

$$\frac{\partial \ln \tau}{\partial t} = -\frac{1}{\rho} \frac{\partial \rho}{\partial t} - \frac{1}{2T} \frac{\partial T}{\partial t} , \qquad (9.20)$$

$$\frac{\partial \ln \tau}{\partial x} = -\frac{1}{\rho} \frac{\partial \rho}{\partial x} - \frac{1}{2T} \frac{\partial T}{\partial x}.$$
(9.21)

Therefore, in linear acoustics, terms containing derivatives of $\ln \tau$ contribute nothing to the first-order equations.

Using the representations (9.7)-(9.9) we now arrive at a system of equations

$$\mathbf{i}\omega s - k'v - \tau \left[-\omega^2 s + \frac{p_0}{\rho_0} k'^2 (s+\eta) - 2\mathbf{i}\omega k'v \right] = 0, \quad (9.22)$$
$$\mathbf{i}\omega v - \frac{p_0}{\rho_0} k' (s+\eta)$$

$$-\tau \left[-\omega^2 v - 2i\omega \frac{p_0}{\rho_0} k'(s+\eta) + 3 \frac{p_0}{\rho_0} k'^2 v \right] = 0, \quad (9.23)$$
$$3i\omega(s+\eta) - 5k'v - \tau \left[-3\omega^2(s+\eta) \right]$$

$$+5\frac{p_0}{\rho_0}k'^2(s+2\eta) - 10i\omega k'v\bigg] = 0.$$
 (9.24)

If the rank of matrix equals the number of equations, then the system of homogeneous algebraic equations (9.22) - (9.24)has only a trivial solution. The requirement that there be a nonzero solution to this system is that its determinant must be zero:

$$\begin{vmatrix} i\omega + \omega^{2}\tau - \tau \frac{p_{0}}{\rho_{0}} k'^{2} & -\tau \frac{p_{0}}{\rho_{0}} k' \\ -\frac{p_{0}}{\rho_{0}} k' + 2i\omega\tau \frac{p_{0}}{\rho_{0}} k' & -\frac{p_{0}}{\rho_{0}} k' + 2i\omega\tau \frac{p_{0}}{\rho_{0}} k' , \\ 3i\omega + 3\omega^{2}\tau - 5\tau \frac{p_{0}}{\rho_{0}} k'^{2} & 3i\omega + 3\omega^{2}\tau - 10\tau \frac{p_{0}}{\rho_{0}} k'^{2} \\ & -k + 2i\omega\tau k' \\ i\omega + \omega^{2}\tau - 3\tau \frac{p_{0}}{\rho_{0}} k'^{2} \\ & -5k' + 10i\omega\tau k' \end{vmatrix} = 0,$$

giving an algebraic equation of the sixth order in the wave number k':

$$5\tau^{3} \frac{p_{0}^{3}}{\rho_{0}^{3}} k^{\prime 6} - \frac{p_{0}^{2}}{\rho_{0}^{2}} \Big[5i\omega\tau^{2} + 5\omega^{2}\tau^{3} + \frac{5}{3}\tau \Big] k^{\prime 4} + \frac{p_{0}}{\rho_{0}} \Big[\frac{5}{3} i\omega + 2\omega^{2}\tau - \frac{2}{3} i\omega^{3}\tau^{2} - \frac{1}{3} \omega^{4}\tau^{3} \Big] k^{\prime 2} + i\omega^{3} + 3\omega^{4}\tau - 3i\omega^{5}\tau^{2} - \omega^{6}\tau^{3} = 0.$$
(9.25)

This equation reduces to the dimensionless form

$$3a^{3}\chi^{2}\hat{k}^{6} - [3ia^{2} + 3a^{3} + a]\chi\hat{k}^{4} + \left[i + \frac{6}{5}a - \frac{2}{5}ia^{2} - \frac{1}{5}a^{3}\right]\hat{k}^{2} + \frac{3}{5\chi}i + \frac{9}{5\chi}a - \frac{9}{5\chi}a^{2} - \frac{3}{5\chi}a^{3} = 0, \qquad (9.26)$$

where we have introduced the dimensionless wave number $\hat{k} = k' c_0 / \omega$ with the characteristic velocity

$$c_0 = \sqrt{\gamma \, \frac{p_0}{\rho_0}} \,. \tag{9.27}$$

-

The separation of the real from imaginary part in Eqn (9.26) according to the equality

$$\hat{k} = \alpha + \mathbf{i}\beta\,,\tag{9.28}$$

now yields the system of equations for α and β :

$$3a^{3}\chi^{2}(\alpha^{2} - \beta^{2})(\alpha^{4} + \beta^{4} - 14\alpha^{2}\beta^{2}) + 12\alpha\beta a^{2}(\alpha^{2} - \beta^{2})\chi - (3a^{3} + a)\chi(\alpha^{4} + \beta^{4} - 6\alpha^{2}\beta^{2}) + (\alpha^{2} - \beta^{2})\left(\frac{6}{5}a - \frac{1}{5}a^{3}\right) - 2\alpha\beta\left(1 - \frac{2}{5}a^{2}\right) + \frac{9}{5\chi} - \frac{3}{5\chi}a^{3} = 0,$$
(9.29)

$$6a^{3}\chi^{2}\alpha\beta(3\alpha^{4} + 3\beta^{4} - 10\alpha^{2}\beta^{2}) - 3a^{2}\chi(\alpha^{4} + \beta^{4} - 6\alpha^{2}\beta^{2}) - 4(3a^{3} + a)\chi\alpha\beta(\alpha^{2} - \beta^{2}) + \left(1 - \frac{2}{5}a^{2}\right)(\alpha^{2} - \beta^{2}) + 2\alpha\beta\left(\frac{6}{5}a - \frac{1}{5}a^{3}\right) + \frac{3}{5\chi} - \frac{9}{5\chi}a^{2} = 0.$$
(9.30)

From Eqn (9.7) it follows

$$s = \bar{s} \exp\left(-\omega \frac{\alpha}{c_0} x\right) \exp\left[i\omega\left(t - \frac{\beta}{c_0} x\right)\right],$$

showing that the factor α characterizes the attenuation of sound and that $\beta = c_0/c$ is the ratio of the classical Eulerian speed of sound to its calculated value.

Let us now consider two asymptotic solutions to Eqns (9.29) and (9.30).

(1) If $a = \omega \tau \to 0$, then in the limiting case a = 0 it follows from Eqns (9.29) and (9.30) that

$$\hat{k}^2 = -\frac{3}{5}\,\chi^{-1}\,.\tag{9.31}$$

Using the value

$$\chi = \frac{5}{3} \,, \tag{9.32}$$

for a monatomic gas [see Eqn (9.4)], one is led to the classical Euler limit

$$k' = \pm i \frac{\omega}{c_0} \,. \tag{9.33}$$

The wave number k' proves to be imaginary; for the density perturbation, for example, the solution is written as

$$s = \bar{s} \exp\left[i\omega\left(t \pm \frac{x}{c_0}\right)\right].$$
(9.34)

Thus, in the classical Euler description sound is unattenuated and its velocity remains constant and equal to c_0 [cf. Eqn (9.27)]. In other words, for oscillations travelling in the positive x direction one obtains

$$\alpha = 0, \qquad \beta = 1. \tag{9.35}$$

(2) If $a \to \infty$, then it follows from Eqn (9.26) that

$$\hat{k}^6 - \frac{5}{3}\hat{k}^4 - \frac{5}{27}\hat{k}^2 = \frac{25}{27}, \qquad (9.36)$$

or [see Eqns (9.29) and (9.30)]

$$-x(x^{2} - 12y) - \frac{5}{3}x^{2} + \frac{20}{3}y + \frac{5}{27}x = \frac{25}{27},$$

$$3x^{2} - 4y + \frac{10}{3}x = \frac{5}{27},$$
(9.37)

where

$$\beta^2 - \alpha^2 = x, \qquad \alpha^2 \beta^2 = y.$$
 (9.38)

From Eqn (9.37), one finds

$$x^{3} + \frac{5}{3}x^{2} + \frac{35}{54}x - \frac{25}{162} = 0, \qquad (9.39)$$

and the asymptotic solution then follows readily as

$$\alpha = 0.509, \quad \beta = 0.650.$$
 (9.40)

Figures 8 and 9 plot the dimensionless velocity of sound β and the dimensionless attenuation rate α , as calculated by the generalized Euler equations [31, 63], the Navier–Stokes equations, and the generalized Navier–Stokes equations, and compares the results with the experimental data of Greenspan [66], and Meyer and Sessler [67]. Detailed general-



Figure 8. Comparison of observed (symbols) and calculated (lines) dimensionless velocity of sound $\beta = c_0/c$ as a function of the Reynolds number analogue *r*: *1*, generalized Euler equation; *2*, generalized Navier – Stokes equation; *3*, Navier – Stokes equation. Open circles, data by Greenspan; filled circles, data by Meyer and Sessler.



Figure 9. Comparison of observed (symbols) and calculated (lines) dimensionless attenuation rate α as a function of the Reynolds number analogue *r*: *I*, generalized Euler equation; *2*, generalized Navier–Stokes equation; *3*, Navier–Stokes equation; *4*, Burnett equation; *5*, super-Burnett equation; *6*, moment equations (the number of moments N = 105). Open circles, data by Greenspan; filled circles, data by Meyer and Sessler.

ized Navier – Stokes calculations are given elsewhere [64] and they are too cumbersome to present here.

We now proceed to discuss the numerical results obtained from the generalized hydrodynamical equations and to make comparisons with available published data. We will also consider some aspects of the method of moments as applied to the Boltzmann equations used in the sound propagation problem. We will base our analysis on the results of Sirovich and Thurber [65], presented in Figs 10 through 12 with necessary notational changes.

Figure 10 compares the numerically calculated dimensionless velocity of sound $\beta = c_0/c$ and dimensionless attenuation rate α as functions of the Reynolds number analogue *r* for the eight- and eleven-moment models using the interaction potential of Maxwellian molecules and that of the hard-sphere models. Notice that the two models yield very close results.

Figures 11 and 12 plot similar data for hard spheres and Maxwellian molecules and compare them with the experimental data of Greenspan [66] and Meyer and Sessler [67] on monatomic gases. Also shown are Navier – Stokes results and those obtained by Pekeris et al. [68, 69] in their unprecedently voluminous computations using the 105- and 483-moment models.

A comparison of the experimental data with the theoretical results obtained with the Boltzmann equations suggests what appears at first sight to be a paradoxical conclusion: the more accurate a theoretical model the worse its agreement with experiment. We see indeed that the hard-sphere model of Sirovich and Thurber [65] works better with eight moments than with eleven, and that the 105-moment results of Pekeris et al. [68, 69] are much poorer.

Considering the weak correlation between the molecular interaction model and the velocity of sound and attenuation rate calculations, the results of the 483-moment computations for the Maxwellian molecules within the range r < 1 should



Figure 10. Comparison of the velocity of sound (a) and the attenuation rate (b) as calculated from the Boltzmann equation for two models: *1*, 11-moment hard-sphere model; *2*, 11-moment model of Maxwellian molecules; *3*, 8-moment hard-sphere model; *4*, 8-moment model of Maxwellian molecules.



Figure 11. Comparison of observed (symbols) and calculated (lines) velocities of sound (a) and attenuation rates (b) as calculated from the Boltzmann equation for the hard-sphere model: *1*, 11-moment model; *2*, 8-moment model; *3*, 105-moment model; *4*, Navier–Stokes equation. Open circles, data by Greenspan; filled circles, data by Meyer and Sessler.



Figure 12. Comparison of observed (symbols) and calculated (lines) velocities of sound (a) and attenuation rates (b) as calculated from the Boltzmann equation for the model of Maxwellian molecules: *I*, 11-moment model; *2*, 8-moment model; *3*, 483-moment model; *4*, Navier – Stokes equation. Open circles, data by Greenspan; filled circles, data by Meyer and Sessler.

be viewed as simply catastrophic. (Note that as the number of the moments used increases, the 'critical' number r decreases [65], apparently raising hopes for a better final result.)

A similar situation exists with regard to the hydrodynamic results: while the Navier–Stokes equations are totally invalid for r < 1, 'corrected' models (e.g., the Burnett equation) are even less successful. It can be argued that, paradoxically though it may seem, the best classical theory approach is to employ the Euler equation which, although yielding zero attenuation and a constant velocity of sound, at least does not involve divergences or nonphysical 'critical' points.

Viewed in the context of the generalized Boltzmann kinetic theory, this effect has a very clear origin. Let us introduce the Knudsen number as the ratio of λ/λ_b , the mean free path of hard-sphere particles to the wavelength

$$\lambda_{\rm b} = 2\pi \, \frac{c_0}{\omega} \,. \tag{9.41}$$

Since in the hard-sphere model

$$\lambda = \frac{1}{\sqrt{2}\pi n\sigma^2}, \qquad \mu = \frac{5}{16}\frac{\sqrt{mkT}}{\sqrt{\pi}\sigma^2}, \qquad (9.42)$$

where σ is the particle diameter, it follows from Eqns (9.2) and (9.3) that

$$Kn = \frac{\lambda_b}{\lambda} = \frac{8}{5\pi\sqrt{2\pi\gamma}} \frac{1}{r} .$$
(9.43)

In this case, the ratio of the heat capacities $\gamma = C_p/C_V$ at constant pressure and constant volume is 5/3, and using Eqn (9.42) we can recalculate the scale of the Reynolds number analogue *r* to an equivalent scale of the Knudsen number as shown in Figs 10–12.

Thus, discrepancies between the experiment and the 'revised' theoretical models based on the Boltzmann equations start to appear for Knudsen number values $Kn \sim 1$. This is to be expected because the additional terms in the kinetic equation of the generalized Boltzmann theory first become comparable in magnitude and then start to dominate the terms on the left-hand side of the Boltzmann equations as the Knudsen number increases. This means, in particular, that neither the Burnett equations nor, less still, super-Burnett equations hold promise for higher Knudsen number computations.

The generalized Boltzmann equation performs much better. The generalized Euler equations and Navier–Stokes equations give quite satisfactory agreement with the experimental data over the entire range of the Knudsen number, including the asymptotic regions. The generalized Navier– Stokes equations fit the experimental points better than the generalized Euler equations. Another important point about this result is that it is obtained from the hydrodynamical equations; this raises hope for a through computation of hydrodynamic flows including shock layers, shock waves, and intermediate Knudsen numbers, thus eliminating the necessity of coupling the hydrodynamic and free-molecular solutions.

Coupling problems of this kind are discussed widely in the scientific literature (see, e.g., Refs [70, 71]). In the next section we will see that the generalized hydrodynamical equations make it possible to perform accurate through computations via the shock wave or, in other words, to examine the structure of the shock wave.

10. Shock wave structure examined with the generalized equations of fluid dynamics

Let us consider the structure of the shock wave in a monatomic gas [31, 72] based on the solution of the general-

ized hydrodynamical equations. The solution of the usual gas-dynamic equations in this case is given by discontinuous density, velocity, and temperature functions interrelated by the Rankine-Hugoniot equations.

This classical problem of kinetic theory has long become a kind of a testing ground for approximate kinetic theories as well as for methods of solving the Boltzmann equation. Note that although the solution of this problem has also been obtained with the Navier–Stokes equations, at Mach numbers not too close to unity the conditions for the applicability of the Navier–Stokes equations (small variations of hydrodynamical quantities over the molecular mean free path) are of course not fulfilled, and a qualitative description of the transition layer is the most that seems achievable. (In this case the viscous terms in the Navier–Stokes equations play the same role as the artificial viscosity terms which are introduced into the Euler equations in shock wave calculations.)

The generalized Euler equations in the one-dimensional steady case are [see Eqns (7.8) - (7.10)]

$$\frac{\mathrm{d}}{\mathrm{d}x} \left\{ \rho v_0 - \tau^{(0)} \, \frac{\mathrm{d}}{\mathrm{d}x} (\rho v_0 + p) \right\} = 0 \,, \tag{10.1}$$

$$\frac{\mathrm{d}}{\mathrm{d}x} \left\{ \rho v_0^2 + p - \tau^{(0)} \frac{\mathrm{d}}{\mathrm{d}x} (\rho v_0^3 + 3pv_0) \right\} = 0, \qquad (10.2)$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\left\{\rho v_0^3 + 5pv_0 - \tau^{(0)} \frac{\mathrm{d}}{\mathrm{d}x}\left(\rho v_0^4 + 8pv_0^2 + 5\frac{p^2}{\rho}\right)\right\} = 0.$$
(10.3)

Recall that in the hard-sphere model $\tau^{(0)}p = 0.8\mu$ in the firstorder approximation within the framework of the Enskog method.

Equations (10.1)-(10.3) in the one-dimensional steady case are readily integrated once to yield

$$\rho v_0 = \tau^{(0)} \frac{\mathrm{d}}{\mathrm{d}x} (p + \rho v_0^2) + C_1 , \qquad (10.4)$$

$$p + \rho v_0^2 = \tau^{(0)} \frac{\mathrm{d}}{\mathrm{d}x} \left[v_0 (3p + \rho v_0^2) \right] + C_2 \,, \tag{10.5}$$

$$v_0(5p + \rho v_0^2) = \tau^{(0)} \frac{\mathrm{d}}{\mathrm{d}x} \left(8pv_0^2 + 5\frac{p^2}{\rho} + \rho v_0^4 \right) + C_3. \quad (10.6)$$

To integrate Eqns (10.1) - (10.3), it is necessary to specify two boundary conditions for the hydrodynamical velocity, density, and pressure. These are the so-called Hugoniot conditions. The constants C_1 , C_2 and C_3 for Eqns (10.4) -(10.6) are determined by the conditions before the shock wave:

$$(\rho v_0)_{\rm b} = C_1 \,, \tag{10.7}$$

$$(p + \rho v_0^2)_{\rm b} = C_2 \,, \tag{10.8}$$

$$\left[v_0(5p + \rho v_0^2)\right]_{\mathbf{b}} = C_3 \,, \tag{10.9}$$

where the subscript 'b' refers to the flow before the shock wave.

However, the numerical integration of Eqns (10.4) - (10.6) is complicated by the necessity of satisfying the boundary conditions at the opposite end of the integration region. A simpler approach in this case is to solve the boundary value problem directly, by applying the sweep method of solving ordinary differential equations of second order. This is exactly what V Polev and the present author did in 1988 [72].

Let us define the width of the shock wave by the relation

$$d = \frac{\rho_{\rm a} - \rho_{\rm b}}{\left(\mathrm{d}\rho/\mathrm{d}x\right)_{\rm max}}\,,\tag{10.10}$$

where the subscript 'a' refers to the flow parameters after the shock wave, and $(d\rho/dx)_{max}$ corresponds to the maximum values of the density gradient in the shock wave.

Let us next define the dimensionless shock wave width

$$\bar{\delta} = \frac{\lambda_{\rm b}}{d} \,, \tag{10.11}$$

where λ_b is the mean free path in the region before the shock. For the hard-sphere model

$$\lambda_{\rm b} = \frac{m}{\sqrt{2}\,\pi\rho_{\rm b}\sigma^2}\,,\tag{10.12}$$

or, using Eqns (9.3) and (9.42), one arrives at

$$\lambda_{\rm b} = \frac{16}{5} \sqrt{\frac{5}{6\pi}} \frac{\mu_{\rm b}}{c_{\rm b}\rho_{\rm b}} \,, \tag{10.13}$$

where c_b is the velocity of sound before the shock as calculated in the Euler approximation. It is also useful to define the dimensionless density

$$\bar{\rho} = \frac{\rho - \rho_{\rm b}}{\rho_{\rm a} - \rho_{\rm b}} \,. \tag{10.14}$$

Figure 13 plots the dimensionless shock wave width δ as a function of the Mach number M. We note that the theoretical curves *1*, *2*, and *3* (computed with the generalized Euler equations, the generalized Navier–Stokes equations, and the ordinary Navier–Stokes equations, respectively) agree reasonably well with the experimental data of Schmidt [73]. Curves *1* and *2* lie somewhat above the experimental points, the generalized Navier–Stokes calculations giving a better fit. Notice that the Navier–Stokes results (curve *3*) become unsatisfactory for M \gtrsim 1.6.

The use of the Grad method also has proved unsatisfactory. Grad himself used the thirteen-moment approximation to determine the shock wave structure [74]. He found that a solution to this problem does not exist for M > 1.65, and Holway later established [75] that the Grad series for the



Figure 13. Comparison of observed (experimental points by Schmidt [73]) and calculated (lines) dimensionless shock wave width $\bar{\delta}$ as a function of the Mach number M: *1*, generalized Euler equations; *2*, generalized Navier–Stokes equations; *3*, Navier–Stokes equations.

distribution function in the Boltzmann equation diverges when M > 1.85.

It is important to note that our results on shock wave structure were obtained in the framework of the generalized hydrodynamical equations, which leads to the expectation that these equations may be used effectively in through calculations for arbitrary Mach and Knudsen numbers.

This brings to an end our presentation of the generalized Boltzmann kinetic theory. The results outlined in this paper are only a small part of what has been done since work on the theory began over 10 years ago. And, as a final general remark, many years of experience with the generalized Boltzmann equation and its applications indicate that it provides an exceptionally effective tool for treating many physical problems in cases where classical theory fails.

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