METHODS OF NONLINEAR KINETICS

Key words:
Boltzmann equation, H theorem, kinetic models, Bhatnagar-Gross-Krook model, quasi-equilibrium approximation, Hilbert method, Chapman-Enskog method, Grad moment method, method of invariant manifold, Discrete velocity models, Direct simulation.

Contents:

Nonlinear kinetics studies time-dependent processes of statistical physics through nonlinear equations.

1. The Boltzmann equation

The **Boltzmann equation** is the first and most famous nonlinear kinetic equation introduced by the great Austrian physicist Ludwig Boltzmann in 1872. This equation describes dynamics of a moderately rarefied gas, taking into account for the two processes, the free flight of the particles, and their collisions. In its original version, the Boltzmann equation has been formulated for particles represented by hard spheres. The physical condition of rarefaction means that only pair collisions are taken into account, a mathematical specification of which is given by the **Grad-Boltzmann limit:** if N is the number of particles, and σ is the diameter of the hard sphere, then the Boltzmann equation is expected to hold when N tends to infinity, σ tends to zero, $N\sigma^3$ (the volume occupied by the particles) tends to zero, while $N\sigma^2$ (the total collision cross section) remains constant. The microscopic state of the gas at time t is described by the one-body distribution function $P(\mathbf{x},\mathbf{v},t)$, where $\mathbf{x}$ is the position of the center of the particle, and $\mathbf{v}$ is the velocity of the particle. The distribution function P is the probability density of finding the particle at time t within the infinitesimal phase space volume $d\mathbf{x}d\mathbf{v}$ centered at the phase point $(\mathbf{x},\mathbf{v})$. The collision mechanism of two hard spheres is presented by a relation between the velocities of the particles before [$\mathbf{v}$ and $\mathbf{w}$] and after [$\mathbf{v}'$ and $\mathbf{w}'$] their impact:

$\mathbf{v}' = \mathbf{v} - \mathbf{n}(\mathbf{n}, \mathbf{v} - \mathbf{w})$,

$\mathbf{w}' = \mathbf{w} + \mathbf{n}(\mathbf{n}, \mathbf{v} - \mathbf{w})$,

where $\mathbf{n}$ is the unit vector along $\mathbf{v} - \mathbf{v}'$. Transformation of the velocities conserves the total momentum of the pair of colliding particles ($\mathbf{v}' + \mathbf{w}' = \mathbf{v} + \mathbf{w}$), and the total kinetic energy ($\mathbf{v}'^2 + \mathbf{w}'^2 = \mathbf{v}^2 + \mathbf{w}^2$). The Boltzmann equation reads:

$$\frac{\partial P}{\partial t} + \left(\mathbf{v}, \frac{\partial P}{\partial \mathbf{x}}\right) = N\sigma^2 \int_{R^3} \int_{B^-} (P(\mathbf{x}, \mathbf{v}', t)P(\mathbf{x}, \mathbf{w}', t) - P(\mathbf{x}, \mathbf{v}, t)P(\mathbf{x}, \mathbf{w}, t))|(\mathbf{w} - \mathbf{v}, \mathbf{n})|d\mathbf{w}d\mathbf{n}, \qquad (1)$$

where integration in $\mathbf{n}$ is carried over the unit sphere R^3, while integration in $\mathbf{w}$ goes over a hemisphere $B^- = \{\mathbf{w} | (\mathbf{w} - \mathbf{v}, \mathbf{n}) < 0\}$. This hemisphere corresponds to the particles entering the collison. The nonlinear integral operator on the right of Eq. (1) is nonlocal in the velocity variable and local in space. The Boltzmann equation for arbitrary hard-core interaction is a generalization of the Boltzmann equation for hard spheres under the proviso that the true infinite-range interaction potential between the particles is cut-off at some distance. This generalization amounts to a replacement,

$$\sigma^2 |(\mathbf{w} - \mathbf{v}, \mathbf{n})|d\mathbf{n} \to B(\theta, |\mathbf{w} - \mathbf{v}|)d\theta d\varepsilon, \qquad (2)$$

where function B is determined by the interaction potential, and vector $\mathbf{n}$ is identified with two angles, θ and ε. In particular, for potentials proportional to the n-th inverse power of the distance, function B reads,

$$B(\theta, |\mathbf{v} - \mathbf{w}|) = \beta(\theta)|\mathbf{v} - \mathbf{w}|^{(n-5)/(n-1)}. \qquad (3)$$

In the special case n=5, function B is independent of the magnitude of the relative velocity (**Maxwell molecules**). Maxwell molecules occupy a distinct place in the theory of the Boltzmann equation, they provide exact results. Three most important findings for the Maxwell molecules are mentioned here:

1. The exact spectrum of the linearized Boltzmann collision integral, found by Truesdell and Muncaster,
2. Exact transport coefficients found by Maxwell even before the Boltzmann equation was formulated,
3. Exact solutions to the space-free model version of the nonlinear Boltzmann equation. Pivotal results in this domain belong to Galkin who has found the general solution to the system of moment equations in a form of a series expansion, to Bobylev, Krook and Wu who have found an exact solution of a particular elegant closed form, and to Bobylev who has demonstrated the complete integrability of this dynamic system.

It is customary to write the Boltzmann equation using another normalization of the distribution function, $f(\mathbf{x}, \mathbf{v}, t)d\mathbf{x}d\mathbf{v}$, taken in such a way that function f is compliant with the definition of the hydrodynamic fields: **the mass density** ρ, **the momentum density** $\rho\mathbf{u}$, and **the energy density** ε :

$$\begin{aligned} &\int f(\mathbf{x}, \mathbf{v}, t)md\mathbf{v} = \rho(\mathbf{x}, t) \\ &\int f(\mathbf{x}, \mathbf{v}, t)\mathbf{v}md\mathbf{v} = \rho\mathbf{u}(\mathbf{x}, t) \\ &\int f(\mathbf{x}, \mathbf{v}, t)m\frac{v^2}{2}d\mathbf{v} = \varepsilon(\mathbf{x}, t) \end{aligned} \qquad (4)$$

Here m is the particle's mass.

The Boltzmann equation for the distribution function f reads,

$$\frac{\partial f}{\partial t} + (\mathbf{v}, \frac{\partial}{\partial \mathbf{x}} f) = Q(f, f), \tag{5}$$

where the nonlinear integral operator on the right is the Boltzmann **collision integral**,

$$Q = \int_{R^3} \int_{B^-} (f(\mathbf{v}')f(\mathbf{w}') - f(\mathbf{v})f(\mathbf{w}))B(\theta, \mathbf{v})d\mathbf{w}d\theta d\varepsilon . \tag{6}$$

Finally, we mention the following form of the Boltzmann collision integral (sometimes referred to as the **scattering** or the **quasi-chemical** representation)

$$Q = \int W(\mathbf{v}, \mathbf{w} | \mathbf{v}', \mathbf{w}')[f(\mathbf{v}')f(\mathbf{w}') - f(\mathbf{v})f(\mathbf{w})]d\mathbf{v}d\mathbf{w}', \tag{7}$$

where W is a generalized function which is called the probability density of the elementary event

$$W = w(\mathbf{v}, \mathbf{w} | \mathbf{v}'\mathbf{w}')\delta(\mathbf{v} + \mathbf{w} - \mathbf{v}' - \mathbf{w}')\delta(v^2 + w^2 - v'^2 - w'^2) . \tag{8}$$

Generalized function W has the following symmetries:

$$W(\mathbf{v}', \mathbf{w}' | \mathbf{v}, \mathbf{w}) \equiv W(\mathbf{w}', \mathbf{v}' | \mathbf{v}, \mathbf{w}) \equiv W(\mathbf{v}', \mathbf{w}' | \mathbf{w}, \mathbf{v}) \equiv W(\mathbf{v}, \mathbf{w} | \mathbf{v}', \mathbf{w}') \tag{9}$$

The first two identities reflect the symmetry of the collision process with respect to labeling the particles whereas the last identity is the celebrated **detail balance** condition which is underpinned by the time-reversal symmetry of the microscopic (Newton's) equations of motion. The basic properties of the Boltzmann equation are:

1. **Additive invariants of collision operator**:

$$\int Q(f, f)\{1, \mathbf{v}, v^2\}dv = 0 \tag{10}$$

for any function f, assuming integrals exist. Identity (10) reflects the fact that the number of particles, three components of particle's momentum and the particle's energy is conserved in the collision. Conservation laws (10) imply that the local hydrodynamic fields (4) can change in time only due to redistribution in space.

2. Zero point of the integral ($Q=0$) satisfy the equation (which is also called the **detailed balance**): For almost all velocities,

$$f(\mathbf{v}', \mathbf{x}, t)f(\mathbf{w}', \mathbf{x}, t) = f(\mathbf{v}, \mathbf{x}, t)f(\mathbf{w}, \mathbf{x}, t) .$$

3. Boltzmann's **local entropy production inequality**:

$$\sigma(\mathbf{x}, t) = k_B \int \ln f Q(f, f)d\mathbf{v} \le 0 \tag{11}$$

for any function f, assuming integrals exist. Dimensional **Boltzmann's constant** ($k_B \approx 6 \cdot 10^{-23} JK^{-1}$) in this expression serves for a recalculation of the energy units into the absolute temperature units. Moreover, equality sign takes place if $\ln f$ is a linear combination of the additive invariants of collision.

Distribution functions f whoes logarithm is a linear combination of additive collision invariants, with coefficients dependent on **x,** are called **local Maxwell distribution functions** f_{LM}

$$f_{LM} = \rho m^{-m}\left(\frac{2\pi k_B T}{m}\right)^{-3/2} \exp\left\{-\frac{m(\mathbf{v}-\mathbf{u})^2}{2k_B T}\right\}. \tag{12}$$

Local Maxwellians are parametrized by values of five scalar functions, ρ, **u** and T. This parametrization is consistent with the definitions of the hydrodynamic fields (4) $\int f_{LM}\left\{m, m\mathbf{v}, \frac{mv^2}{2}\right\} = \{\rho, \rho\mathbf{u}, \varepsilon\}$ provided the relation between the energy and the kinetic temperature T, holds, $\varepsilon = \frac{3}{2}\frac{\rho}{mk_B T}$.

4. Boltzmann's **H theorem**: The function

$$S[f] = -k_B \int f \ln f d\mathbf{v} \tag{13}$$

is called the **entropy density**. The **local H theorem** for distribution functions independent of space states that the rate of the entropy density increase is equal to the entropy production,

$$\frac{dS}{dt} = -\sigma. \tag{14}$$

Thus, if no space dependence is concerned, the Boltzmann equation describes relaxation to the unique global Maxwellian (whose parameters are fixed by initial conditions), and the entropy density grows monotonically along with solutions. Mathematical specifications of this property has been initialized by Carleman, and many estimations of the entropy growth were obtained over the past two decades. In the case of space-dependent distribution functions, the local entropy density obeys the **entropy balance equation**:

$$\frac{\partial S(\mathbf{x},t)}{\partial t} + \left(\frac{\partial}{\partial \mathbf{x}}, \mathbf{J_S}(\mathbf{x},t)\right) = -\sigma(\mathbf{x},t). \tag{15}$$

Where $\mathbf{J_S}$ is the entropy flux, $\mathbf{J_S}(\mathbf{x},t) = -k_B \int ln\, f(\mathbf{x},t)\mathbf{v} f(\mathbf{x},t) d\mathbf{v}$. For suitable boundary conditions, such as, specularly reflecting or at the infinity, the entropy flux gives no contribution to the equation for the **total entropy**, $S_{tot} = \int S(\mathbf{x},t) d\mathbf{x}$ and its rate of changes is then equal to the total entropy production $\sigma_{tot} = \int \sigma(\mathbf{x},t) d\mathbf{x}$ (the **global H theorem**). For more general boundary conditions which maintain the entropy influx the global H theorem needs to be modified. A detailed discussion of this question is given by Cercignani.

The local maxwellian is also specified as the maximizer of the Boltzmannrs entropy function (13), subject to fixed hydrodynamic constraints (4). For this reason, the local Maxwellian is also termed the local equilibrium distribution function.

Linearization of the Boltzmann integral around the local equilibrium results in the linear integral operator,

$$Lh(\mathbf{v}) = \int W(\mathbf{v},\mathbf{w}|\mathbf{v}',\mathbf{w}') f_{LM}(\mathbf{v}) f(\mathbf{w}) \left[\frac{h(\mathbf{v}')}{f_{LM}(\mathbf{v}')} + \frac{h(\mathbf{w}')}{f_{LM}(\mathbf{w}')} - \frac{h(\mathbf{v})}{f_{LM}(\mathbf{v})} - \frac{h(\mathbf{w})}{f_{LM}(\mathbf{w})} \right] d\mathbf{w}' d\mathbf{v}' d\mathbf{w} .$$

Linearized collision integral is symmetric with respect to scalar product defined by the second derivative of the entropy functional,

$$\int f_{LM}^{-1}(\mathbf{v}) g(\mathbf{v}) Lh(\mathbf{v}) d\mathbf{v} = \int f_{LM}^{-1}(\mathbf{v}) h(\mathbf{v}) Lg(\mathbf{v}) d\mathbf{v},$$

nonpositively definite

$$\int f_{LM}^{-1}(\mathbf{v}) h(\mathbf{v}) Lh(\mathbf{v}) d\mathbf{v} \le 0,$$

where equality sign takes place if the function hf_{LM}^{-1} is a linear combination of collision invariants, which characterize the null-space of the operator *L*. Spectrum of the linearized collision integral is well studied in the case of small angle cut-off.

2. Phenomenology of the Boltzmann equation

Boltzmann's original derivation of his collision integral was based on a phenomenological 'bookkeeping' of the **gain** and of the **loss** of probability density in the collision process. This derivation postulates that the rate of gain *G* equals

$$G = \int W^{+}(\mathbf{v},\mathbf{w}|\mathbf{v}',\mathbf{w}') f(\mathbf{v}) f(\mathbf{w}) d\mathbf{v}' d\mathbf{w}' d\mathbf{w} .$$

While the rate of loss is

$$L = \int W^{-}(\mathbf{v},\mathbf{w}|\mathbf{v}',\mathbf{w}') f(\mathbf{w}) f(\mathbf{w}) d\mathbf{v}' d\mathbf{w}' d\mathbf{w} .$$

The form of the the gain and of the loss, containing products of one-body distribution functions in place of the two-body distribution, constitutes the famous *Stosszahlansatz*. The Boltzmann collision integral follows now as (*G-L*), subject to the detail balance for the rates of individual collisions,

$$W^{+}(\mathbf{v},\mathbf{w}|\mathbf{v}',\mathbf{w}') = W^{-}(\mathbf{v}',\mathbf{w}'|\mathbf{v},\mathbf{w}) .$$

This representation for interactions different from hard spheres requires also the cut-off of functions β (3) at small angles. The gain-loss form of the collision integral makes it evident that the detail balance for the rates of individual collisions is sufficient to prove the local H theorem. A weaker condition which is also sufficient to establish the H theorem was first derived by Stueckelberg (so-called **semi-detailed balance**), and later generalized **to inequalities of concordance**:

$$\int d\mathbf{v}' \int d\mathbf{w}' (w^{+}(\mathbf{v},\mathbf{w},\mathbf{v}',\mathbf{w}') - w^{-}(\mathbf{v},\mathbf{w},\mathbf{v}',\mathbf{w}')) \ge 0,$$

$$\int d\mathbf{v} \int d\mathbf{w} (w^{+}(\mathbf{v},\mathbf{w},\mathbf{v}',\mathbf{w}') - w^{-}(\mathbf{v},\mathbf{w},\mathbf{v}',\mathbf{w}')) \le 0 .$$

The semi-detailed balance follows from these expressions if the inequality signes are replaced by equalities.
The pattern of Boltzmann's phenomenological approach is often used in order to construct nonlinear kinetic models. In particular, **nonlinear equations of chemical kinetics** are based on this idea: If *n* chemical species A_i participate in a complex chemical reaction,

$$\sum_i \alpha_{si} A_i \leftrightarrow \sum_i \beta_{si} A_i .$$

Where α_{si} and β_{si} are nonnegative integers (stoichiometric coefficients) then equations of chemical kinetics for the concentrations of species c_j are written

$$\frac{dc_i}{dt} = \sum_{s=1}^{n} (\beta_{si} - \alpha_{si}) \left[\varphi_s^+ \exp\left(\sum_{j=1}^{n} \frac{\partial G}{\partial c_j}, \alpha_s \right) - \varphi_s^- \exp\left(\sum_{j=1}^{n} \frac{\partial G}{\partial c_j}, \beta_s \right) \right].$$

Functions φ_s^+ and φ_s^- are interpreted as constants of the direct and of the inverse reactions, while g is an analog of the Boltzmannrs entropy function.
Modern derivation of the Boltzmann equation, initialized by the seminal work of N.N.Bogoliubov, seek a replacement condition, and which would be more closely related to many-particle dynamics. Such conditions are applied to the N-particle Liouville equation should factorize in the remote past, as well as in the remote infinity (the hypothesis of weakening of correlations). Different conditions has been formulated by D.N.Zubarev, J.Lewis and others. The advantage of these formulations is the possibility to systematically find corrections not included in the Stosszahlansatz.

3. Kinetic models

Mathematical complications caused by the nonlinearly Boltzmann collision integral are traced back to the *Stosszahlansatz.* Several approaches have developed in order to simplify the Boltzmann equation. Such simplifications are termed kinetic models. Various kinetic models preserve certain features of the Boltzmann equation, while scarifying the rest of them.
The most well known kinetic model which preserve the H theorem is the nonlinear Bhatnagar-Gross-Krook model (BGK). The BGK collision integral reads:

$$Q_{BGK} = -\frac{1}{\tau}(f - f_{LM}(f)).$$

The time parameter $\tau > 0$ is interpreted as a characteristic relaxation time to the local Maxwellian. The BGK is a nonlinear operator: Parameters of the local Maxwellian are identified with the values of the corresponding moments of the distribution function *f*. This nonlinearly is of 'lower dimension' than in the Boltzmann collision integral because $f_{LM}(f)$ is a nonlinear function of only the moments of *f* whereas the true Boltzmann collision integral is nonlinear in the distribution function *f* itself. This type of simplification introduced by the BGK approach is closely related to the family of so-called mean-field approximations in statistical mechanics. By its construction, the BGK collision integral preserves the following three properties of the Boltzmann equation: additive invariants of collision, uniqueness of the equilibrium, and the H theorem.
A class of kinetic models which generalized the BGK model to **quasi-equilibrium approximations** of a general form is described as follows. The quasi-equilibrium for the set of linear functionales *M(f)* is a

distribution function $f^*(\mathbf{v}, M)$ which maximizes the entropy under fixed values of functions M. The Quasi-equilibrium (QE) models are characterized by the collision integral,

$$Q_{QE}(f) = -\frac{1}{\tau}[f - f^*(\mathbf{v}, M(f))] + Q_B(f^*(\mathbf{v}, M(f)), f^*(\mathbf{v}, M(f))).$$

Same as in the case of the BGK collision integral, operator Q_{QE} is nonlinear in the moments M. The QE models preserve the following properties of the Boltzmann collision operator: additive invariants, uniqueness of the equilibrium, and the H theorem, provided the relaxation time τ to the quasi-equilibrium is sufficiently small.

A different nonlinear model was proposed by Lebowitz, Frisch and Helfand:

$$Q_D = D\left\{\frac{\partial}{\partial \mathbf{v}}\frac{\partial}{\partial \mathbf{v}} f + \frac{m}{k_B T}\frac{\partial}{\partial \mathbf{v}}((\mathbf{v}-\mathbf{u})f)\right\}.$$

The collision integral has the form of the self-consistent Fokker-Planck operator, describing diffusion (in the velocity space) in the self-consistent potential. Diffusion coefficient $D > 0$ may depend on the distribution function f. Operator Q_D preserves the same properties of the Boltzmann collision operator as the BGK model.

Kinetic BGK model has been used for obtaining exact solutions of gasdynamic problems, especially its linearized form for stationary problems. Linearized BGK collision model has been extended to model more precisely the linearized Boltzmann collision integral.

4. Methods of reduced description

One of the major issues raised by the Boltzmann equation was problem of the reduced description. Equations of hydrodynamics constitute a closet set of equations for the hydrodynamic field (local density, local momentum, and local temperature). From the standpoint of the Boltzmann equation, these quantities are low-order moments of the one-body distribution function, or, in other words, the macroscopic variables. The problem of reduced description consists in giving an answer to the following two questions:

1. What are the conditions under which the macroscopic description sets in?
2. How to derive equations for the macroscopic variables from kinetic equations?

The classical methods of reduced description for the Boltzmann equation are: the Hilbert method, the Chapman-Enskog method, and the Grad moment method

4.1. The Hilbert method

In 1911, David Hilbert has introduced the notion of normal solutions $f_H(\mathbf{v}, n(\mathbf{r},t), \mathbf{u}(\mathbf{r},t), T(\mathbf{r},t))$ that is, solution to the Boltzmann equation which depend on space and time only through five hydrodynamic fields.

The normal solution are found from a singularly perturbed Boltzmann equation,

$$D_t f = \frac{1}{\varepsilon} Q(f, f), \tag{16}$$

where ε is a small parameter, and $D_f f \equiv \frac{\partial}{\partial t} f + (\mathbf{v}, \frac{\partial}{\partial \mathbf{r}}) f$. Physically, parameter ε corresponds to the Knudsen number, the ratio between the mean free path of the molecules between collisions, and the characteristic scale of variation of the hydrodynamic fields. In the Hilbert method, one seeks functions $n(\mathbf{r},t), \mathbf{u}(\mathbf{r},t), T(\mathbf{r},t)$, such that the normal solution in the form of the Hilbert expansion,

$$f_H = \sum_{i=0}^{\infty} \varepsilon^i f_H{}^{(i)} \tag{17}$$

satisfies the Eq.(16) them by term. Hilbert was able to demonstrate that this is formally possible.
Substituting (17) into (16), and matching various order in ε, we have the sequence of integral equations

$$Q(f_H^{(0)}, f_H^{(0)}) = 0, \tag{18}$$

$$Lf_H^{(1)} = D_t f_H^{(0)} \tag{19}$$

$$Lf_H^{(2)} = D_t f_H^{(1)} - Q(f_H{}^{(0)}, f_H^{(1)}) \tag{20}$$

and so on for higher orders.
Here *L* is the linearized collision integral. From Eq.(18), it follow that $f_H^{(0)}$ is the local Maxwellian with parameters not yet determined. The Fredholm alternative, as applied to the second Eq. (19) results in
a) Solvability condition

$$\int D_t f_H^{(0)} \{1, \mathbf{v}, v^2\} d\mathbf{v} = 0,$$

which is the set of compressible Euler equations of non-viscid hydrodynamics. Solution to the Euler equation determine the parameters of Maxwellian $f_H^{(0)}$.
b) General solution $f_H^{(1)} = f_H^{(1)1} + f_H^{(1)2}$, where $f_H^{(1)1}$ is the special solution to the linear integral equation (19), and $f_H^{(1)2}$ is yet undeterminal linear combination of the additive invariants of collision.
c) Solvability condition to the next equation (19) determines coefficients of the function $f_H^{(1)2}$ in terms of solutions to the linear hyperbolic differential equations

$$\int D_t (f_H^{(1)1} + f_H^{(1)2}) \{1, \mathbf{v}, v^2\} d\mathbf{v} = 0.$$

Hilbert was able to demonstrate that this procedure of constructing the normal solution can be carried out to arbitrary order n, where the function $f_H^{(n)}$ is determined from the solvability condition at the next, (n+1)-th order. In order to summarize, implementation of the Hilbert method requires solutions for the function $n(\mathbf{r},t)$, $\mathbf{u}(\mathbf{r},t)$ and $T(\mathbf{r},t)$ obtained from a sequence of partial differential equations.

4.2. The Chapman-Enskog method

A completely different approach to reduced description has been invented in 1917 by David Enskog, and (independently) by Sidney Chapman. The key innovation was to seek an expansion of the time derivatives of the hydrodynamic variables rather than seeking the time-space dependencies of these functions in the Hilbert method.
The Chapman-Enskog method start also with the singularly perturbed Boltzmann equation, and the expansion

$$f_{CE} = \sum_{n=0}^{\infty} \varepsilon^n f_{CE}^{(n)}.$$

However, procedure of evaluation of the functions $f_{CE}^{(n)}$ differs completely from the Hilbert method.

$$Q(f_{CE}^{(0)}, f_{CE}^{(0)}) = 0, \tag{21}$$

$$Lf_{CE}^{(1)} = -Q(f_{CE}^{(0)}, f_{CE}^{(0)}) + \frac{\partial^{(0)}}{\partial t} f_{CE}^{(0)} - v \frac{\partial}{\partial r} f_{CE}^{(0)}. \tag{22}$$

Operator $\frac{\partial^{(0)}}{\partial t}$ is defined from the expansion of the right hand side of hydrodynamic equation

$$\frac{\partial^{(0)}}{\partial t}\{\rho,\rho\mathbf{u},e\}\equiv-\int\left\{m,m\mathbf{v},\frac{mv^2}{2}\right\}\mathbf{v}\frac{\partial}{\partial r}f^{(0)}d\mathbf{v}, \tag{23}$$

from Eq. (21), function $f_{CE}^{(0)}$ is again the local Maxwellian, whereas (23) is the Euler equations and $\frac{\partial^{(0)}}{\partial t}$ acts on various functions $g(\rho,\rho\mathbf{u},E)$ according to the chain rule,

$$\frac{\partial^{(0)}}{\partial t}g=\frac{\partial g}{\partial\rho}\frac{\partial^{(0)}}{\partial t}\rho+\frac{\partial g}{\partial(\rho\mathbf{u})}\frac{\partial^{(0)}}{\partial t}\rho\mathbf{u}+\frac{\partial g}{\partial e}\partial_t^{(0)}e,$$

while the time derivatives $\frac{\partial^{(0)}}{\partial t}$ of the hydrodynamic fields are expressed using the right hand side of Eq. (23).

The result of the Chapman-Enskog definition of the time derivative $\frac{\partial}{\partial t}$, is that the Fredholm alternative is satisfied by the right hand side of Eq. (22). Finally, the solution to the homogeneous equation is set to be zero by the requirement that the hydrodynamic variables as defined by the function $f_{CE}^{(0)}+\varepsilon f_{CE}^{(1)}$ coincide with the parameters of the local Maxwellian $f_{CE}^{(0)}$:

$$\int\left\{1,\mathbf{v},v^2\right\}f_{CE}^{(1)}d\mathbf{v}=0.$$

The first correction $f_{CE}^{(1)}$ of the Chapman-Enskog method adds the terms

$$\frac{\partial^{(1)}}{\partial t}\{\rho,\rho\mathbf{u},e\}=-\int\left\{m,m\mathbf{v},\frac{mv^2}{2}\right\}\mathbf{v}\frac{\partial}{\partial r}f_{CE}^{(1)}d\mathbf{v}$$

to the time derivatives of the hydrodynamic fields. These terms correspond to the dissipative hydrodynamics where viscous momentum transfer and heat transfer are in the Navier-Stokes and Fourier form, which are obtained with a very good accuracy for a variety of specific particle's interaction.

The Chapman-Enskog method was the first true success of the Boltzmann equation since it had made it possible to derive macroscopic equation without a priori guessing (the generalization of the Boltzmann equation onto mixtures has predicted existence of the thermodiffusion before it has been found experimentally), and to express the kinetic coefficient in terms of microscopic particle's interaction.

However, higher-order corrections of the Capman-Enskog method, resulting in hydrodynamic equations with derivatives (Burnett hydrodynamic equations) face serve difficulties both from the theoretical, as well as from the practical sides.

In particular, they result in unphysical instabilities of the equilibrium.

4.3. The Grad moment method

In 1949, Harold Grad has extended the basic assumption behind the Hilbert and Chapman-Enskog method (the space and time dependence of the normal solutions is mediated by the five hydrodynamic moments). A physical rationale behind the Grad moment method is an assumption of the decomposition of motion (i). During the time of order τ, a set of distinguished moments M' (which include the hydrodynamic moments and a subset of higher-order moment) does not change significantly as compared to the rest of the moments M'' (the fast evolution) (ii). Towards the end of the fast

evolution, the values of the moments M'' become unambiguously determined by the values of the distinguished moments M', and (iii). On the time of order $\theta >> \tau$, dynamics of the distribution function is determined by the dynamics of the distinguished moments while the rest of the moments remains to be determined by the distinguished moments (the slow evolution period).

Implementation of this picture requires an ansatz for the distribution function in order to represent the set of states visited in the course of the slow evolution. In Grad's method, these representative sets are finite-order truncations of an expansion of the distribution functions in terms of Hermit velocity tensors:

$$f_C(M', \mathbf{v}) = f_{LM}(\rho, \mathbf{u}, E, \mathbf{v})\left[1 + \sum_{\{\alpha\}}^{N} a_{\{\alpha\}}(M') H_{\{\alpha\}}(\mathbf{v} - \mathbf{u})\right] \tag{24}$$

where $H_{\{\alpha\}}(\mathbf{v} - \mathbf{u})$ are various Hermit tensor polynomials, orthogonal with the weight f_{LM}, while coefficient $a_{\{\alpha\}}(M')$ are known functions of the distinguished moments M', and N is the highest order of M'. Other moments are functions of M': $M'' = M''(f_C(M'))$.

Slow evolution of distinguished moments is found upon substitution of Eq. (24) into the Boltzmann equation and finding the moments M' of the resulting expression (Grad's moment equations). Following Grad, this extremely simple approximation can be improved by extending the list of distinguished moments. The most well known is Grad's thirteen-moment approximation where the set of distinguished moments consists of five hydrodynamic moments, five components of the traceless stress tensor $\sigma_{ij} = \int m\left[(v_i - u_i)(v_j - u_j) - \frac{1}{3}\delta_{ij}(\mathbf{v} - \mathbf{u})^2\right] f d\mathbf{v}$, and of the three components of the heat flux vector $q_i = \int (v_i - u_i)\frac{m}{2}(\mathbf{v} - \mathbf{u})^2 f d\mathbf{v}$.

The time evolution hypothesis cannot be evaluated for its validity within the framework of Grad's approach. It is not surprising therefore that Grad's methods failed to work in situations where it was (unmotivatedly) supposed to, primarily, in the phenomena with sharp time-space dependence such as the strong shock wave. On the other hand, Grad's method was quite successful for describing transition between parabolic and hyperbolic propagation, in particular the second sound effect in massive solids at low temperatures, and, in general, situations slightly deviating from the classical Navier-Stokes-Fourier domain. Finally, the Grad method has been important background for development of phenomenological nonequilibrium thermodynamics based on hyperbolic first-order equation, the so-called EIT (extended irreversible thermodynamics).

4.4. Special approximations

Special approximation of the solutions to the Boltzmann equation has been found for several problems, and which perform better than results of «regular» procedures. The most well known is the ansatz introduced independently by Mott-Smith and Tamm for the strong shock wave problem: The (stationary) distribution function is thought as

$$f_{TMS}(a(x)) = (1 - a(x))f_+ + a(x)f_-, \tag{25}$$

where $f_\pm$ are up- and downstream Maxwell distribution functions, whereas $a(x)$ is an undermined scalar function of the coordinate along the shock tube.

Equation for function $a(x)$ has to be found upon substitution of Eq.(25) into the Bolltzmann equation, and upon integration with some velocity-dependent function $\varphi(\mathbf{v})$.

Two general problems arise with the special approximation thus constructed: which function $\varphi(\mathbf{v})$ should be taken, and how to find correction to the Ansatz like Eq. (25).

4.5. The method of invariant manifold

The general approach problem of reduced description for dissipative system was recognized as the problem of finding stable invariant manifolds in the space of distribution function. The notion of invariant manifold generalizes the normal solution in the Hilbert and in the Chapman-Enskog method, and the finite-moment sets of distribution function in the Grad method: If Ω is a smooth manifold in the space of distribution function, and if f_Ω is an element of Ω, then Ω is invariant with respect to the dynamic system

$$\frac{\partial f}{\partial t} = J(f) \tag{26}$$

if

$$J(f_\Omega) \in T\Omega, \text{ for all } f_\Omega \in \Omega, \tag{27}$$

where $T\Omega$ is the tangent bundle of the manifold Ω. Application of the invariant manifold idea to dissipative systems is based on *iterations*, progressively improving the *initial approximation* consist of the iteration procedure the following steps:

1. Thermodynamic projector

Given a manifold Ω (not obligatory invariant), the macroscopic dynamics on this manifold is defined by *the macroscopic vector field,* which is the result of a projection of vector $J(f_\Omega)$ onto the tangent bundle $T\Omega$. The thermodynamic projector P^*_Ω takes advantage of dissipativity:

$$ker\, P^*_{f_\Omega} \subseteq D_f S\big|_{f_\Omega} \bullet. \tag{28}$$

This condition of thermodynamicity means that each state of the manifold Ω is regarded as the result of decomposition of motions occurring near Ω: The state f_Ω is the maximum entropy state on the set of states $f_\Omega + ker\, P^*_{f_\Omega}$. Condition of thermodynamicity does not define projector P^*_Ω completely; rather, it is the condition that should be satisfied by any projector used to define macroscopic vector field $J'_\Omega = P^*_\Omega J(f_\Omega)$. For, once the condition (25) is met, the macroscopic vector field preserves dissipativity of the original microscopic vector field *J(f)*:

$$DS\big|_{f_\Omega} \bullet P^*_\Omega(J(f_\Omega)) \geq 0 \text{ for all } f_\Omega \in \Omega.$$

The thermodynamic projector is the formalization of the assumption that Ω is the manifold of slow motion: if a fast relaxation takes place at least in a sufficiently small neighborhood of Ω, then the states visited in this process before arriving at f_Ω belong to $ker\, P^*_\Omega$. In general, P^*_Ω depends in a non-trivial way on f_Ω.

2. Iterations for the invariance condition

The invariance condition for the manifold Ω reads

$$P_\Omega J(f_\Omega) - J(f_\Omega) = 0,$$

here P_Ω is arbitrary (not obligatory thermodynamic) projector onto the tangent bundle of Ω. The invariance condition is considered as an equation which is solved iteratively, starting with initial approximation Ω_0. On the (n+1)th iteration, the correction $f^{(n+1)} = f^{(n)} + \delta f^{(n+1)}$ is found from linear equations,

$$\begin{aligned} D_f J^*{}_n \delta f^{(n+1)} &= P^*{}_{(n)} J(f^{(n)}) - J(f^{(n)}), \\ P^*{}_{(n)} \delta f^{(n+1)} &= 0, \end{aligned} \tag{29}$$

here $D_f J^*{}_n$ is the linear selfadjoint operator with respect to the scalar product by the second differential of the entropy $D_f^2 S\big|_{f^{(n)}}$.

Together with the above-mentioned principle of thermodynamic projecting, *the selfadjoint linearization* implements the assumption about the decomposition of motions around the n'th approximation. The selfadjoint linearization of the Boltzmann collision integral around a distribution function *f* is given by the formula,

$$D_f J^* \delta f =$$

$$\int w(\mathbf{v}', \mathbf{w}', \mathbf{v}, \mathbf{w}) \frac{f(\mathbf{v}) f(\mathbf{w}) + f(\mathbf{v}') f(\mathbf{w}')}{2} \left\{ \frac{\delta f(\mathbf{w}')}{f(\mathbf{w}')} + \frac{\delta f(\mathbf{v}')}{f(\mathbf{v}')} - \frac{\delta f(\mathbf{w})}{f(\mathbf{w})} - \frac{\delta f(\mathbf{v})}{f(\mathbf{v})} \right\} d\mathbf{v}' d\mathbf{w}' d\mathbf{w}. \tag{30}$$

If $f = f_{LM}$, the selfadjoint operator (30) becomes the familiar linearized collision integral.

The method of invariant manifold is the iterative process:

$$(f^{(n)}, P^{*(n)}) \xrightarrow{(1)} (f^{(n+1)}, P^{*(n)}) \xrightarrow{(2)} (f^{(n+1)}, P^{*(n+1)}).$$

On each 1-st part of the method, the linear equation (30) are solved with the projector known from the previous iteration. On each 2-nd part, the projector is updated, following the thermodynamic construction.

The method of invariant manifold can be further simplified if smallness parameters are known.

The proliferation of the procedure in comparison to the Chapman-Enskog method is essentially twofold: first, the projector is made dependent on the manifold. This enlarges the set of admissible approximations.

Second, the method is based on iteration rather than a series expansion in a smallness parameter. Importance of iteration procedures is well understood in physics, in particular, in the renormalization group approach to reducing the description in equilibrium statistical mechanics, and in the Kolmogorov-Arnold-Moser theory of finite-dimensional Hamiltonian systems.

4.6. Quasi-equilibrium approximations

Important generalization of the Grad moment method is the concept of quasi-equilibrium approximations already mentioned above. The quasi-equilibrium distribution function for a set of distinguished moment M' maximizes the entropy density *S* for fixed M'. The quasi-equilibrium manifold $\Omega^*(M)$ is the collection of the quasi-equilibrium distribution functions for all admissible

values of M. The quasi-equilibrium approximation is the simplest and extremely useful (not only in the kinetic theory itself) implementation of the hypothesis about a decomposition: If M' are considered as slow variables, then states which could be visited in the course of rapid motion in the neighbored of $\Omega^*(M')$ belong to the planes $\Gamma_{M'} = \left\{ f \middle| m'(f - f^*(M')) = 0 \right\}$. In this respect, the thermodynamic construction in the method of invariant manifold is a generalization of the quasi-equilibrium approximation where the given manifold is equipped with a quasi-equilibrium structure by choosing appropriately the macroscopic variables of the slow motion. In contrast to the quasi-equilibrium, the macroscopic variables thus constructed are not obligatory moments. A text book example of the quasi-equilibrium approximation is the generalized Gaussian function for $M' = \left\{ \rho, \rho \mathbf{u}, \widehat{P} \right\}$ where $P_{ij} = \int v_i v_j f d\mathbf{v}$ is the pressure tensor.

The thermodynamic projector for a quasi-equilibrium approximation was first introduced by B. Robertson (in a different context of conservative dynamics and for a special case of the Gibbs-Shannon entropy).

$$P^*_{M'} \bullet = \sum_i \frac{\partial f^*}{\partial M'_i} \int m_i \bullet d\mathbf{v},$$

where $M'_i = \int m_i f d\mathbf{v}$. The quasi-equilibrium approximation does not exist if the highest order moment is an odd polynomial of velocity (therefore, there exists no quasi-equilibrium for thirteen Grad's moments). Otherwise, the Grad moment approximation is the first-order expansion of the quasi-equilibrium around the local Maxwellian.

5. Discrete velocity models

If the number of microscopic velocities is reduced drastically to only a finite set, the resulting discrete velocity, continuous time and continuous space models can still mimic the gas-dynamic flows. This idea was introduced in Broadwell's paper in 1963 to mimic the strong shock wave.

Further important development of this idea was due to Cabannes and Gatignol in seventies who introduced a systematic class of discrete velocity models. The structure of the collision operators in the discrete velocity models mimics the polynomial character of the Boltzmann collision integral. Discrete velocity models are implemented numerically by using the natural operator splitting in which each update due to free flight is followed by the collision update, the idea which dates back to Grad. One of the most important recent results is the proof of convergence of the discrete velocity models with pair collisions to the Boltzmann collision integral.

6. Direct simulation

Besides the analytical approach since mid of 1960s, direct numerical simulation of Boltzmann-type nonlinear kinetic equations have been developed. The basis of the approach is a representation of the Boltzmann gas by a set of particles whose dynamics is modeled as a sequence of free propagation and collisions. The modeling of collisions uses a random choice of pairs of particles inside the cells of the space, and changing the velocities of these pairs in such a way as to comply with the conservation laws, and in accordance with the kernel of the Boltzmann collision integral. At present, there exists a variety of this scheme known under the common title of the direct simulation Monte-Carlo method. The DSMC, in particular, provides data for tests of various analytical theories.

7. Lattice Gas and Lattice Boltzmann models

Since mid of 1980s, the kinetic theory based approach to simulation of complex macroscopic phenomena such as hydrodynamics has been developed. The main idea of the approach is construction of minimal kinetic system in such a way that their long-time and large-scale limit matches the desired macroscopic equations. For this purpose, the fully discrete (in time-space-velocity) nonlinear kinetic equations are considered on sufficiently isotropic lattices, where the links represent the discrete velocities of fictitious particles. In the earlier version of the lattice methods, the particle-based picture has been exploited, subject to the exclusion rule (one or zero particle per lattice link) [the Lattice gas model]. Most of the present versions use the distribution function picture, where populations of the links are real [the Lattice Boltzmann model]. Discrete-time dynamics consists of a propagation step where populations are transmitted to adjacent links and collision step where populations of the links at each node of the lattice are equilibrated by a certain rule. Most of the present versions use the BGK-type equilibration, where the local equilibrium is constructed in such a way as to match desired macroscopic equations. The Lattice Boltzmann method is potentially useful approach for computational fluid dynamics, effectively compliant with parallel architectures. The proof of the H theorem for the Lattice gas models is based on the semi-detailed (or Stueckelberg's) balance principle. For the basic case of the Navier-Stokes equation, the proof of the H theorem in the framework of the Lattice Boltzmann has been only very recently achieved.

8. Other kinetic equations

8.1. The Enskog equation for hard spheres

The Enskog equation for hard spheres is an extension of the Boltzmann equation to moderately dense gases. The Enskog equation explicitly takes into account the nonlocality of collisions through a two-fold modification of the Boltzmann collision integral: First, the one-particle distribution functions are evaluated at the locations of the centers of spheres, separated by the non-zero distance at the impact. This makes the collision integral nonlocal in space. Second, the equilibrium pair distribution function at the contact of the spheres enhances the scattering probability. The proof of the H theorem for the Enskog equation has posed certain difficulties, and has led to a modification of the collision integral.
Methods of solution of the Enskog equation are immediate generalizations of those developed for the Boltzmann equation.

8.2. The Vlasov equation

The Vlasov equation (or kinetic equation for a self-consistent force) is the nonlinear equation for the one-body distribution function, which takes into account a long-range interaction between particles:

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

where $\mathbf{F}(\mathbf{r}) = \int \Phi(|\mathbf{r}-\mathbf{r}'|)\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|} n(\mathbf{r}')d\mathbf{r}'$ is the self-consistent force. In this expression $\Phi(|\mathbf{r}-\mathbf{r}'|)\frac{\mathbf{r}-\mathbf{r}'}{|\mathbf{r}-\mathbf{r}'|}$ is the microscopic force between the two particles, and $n(\mathbf{r}')$ is the density of particles, defined self-consistently, $n(\mathbf{r}') = \int f(\mathbf{r}'\mathbf{v})d\mathbf{v}$.

The Vlasov equation is used for a description of collisionless plasmas in which case it is completed by a set of Maxwell equation for the electromagnetic field. It is also used for a description of the gravitating gas.
The Vlasov equation is an infinite-dimensional Hamiltonian system. Many special and approximate (wave-like) solutions to the Vlasov equation are known and they describe important physical effects. One of the most well known effects is the Landau damping:
The energy of a volume element dissipates with the rate

$$Q \approx -|E|^2 \frac{\omega(k)}{k^2} \frac{df_0}{dv}\bigg|_{v=\varpi/k},$$

where f_0 is the Maxwell distribution function, $|E|$ is the amplitude of the applied monochromatic electric field with the frequency $\omega(k)$, k is the wave vector. The Landau damping is thermodynamically reversible effect, and it is not accompanied with an entropy increase. Thermodynamically reversed to the Landau damping is the plasma echo effect.

8.3. The Smoluchowski equation

Diffusion of particles combined with theses reaction has been first studied by R. von Smoluchowski. The simplest (phenomenological) models for concentration c_i of particles of the i-th species are described with reaction type equations:

$$\partial_t c_i(\mathbf{x},t) = D_i \nabla^2 c_i + P_i(c),$$

where D_i>0 are diffusion coefficients, whereas $P_i(c)$ are reaction rates, usually given by mass action low or its generalizations. At present time, there exist a large number of generalizations of the Smoluchowski equation, including formulations on the level of tow-body distribution functions, coupling to hydrodynamic equation, etc.

Modern development of nonlinear kinetics follows the route of specific numerical methods, such as direct simulations. An opposite tendency is also clearly observed, and the kinetic theory based schemes are increasingly used for development of numerical methods in mechanics of continuous media.

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