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General approach to constructing models of the Boltzmann equation

Alexander N. Gorban[1] and Iliya V. Karlin[1]

Nonequilibrium Systems Laboratory, Computing Center, Russian Academy of Sciences, 660 036 Krasnoyarsk-36, Russian Federation

The problem of thermodynamic parameterization of an arbitrary approximation of reduced description is solved. On the base of this solution a new class of model kinetic equations is constructed that gives a model extension of the chosen approximation to a kinetic model. Model equations describe two processes: rapid relaxation to the chosen approximation along the planes of rapid motions, and the slow motion caused by the chosen approximation. The H-theorem is proved for these models. It is shown, that the rapid process always leads to entropy growth, and also a neighborhood of the approximation is determined inside which the slow process satisfies the H-theorem. Kinetic models for Grad moment approximations and for the Tamm–Mott–Smith approximation are constructed explicitly. In particular, the problem of concordance of the ES-model with the H-theorem is solved.

1. Introduction

In this paper we develop a new method of constructing kinetic models for the Boltzmann equation. This method gives a model extension of an arbitrary approximation of reduced description. These kinetic models are concordant with the H-theorem. One of the principal ideas of our method is a specific thermodynamic parametrization of an arbitrary approximation.

In this section we pose the problem of kinetic modeling and outline a way to solve it.

One can distinguish two points of view on the idea of using kinetic models:
(1) A simplification of the Boltzmann kinetic equation.
(2) An extension of the approximate reduced (macroscopic) description.
  We undergo the second of these viewpoints as more constructive.
  As a rule, model kinetic equations of the following type are used [1]:

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[1] E-mail: amse@cckr.krasnoyarsk.su.

$$\frac{df}{dt} = -\tau^{-1}[f - \tilde{f}(f)] \, . \tag{1.1}$$

Here $d/dt = \partial/\partial t + \Sigma_{i=1}^{3} v_i \, \partial/\partial x_i$ represents the substantial derivative, and τ is the time of relaxation to the states $\tilde{f}(f)$. The distribution $\tilde{f}(f)$ is related to the distribution f by some integral relationships.

The choice of $\tilde{f}(f)$ as the local equilibrium distribution $f_0(f)$ results in the well-known BGK-model [1]. This latter preserves all main properties of the Boltzmann equation, i.e. the conservation laws and the H-theorem. One can consider the BGK-model as the model extension of Euler dynamics.

Attempts to choose $\tilde{f}(f)$, different from $f_0(f)$, result in a discrepancy with the H-theorem. For example, in the ES-model [1] $\tilde{f}(f)$ is

$$\tilde{f}(f) = n \, \pi^{-3/2} (\det \alpha)^{1/2} \exp\left(- \sum_{i,j=1}^{3} \alpha_{ij} (v_i - u_i)(v_j - u_j) \right) . \tag{1.2}$$

The matrix α_{ij} is chosen in order that the correct Prandtl number values are obtained and the conservation laws are satisfied. However, as it was noticed in ref. [1], one can neither prove, nor reject the H-theorem for eq. (1.1) with $\tilde{f}(f)$ (1.2).

We now suppose that an approximation of reduced description is chosen. This means that a manifold $\{f(a)\}$ is fixed in the space of distributions F. This manifold consists of distributions $f(a)$, and a represents coordinates on the manifold. We wish to extend this approximation to a kinetic model.

Looking ahead, we can assume that this model will describe two processes: relaxation to the manifold $\{f(a)\}$ and the motion along the manifold $\{f(a)\}$. The latter motion should be obtained from the Boltzmann equation, while the relaxation to $\{f(a)\}$ will be described by a model term of the type of (1.1).

The model would concur for physical sense only if the H-theorem will be valid in both of these processes.

Here we arrive at two general problems:
(1) The problem of thermodynamic parameterization of the manifold $\{f(a)\}$. This means that we should determine the dynamics on the manifold $\{f(a)\}$ from the Boltzmann equation in order that the H-theorem would be preserved.
(2) The problem of preservation of the H-theorem in the model relaxation.

We stress here that the first of these problems is important already by itself. One can also pose this problem in the form of the question: how and onto which macroscopic variables should one perform the projecting of the Boltzmann equation? In fact, there are a number of possible answers to this question. Which projector would make physical sense?

The answer is not evident especially when the reduced description is defined

only by the coordinates on the manifold $\{f(a)\}$. An example of this situation gives the well-known Mott–Smith approximation in the shock wave theory [1]. The choice of the "natural" projector is recognized as one of the main unsolved problems of the Mott–Smith kinetics. It is evident that the solution of the second problem is impossible without the solution of the first problem.

In this paper we solve both of these problems for an almost arbitrary manifold $\{f(a)\}$. The main idea is to act as if a decomposition of slow and rapid motions corresponds to the manifold $\{f(a)\}$. Then the increase of the entropy in the rapid process results in the essentially unique thermodynamic parameterization and shows explicitly along which manifolds the system relaxes in the neighborhood of the states $f(a)$. After this latter structure would be obtained, we will model the rapid relaxation in the manner of (1.1).

In the next section we introduce a general method of thermodynamic parameterization. As an example we solve the classical problem of obtaining the Mott–Smith dynamics. In section 3 we construct quasi-equilibrium models, and we prove the H-theorem for them in section 4. In section 5 we consider some examples of these models.

2. Thermodynamic parameterization

Our basic idea is to act as if a times hierarchy hypothesis corresponds to the chosen approximation $\{f(a)\}$. This means that a "rapid" relaxation occurs to the states $f(a)$ in a neighborhood of the manifold $\{f(a)\}$, and then the "slow" motion along $\{f(a)\}$ takes place. The rapid motion determines the direction of projecting. The choice of the projector is determined by the fact that the H-function decreases in rapid relaxation. Therefore, the state f will be able to relax into the state $f(a)$ at the end of rapid motion if f belongs to the hyperplane $\Gamma_{f(a)}$, the latter being orthogonal to the gradient of the H-function $D_f H[f]$ at the point $f(a)$. We call $\Gamma_{f(a)}$ the hyperplane of rapid motion. We use the H-function $\int f(\ln f - 1)\, d^3v$. Then $D_f H[f] = \ln f$, and $\Gamma_{f(a)}$ is defined according to the equation

$$\Gamma_{f(a)} = \left\{ f \,\middle|\, \int [f - f(a)]\ln f(a)\, d^3v = 0 \right\}. \tag{2.1}$$

We assume that $\{f(a)\}$ is not tangent to a level of the H-function at any point $f(a) \in \{f(a)\}$.

Due to the strict convexity of the H-function, the point $f(a)$ is the only point of minimum of the H-function on the hyperplane of rapid motions $\Gamma_{f(a)}$. In other words, $f(a)$ coincides with the solution of the variational problem

$$H[f] \to \min \qquad \text{for} \int f \ln f(a) \, \mathrm{d}^3 v = \int f(a) \ln f(a) \, \mathrm{d}^3 v \, . \tag{2.2}$$

The latter statement can be easily checked by the Lagrange multiplier method.

Thus, the hypothesis of the times hierarchy means that the H-function decreases during the relaxation, and its points of minimum occur on the manifolds of rapid motions. The gradient of the H-function is normal to this manifold of rapid motions at the point of minimum. Therefore, in the linear approximation the equation $\int f \ln f(a) \, \mathrm{d}^3 v = \int f(a) \ln f(a) \, \mathrm{d}^3 v$ is valid for those distributions f which relax to the state $f(a)$ in rapid processes.

We finish the constructing of the projector by choosing macroscopic parameters M which define a coordinate system on the manifold $\{f(a)\}$. As a rule, it is sufficient to add some linear functionals $M(f) = \int m(v) \, f \, \mathrm{d}^3 v$ to the functionals $m^*_{f(a)}(f) = \int f \ln f(a) \, \mathrm{d}^3 v$. Then the manifold $\{f(a)\}$ will be parameterized by the macroscopic parameters $m^*_{f(a)}(f(a))$ and $M(f(a))$. The notation $M^*_{f(a)}(f)$ will stand for the set of functionals $m^*_{f(a)}(f)$ and $M(f)$.

Remark 1. It is necessary to distinguish the following three notions: operators $M^*_{f(a)}(f)$, which are defined in a neighborhood of the manifold $\{f(a)\}$; their values, the macroscopic parameters $M^*_{f(a)}(f(a))$; and the coordinates a on the manifold. One can consider the macroscopic parameters $M^*_{f(a)}(f(a))$ as new coordinates on the manifold (i.e. for these coordinates we can write $f^*(M^*_{f(a)}(f(a)))$). The choice of the coordinate system on the manifold does not play an outstanding role while the choice of projector $M^*_{f(a)}(f)$ in the neighborhood of the manifold is principle.

We use the asterisk * in order to stress the thermodynamicity of the chosen parameterization.

The slow dynamics on the manifold $\{f(a)\}$ is governed by equations

$$\frac{\partial M^*_{f(a)}(f(a))}{\partial t} = \mathrm{D}_f M^*_{f(a)}(B(f)) \Big|_{f=f(a)} \, . \tag{2.3}$$

Here $B(f) = -\sum_{i=1}^3 v_i \partial f / \partial x_i + Q(f, f)$ represents the vector field of the Boltzmann equation, and $Q(f, f)$ represents the Boltzmann collision integral. Eqs. (2.3) are obtained by projecting of the vector field of the Boltzmann equation in the point $f(a)$ along the directions $M^*_{f(a)}(f)$.

The functionals $-k_B m^*_{f(a)}$ project the points $f(a)$ into the values of the entropy $S[f(a)]$ and determine the entropy balance equation on the manifold $\{f(a)\}$. Thus, the times hierarchy hypothesis results in the thermodynamic parameterization of the manifold $\{f(a)\}$.

An important particular case occurs when the manifold we consider is a

quasi-equilibrium manifold. This means that $f^*(M)$ is the solution of the problem

$$H[f] \to \min \qquad \text{for } M(f) = M \,. \tag{2.4}$$

Here $M(f)$ is a given operator. Then one does not need a new projector. The quasi-equilibrium manifold $\{f^*(M)\}$ is thermodynamic due to its construction [2–4]: $\ln f^*(M)$ is then a linear combination of $\mathrm{D}_f M(f)|_{f=f(M)}$. Due to (2.2) one can consider an arbitrary manifold as if it were a quasi-equilibrium manifold after the appropriate parameterization.

Remark 2. In spite of the external simplicity of the final results (the entropy balance equation is indeed "natural"), this parameterization has a complicated structure because the functional $m^*_{f(a)}(f)$ is neither the usual moment functional nor the entropy.

The picture of rapid relaxation in the neighborhood of the manifold $\{f(a)\}$ is as follows: the system relaxes along the planes of rapid motions $P_{f(a)}$. The plane of rapid motions $P_{f(a)}$ which includes the point $f(a)$ is the cross section of the hyperplane of rapid motions $\Gamma_{f(a)}$ with the hyperplanes $M(f - f(a)) = 0$. In other words, the equation of the plane of rapid motions is as follows:

$$P_{f(a)} = \{f \mid M^*_{f(a)}(f - f(a)) = 0\} \,. \tag{2.5}$$

It is evident that the state $f(a)$ gives the minimum of the H-function in the plane $P_{f(a)}$ because $f(a)$ is the point of minimum in the "more wide" set (i.e. in the hyperplane $\Gamma_{f(a)}$, see (2.2)). Therefore, $f(a)$ coincides also with the solution of the variational problem

$$H[f] \to \min \qquad \text{for } M^*_{f(a)}(f) = M^*_{f(a)}(f(a)) \,. \tag{2.6}$$

In general, the hyperplanes of rapid motions $\Gamma_{f(a)}$ are nonparallel for different points $f(a)$. The structure of thermodynamic parameterization is sketched in fig. 1. The hyperplane of rapid motions $\Gamma_{f(a)}$ is the only hyperplane where the levels of the H-function "surround" the point $f(a)$. This illustrates the variational principle (2.2).

2.1. Example: The Tamm–Mott–Smith approximation

The following Tamm–Mott–Smith approximation is commonly known in the shock wave problem [1]:

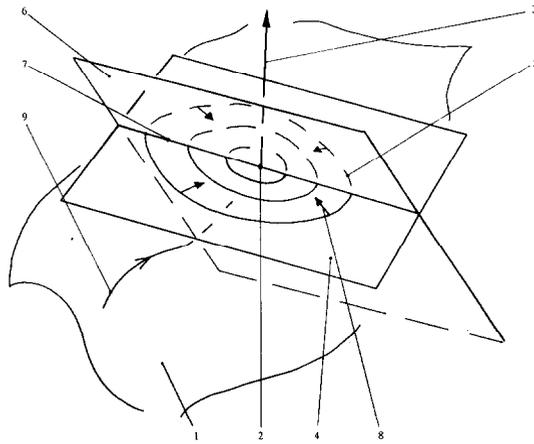$$f(a_-, a_+) = a_- f_- + a_+ f_+ \,. \tag{2.7}$$

Fig. 1. The structure of thermodynamic parameterization. 1 – the manifold $\{f(a)\}$; 2 – the point $f(a)$; 3 – the gradient of the H-function at the point $f(a)$ $(D_f H[f]|_{f=f(a)} = \ln f(a))$; 4 – the hyperplane of rapid motions $\Gamma_{f(a)}$; 5 – the levels of the H-function on the hyperplane $\Gamma_{f(a)}$; 6 – the additional hyperplane $\{f \mid M(f - f(a)) = 0\}$; 7 – the plane of rapid motions $P_{f(a)}$ being the cross-section of the hyperplanes 4 and 6; 8 – the direction of rapid motions on $\Gamma_{f(a)}$; 9 – the direction of slow motion on the manifold $\{f(a)\}$.

Here f_- and f_+ represent Maxwell distributions infinitely far up and down the flow. According to ref. [1], the choice of the "natural" projector is the main unsolved problem of the approximation (2.7).

Thermodynamic parameterization of the approximation (2.7) is determined by the values of the functionals $m^*_{f(a_-,a_+)}(f)$ and of the moment functional $n(f) = \int f\, d^3v$. Then the dynamics of a_- and a_+ are obtained from the equations for the macroscopic variables $m^*_{f(a_-,a_+)}(f(a_-,a_+))$ and $n(f(a_-,a_+))$:

$$\frac{\partial H(a_-,a_+)}{\partial t} + \frac{\partial j_H(a_-,a_+)}{\partial x} = \sigma(a_-,a_+) \,,$$

$$\frac{\partial n(a_-,a_+)}{\partial t} + \frac{\partial j_n(a_-,a_+)}{\partial x} = 0 \,,$$

$$H(a_-,a_+) = \int f(a_-,a_+) \ln f(a_-,a_+)\, d^3v \,,$$

$$j_H(a_-,a_+) = \int v_x f(a_-,a_+) \ln f(a_-,a_+)\, d^3v \,,$$

$$\sigma(a_-,a_+) = \int Q(f(a_-,a_+), f(a_-,a_+)) \ln f(a_-,a_+)\, d^3v \,,$$

$$n(a_-,a_+) = \int f(a_-,a_+)\, d^3v \,,$$

$$j_n(a_-,a_+) = \int v_x f(a_-,a_+)\, d^3v \,. \tag{2.8}$$

The stationary version of the set (2.8) was originally introduced ad hoc in ref. [5]. Here we have shown that eqs. (2.8) are the only equations which make physical sense in the Mott-Smith kinetics.

The plane of rapid motions $P_{f(a_-,\,a_+)}$ for the approximation (2.6) is

$$P_{f(a_-,\,a_+)} = \left\{ f \,\middle|\, \int [f - f(a_-,a_+)]\ln f(a_-,a_+)\,\mathrm{d}^3v = 0 , \right.$$
$$\left. \times \int [f - f(a_-,a_+)]\,\mathrm{d}^3v = 0 \right\} . \tag{2.9}$$

The planes of rapid motions $P_{f(a)}$ (2.5) correspond the distribution f from the neighborhood of $\{f^*(a)\}$ to a distribution $f^*(a((f))$ on $\{f^*(a)\}$. This latter distribution $f^*(a(f))$ represents the state into which the state f transforms in the end of rapid processes. In other words, the equations $M^*_{f(a)}(f - f(a)) = 0$ (2.5) result in the relation $f^*(a(f))$. Further we use sometimes the shortened notation $f^*(f)$ for the function $f^*(a(f))$.

In some cases one requires the explicit expression $f^*(a(f))$. In particular, we will need them in the next section for constructing kinetic models. In order to obtain $f^*(a(f))$ we should solve the equations $M^*_{f(a)}(f - f(a)) = 0$ (2.5) with respect to a (i.e. we have to determine the function $a(f)$). Besides the case of quasi-equilibrium manifolds, the obtaining of $f^*(a(f))$ is not at all simple. Here we represent a method of constructing the function $f^*(a(f))$ by successive approximations.

The zeroth approximation $f^*(a^{(0)}(f))$ is obtained from the equations

$$M^*_f(f - f(a^{(0)})) = 0 . \tag{2.10}$$

Next approximations $f^*(a^{(k)}(f))$, where $k \geqslant 1$, are obtained from the recurrent system

$$M^*_{f(a^{(k-1)})}(f - f(a^{(k)})) = 0 . \tag{2.11}$$

If f is close enough to the manifold $\{f(a)\}$ then this recurrent process converges to the distribution $f^*(a(f))$. Here we do not prove the latter statement.

This recurrent process has a clear geometrical interpretation. At the zeroth approximation (2.10) we take the plane of rapid motions P_f being orthogonal to the gradient of the H-function at the point f, and we search for the point $f(a^{(0)})$ which is the cross section of P_f with the manifold $\{f(a)\}$. At the first iteration (2.11) we project the distribution f onto the manifold $\{f(a)\}$ along the
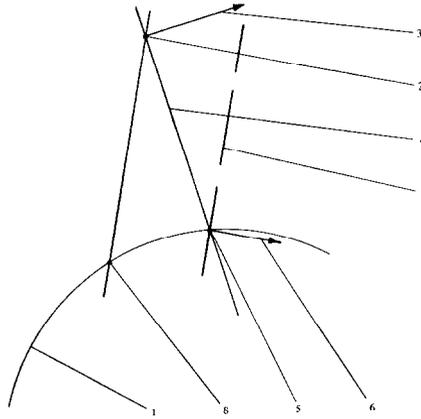
Fig. 2. The constructing of the function f^* (f). 1 – the manifold $\{f(a)\}$; 2 – the point f; 3 – the gradient of the H-function at the point f; 4 – the plane of rapid motions P_f; 5 – the zeroth approximation $f^*(a^{(0)}(f))$; 6 – the gradient of the H-function at the point 5; 7 – the plane of rapid motions $P_{f^*(a^{(0)}(f))}$; 8 – the first approximation $f^*(a^{(1)}(f))$.

direction which is parallel to the plane of rapid motions $P_{f(a^{(0)})}$. Then the procedure is continued. The process (2.10) and (2.11) is sketched in fig. 2.

The procedure (2.10) and (2.11) is the Newton-type method for obtaining the dependence $f^*(f)$. In section 5 we consider the procedure (2.10) and (2.11) for the Mott–Smith approximation.

Thus the choice of the projector $M^*_{f(a)}(f)$ solves the problem of thermodynamicity for the arbitrary approximation of reduced description $\{f(a)\}$. Now we are able to extend the approximation $\{f(a)\}$ to a kinetic model. This extension will model the rapid relaxation along the planes of rapid motions $P_{f(a)}$.

3. Quasi-equilibrium models

According to the previous section we assume that the thermodynamic approximation $\{f^*(a)\}$ is chosen, and the relationship $f^*(f)$ is obtained.

We denote $\delta f = f - f^*(f)$ as the deviation of f from its image in the end of rapid relaxation $f^*(f)$. We stress once again that due to definition of $f^*(f)$ the deviation δf belongs to the appropriate plane of rapid motions.

Assume the model equation to be valid,

$$\frac{d(\delta f)}{dt} = -\tau^{-1} \delta f . \tag{3.1}$$

Eq. (3.1) has a clear sense: the rate of rapid relaxation is proportional to the deviation from the final slow state.

We construct the vector field df/dt in the neighborhood of the manifold $\{f^*(a)\}$ in accordance with the following two assumptions:

(1) The deviation δf decreases according to the simple law (3.1);

(2) On the manifold $\{f^*(a)\}$ the vector field of the model equation coincides with the vector field of the Boltzmann equation, i.e.

$$\frac{df}{dt} = Q(f, f) \qquad \text{if } f \in \{f^*(a)\} \, . \tag{3.2}$$

Clarification. Due to assumption (1), the states relax to the slow manifold. The assumption (2) results in a motion along the manifold, and in a "take-off" from the manifold. In whole, the model vector field describes a motion in the neighborhood of the manifold $\{f^*(a)\}$.

Assumptions (1) and (2) define the vector field unambiguously. The explicit form of the equations is

$$\frac{df}{dt} = J(f, f^*(a(f))) \, ,$$

$$J(f, f^*(a(f))) = -\tau^{-1}[f - f^*(a(f))] + Q(f^*(a(f)), f^*(a(f))) \, . \tag{3.3}$$

Evolution of the state $f^*(a(f))$ is expressed only in terms of the variables $a(f)$:

$$\frac{\partial M^*_{f^*(a(f))}(f^*(a(f)))}{\partial t} = D_f M^*_{f^*(a(f))}(B(f))\Big|_{f=f^*(a(f))} \, . \tag{3.4}$$

Eqs. (3.4) are obtained from (2.3) by substituting the functions $a(f)$. Eqs. (3.3) and (3.4) give the closed set which describes both of the processes mentioned in the introduction.

Macroscopic equations (3.4) are defined in the neighborhood of the manifold $\{f(a)\}$. In the next section we will determine the neighborhood inside which the H-theorem is valid for the equations (3.4).

Now we will make some remarks.

Remark 1. Model equations are simpler than the Boltzmann equation in the following sense: their nonlinearity is expressed only in the terms of some functionals of f but not through the distribution itself. In other words, the "dimension" of nonlinearity in (3.3) is "many times lower" than in the Boltzmann equation, and it may be even finite.

Remark 2. If the manifold $\{f^*\}$ is the local-equilibrium manifold $\{f_0\}$, then the term $Q(f^*(f), f^*(f))$ is identical to zero, and (3.3) coincides with the BGK-model. The planes of rapid motion for the approximation $\{f_0\}$ are

$$P_{f_0} = \left\{ f \,\Big|\, \int m_i(v)\,(f - f_0)\,\mathrm{d}^3 v = 0,\, m_i = 1, v, v^2 \right\}. \tag{3.5}$$

Remark 3. If the set $M^*_{f(a)}(f)$ contains the functionals $\int m_i(v)\,f\,\mathrm{d}^3 v$ (3.4) then the model collision integral (3.3) preserves the conservation laws of the Boltzmann equation.

Remark 4. If the manifold $\{f^*\}$ is the quasi-equilibrium manifold (2.3), and if the functionals $\int m_i(v)\,f\,\mathrm{d}^3 v$ (3.4) are included then $f^*(M(f_0)) = f_0(M(f_0))$. In this case the expression $J(f_0, f^*(f_0))$ is equal to zero, and it is similar to the case of the Boltzmann equation $Q(f_0, f_0) = 0$.

Remark 5. Considering the particular case of quasi-equilibrium approximations (2.4) we mention that the solution of the problem (2.4) does not exist for some $m(f)$ (see elsewhere, for example ref. [2]). For example, if all $m_i(f) \in m(f)$ are usual polynomial moments, and if the degree of the leading polynomial is odd then the quasi-equilibrium distribution $f^*(M)$ cannot be normalized. In order to eliminate these singularities of quasi-equilibrium approximations a general procedure of linearization was developed in ref. [4]. Here we represent the sketch of this procedure for polynomial $m_i(f)$. Firstly, we construct the quasi-equilibrium distribution f_1^* for the restriction m^1, the latter being the set m without the leading odd polynomial m_k. Then, secondly, we solve the following problem in the neighborhood of the manifold f_1^*:

$$\Delta H[\varphi] = H[f_1^*] + \int \varphi f_1^* \ln f_1^*\,\mathrm{d}^3 v + \tfrac{1}{2} \int \varphi^2 f_1^*\,\mathrm{d}^3 v \to \min$$

$$\text{for } \int m^1 f_1^* \varphi\,\mathrm{d}^3 v = 0, \qquad \int m_k f_1^*(1 + \varphi)\,\mathrm{d}^3 v = M_k(f_1^*) + \Delta M_k.$$

This solution results in the approximation $f^* = f_1^*(1 + \varphi)$, $\varphi = \lambda_k m_k\,\Delta M_k$. For this approximation all integrals are converging. In particular, if f_1^* is the local equilibrium then the procedure [4] results in the Grad approximation [6]. Further we assume the solution of the problem (2.4) exists. The method [4] enables one to transfer all results onto arbitrary m.

In the next section we will prove the H-theorem for the model equations (3.3).

4. *H*-theorem for quasi-equilibrium models

Calculating the substantial derivative of the *H*-function induced by (3.3) yields

$$\frac{dH}{dt} = \left(\frac{dH}{dt}\right)_1 + \left(\frac{dH}{dt}\right)_2 ,$$

$$\left(\frac{dH}{dt}\right)_1 = -\tau^{-1} \int \ln f \, [f - f^*(f)] \, d^3v ,$$

$$\left(\frac{dH}{dt}\right)_2 = \int \ln f \, Q(f^*(f), f^*(f)) \, d^3v . \tag{4.1}$$

The derivative $(dH/dt)_1$ is nonpositive for any f. In fact, due to the construction of the distribution $f^*(f)$ we have $\int f \ln f^*(f) \, d^3v = \int f^* \ln f^*(f) \, d^3v$. Therefore, for any f we obtain the inequality

$$\left(\frac{dH}{dt}\right)_1 = -\tau^{-1} \int \ln \frac{f}{f^*(f)} \, [f - f^*(f)] \, d^3v \leq 0 .$$

Note that $(dH/dt)_1$ becomes zero within the whole set f^*, but not only within its local-equilibrium subset.

The term $(dH/dt)_2$ can take both negative and positive values in the general case. We will now define the neighborhood around the point f^*, at which the value $(dH/dt)_2$, is nonpositive.

Let g be some fixed distribution function. It should be determined which f satisfy the following inequality:

$$R(f, g) = \int \ln f \, Q(g, g) \, d^3v \leq 0 . \tag{4.2}$$

We will use a method similar to that discussed in refs. [3,4]. Represent f and g in the form $f = e^\nu$, $g = e^\mu$, and consider a positive functional $\theta_{f,g}[\lambda]$, $\lambda \in \mathbb{R}^1$:

$$\theta_{f,g}[\lambda] = \int \varphi \{ \exp[\mu' + \mu_1' + (1 - \lambda) \, \Delta(\nu)]$$

$$+ \exp[\mu + \mu_1 + (\lambda - 1) \, \Delta(\nu)] \} \, d^3v_1' \, d^3v' \, dv_1^3 \, d^3v . \tag{4.3}$$

Here $\varphi = \varphi(v', v_1'|v, v_1)$ is the kernel of the Boltzmann collision integral, $\Delta(\nu) = \nu + \nu_1 - \nu' - \nu_1'$; the standard notations for variables before and after a collision are used. The kernel φ is supposed to satisfy the detail balancing law.

Since $d\theta_{f,g}[\lambda]/d\lambda|_{\lambda=1} = -\frac{1}{4}R(f, g)$, the inequality (4.2) is equivalent to

$$\frac{\mathrm{d}\theta_{f,g}[\lambda]}{\mathrm{d}\lambda}\bigg|_{\lambda=1} \geq 0 \ . \tag{4.4}$$

Since $\mathrm{d}^2\theta/\mathrm{d}\lambda^2 \geq 0$ for any λ, the functional (4.3) is the convex function of λ for any pair f and g. Moreover, the derivative (4.4) is equal to zero only in the case when $\Delta(\nu) = 0$. In this latter case $\theta_{f,g}$ does not depend on λ.

Due to the convexity of $\theta_{f,g}[\lambda]$, to satisfy the inequality (4.4) it is sufficient that such value $\lambda < 1$ should exist for which

$$\theta_{f,g}[\lambda] \leq \theta_{f,g}[1] \ . \tag{4.5}$$

If $f = g$ (the Boltzmann H-theorem) then the function $\theta_{g,g}[\lambda]$ is symmetric for the point $\lambda = \frac{1}{2}$: for any $\alpha \in \mathbb{R}^1$

$$\theta_{g,g}[\tfrac{1}{2} + \alpha] = \theta_{g,g}[\tfrac{1}{2} - \alpha] \ .$$

Therefore $\theta_{g,g}[1/2]$ is the minimum value of $\theta_{g,g}[\lambda]$ and if g is not a local-equilibrium distribution, then the following strict inequality is valid for $0 < \lambda < 1$:

$$\theta_{g,g}[\lambda] < \theta_{g,g}[1] \ , \qquad 0 < \lambda < 1 \ . \tag{4.6}$$

Hence, choosing an arbitrary value λ in (4.5), where $0 < \lambda < 1$, we obtain the constraint which prescribes the neighborhood of the point g; inside this neighborhood (4.2) is valid. In particular, taking $\lambda = \frac{1}{2}$, we obtain

$$\int \varphi \exp[\mu + \mu_1 - \tfrac{1}{2}\Delta(\nu)]\, \mathrm{d}^3 v_1'\, \mathrm{d}^3 v'\, \mathrm{d}^3 v_1\, \mathrm{d}^3 v$$

$$\leq \int \varphi \exp(\mu + \mu_1)\, \mathrm{d}^3 v_1'\, \mathrm{d}^3 v'\, \mathrm{d}^3 v_1\, \mathrm{d}^3 v \ . \tag{4.7}$$

The inequality (4.7) is strict for $\mu = \nu$, if $\Delta(\mu) \neq 0$.

We represent ν in the form of $\mu + \delta\nu$ and expand (4.7), up to the $\delta\nu$ square terms. The linear part becomes equal to zero, and we obtain

$$\int \varphi(gg_1 g'g_1')^{1/2}[\Delta(\delta\nu)]^2\, \mathrm{d}^3 v_1'\, \mathrm{d}^3 v'\, \mathrm{d}^3 v_1\, \mathrm{d}^3 v \leq 8 d_\varphi(g) \ ,$$

$$d_\varphi(g) = \int \varphi(gg_1)^{1/2}[(gg_1)^{1/2} - (g'g_1')^{1/2}]\, \mathrm{d}^3 v_1'\, \mathrm{d}^3 v'\, \mathrm{d}^3 v_1\, \mathrm{d}^3 v \ . \tag{4.8}$$

The case when g is the local-equilibrium g_0 is singular: $d_\varphi(g_0) = 0$. Then the expression $(dH/dt)_2$ is identical to zero.

Thus, for the quasi-equilibrium model kinetic equations (3.3) the local H-theorem is set: the derivative $(dH/dt)_1$ is nonpositive for any f, and the neighborhood $U(f^*(f))$ exists for the point $f^*(f)$, inside which the derivative $(dH/dt)_2$ is nonpositive. Since $(dH/dt)_2 = 0$ for $f^* = f_0$ only, dH/dt (4.1) becomes equal to zero at local-equilibrium distributions only.

Remark 1. The neighborhood $U(f^*(f))$ of the distribution $f^*(f)$ consists of those distributions f which could be involved into the macroscopic description. The conjunction of the neighborhoods $U(f^*(f))$ for all $f^*(f)$ yields the neighborhood $\{U(f^*(f))\}$ of the manifold $\{f^*(f)\}$. The neighborhood $\{U(f^*(f))\}$ represents the set inside which equations of slow processes (3.4) are applicable.

Remark 2. For $f^* = f_0$ the local H-theorem becomes global: $dH/dt \leq 0$ for any f and τ. If $f^* \neq f_0$, then the relaxation to the state f^* should be rapid enough to satisfy the inequality $dH/dt \leq 0$ for any f. It is sufficient that the inequality $|(dH/dt)_1| > |(dH/dt)_2|$ remains true outside of the neighborhood $U(f^*(f))$.

5. Examples

In this section we represent some examples of quasi-equilibrium models (3.3).

5.1. Example 1: moment hydrodynamics

In this example we consider the manifold which consists of the moment quasi-equilibrium distributions. These distributions are parameterized by the values of moment functionals $M_i(f) = \int m_i(v) f \, d^3v$, where $m_i(v)$ is a polynomial. We denote $M(f)$ as the set of k chosen moment functionals $M_i(f)$: $M(f) = \{M_1(f), \ldots, M_k(f)\}$. We assume that the hydrodynamics parameters (density, flux-velocity vector, and temperature) are included into the set $M(f)$.

The quasi-equilibrium distribution $f^*(f) = f^*(M(f))$ is the solution of the problem (2.4),

$$H[f] \to \min \quad \text{for} \int m_i(v) f \, d^3v = M_i, \quad i = 1, \ldots, k . \tag{5.1}$$

The function $f^*(f) = f^*(M(f))$ obtained depends parametrically on M, which, in turn, is connected with f by the integral relationships (5.1).

Eqs. (3.4) take the form

$$\frac{\partial M_i(f)}{\partial t} + \text{div } j_{M_i}(f) = D_{M_i}(f) \,,$$

$$M_i(f) = \int m_i(v) f \, d^3v \,, \qquad j_{M_i}(f) = \int m_i(v) vf \, d^3v \,,$$

$$D_{M_i}(f) = \int m_i(v) \, Q(f^*(M(f)), f^*(M(f))) \, d^3v \,. \tag{5.2}$$

According to the remark 5 in section 3, the set (5.2) is the direct generalization of the Grad moment equations (see also ref. [2]).

For the decamoment approximation, the set $M(f)$ includes density, the flux-velocity vector, and the tension tensor. The distribution f^* is calculated in ref. [2]:

$$f^* = \frac{n}{(2\pi)^{3/2}} \left(\frac{\rho^3}{\det P_{ij}}\right)^{1/2}$$

$$\times \exp\left(-\frac{\rho}{2} \sum_{i=1}^{3} \sum_{j=1}^{3} (P^{-1})_{ij}(v_i - u_i)(v_j - u_j)\right) . \tag{5.3}$$

Here P_{ij} is the tension tensor.

Remark. The distribution (5.3) is similar to the function $\tilde{f}(f)$ in the ES-model (1.2). This similarity is not only external. Indeed, according to section 2, the hyperplanes of rapid motions for the manifold (1.2) are parallel to those for the manifold (5.3). These manifolds differ only by coordinate systems on the manifolds. Thus, the consideration of sections 3 and 4 solves the old problem of the validity of the H-theorem for the ES-model.

Now we will represent the explicit form of equations (3.3) and (5.2) for the linearized version of the quasi-equilibrium decamoment distributions (5.3). Representing P_{ij} as $P_{ij} = P \delta_{ij} + \sigma_{ij}$, where P is the scalar pressure, Sp $\sigma_{ij} = 0$, and, expanding the exponent into the powers of σ_{ij} up to linear terms, one yields

$$f^* = f_0^*\left(1 + (2k_{\text{B}}PT)^{-1} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij}[(v_i - u_i)(v_j - u_j) - \tfrac{1}{3}\delta_{ij}(v - u)^2]\right). \tag{5.4}$$

Here f_0^* is the local-equilibrium distribution. The distribution (5.4) coincides with the Grad decamoment distribution (see also remark 5 in section 3).

The model extension (3.3) for the approximation (5.4) yields

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i} = -\tau^{-1}[f - f^*(f)] - (2k_{\mathrm{B}}PT)^{-1} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij} L_{ij} ,$$

$$L_{ij} = \int \varphi f_0^* f_{01}^* \Delta[(v_i - u_i)(v_j - u_j) - \tfrac{1}{3}\delta_{ij}(v-u)^2] \, \mathrm{d}^3 v' \, \mathrm{d}^3 v_1' \, \mathrm{d}^3 v_1 . \qquad (5.5)$$

Here we have used notations of section 4. Functions L_{ij} are well investigated in ref. [7] for a wide class of kernels φ. The parameters of the function $f^*(f)$ (5.4) in (5.5) are

$$\rho(f) = m \int f \, \mathrm{d}^3 v , \qquad \rho(f) u_i(f) = m \int v_i f \, \mathrm{d}^3 v ,$$

$$3P(f) = m \int [v - u(f)]^2 f \, \mathrm{d}^3 v ,$$

$$\sigma_{ij}(f) = m \int \{[v_i - u_i(f)][v_j - u_j(f)] - \tfrac{1}{3}\delta_{ij}[v - u(f)]^2\} f \, \mathrm{d}^3 v . \qquad (5.6)$$

Eqs. (5.2) in the situation under consideration coincide with the Grad decamoment system [6]:

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} \frac{\partial(u_i \rho)}{\partial x_i} = 0 ,$$

$$\frac{\partial u_k}{\partial t} + \sum_{i=1}^{3} u_i \frac{\partial u_k}{\partial x_i} + \rho^{-1}\left(\frac{\partial P}{\partial x_k} + \sum_{i=1}^{3} \frac{\partial \sigma_{ik}}{\partial x_i}\right) = 0 ,$$

$$\frac{3}{2}\left(\frac{\partial P}{\partial t} + \sum_{i=1}^{3} u_i \frac{\partial P}{\partial x_i}\right) + \tfrac{5}{2} P \sum_{i=1}^{3} \frac{\partial u_i}{\partial x_i} + \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij} \frac{\partial u_i}{\partial x_j} = 0 ,$$

$$\frac{\partial \sigma_{ik}}{\partial t} + \sum_{s=1}^{3} \frac{\partial(u_s \sigma_{ik})}{\partial x_s} + P\left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} - \frac{2}{3}\delta_{ik} \sum_{s=1}^{3} \frac{\partial u_s}{\partial x_s}\right)$$

$$+ \sum_{s=1}^{3} \left(\sigma_{is} \frac{\partial u_k}{\partial x_s} + \sigma_{ks} \frac{\partial u_i}{\partial x_s} - \frac{2}{3}\delta_{ij}k \sum_{l=1}^{3} \sigma_{ls} \frac{\partial u_l}{\partial x_s}\right) + \mu_\varphi^{-1} P\sigma_{ik} = 0 . \qquad (5.7)$$

Here and in eq. (5.5) parameters are understood as the functionals (5.6), and μ_φ represents the viscosity coefficient in the first approximation of the Chapman–Enskog method.

Eqs. (5.5) and (5.7) combined with (5.6) create the model extension of the Grad decamoment description. They are suitable when the Grad description becomes insufficient. One can also use the model for the functions (5.3). This model is more perfect in comparison with its linearized version (5.5) but it is also more complicated.

Eqs. (5.5) and (5.7) become even more simple if we consider the neigh-

borhood of the equilibrium distribution F^0. Then we can use the representation $f = F^0(1 + \delta)$, where δ is a small deviation. Linearization of (5.5) yields

$$
\begin{aligned}
\frac{\partial \delta}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial \delta}{\partial x_i} = & -\tau^{-1}\left(\delta - \sum_{\alpha=0}^{4} m_\alpha(v)\, (m_\alpha; \delta)\right) \\
& - \tau^{-1}(2k_B P_0 T_0)^{-1} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij}(\delta) \\
& \times [(v_i - u_{0i})(v_j - u_{0j}) - \tfrac{1}{3}\delta_{ij}(v - u_0)^2] \\
& - (2k_B P_0 T_0)^{-1} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij}(\delta) L_{ij} ,
\end{aligned}
$$

$$
L_{ij} = \int \varphi F_1^0 \Delta[(v_i - u_{0i})(v_j - u_{0j}) - \tfrac{1}{3}\delta_{ij}(v - u_0)^2]\, \mathrm{d}^3 v'\, \mathrm{d}^3 v_1'\, \mathrm{d}^3 v_1 . \tag{5.5a}
$$

Here the subindex zero indicates equilibrium values, and brackets denote the scalar product $(\varphi; \psi) = \int F^0 \varphi \psi\, \mathrm{d}^3 v$. Summational invariants m_α are normalized as $(m_\alpha; m_\beta) = \delta_{\alpha\beta}$.

The first term in the right hand side of (5.5a) coincides with the linearized BGK-model. The expression of $\sigma_{ij}(\delta)$ is

$$
\sigma_{ij}(\delta) = m(\delta; (v_i - u_{0i})(v_j - u_{0j}) - \tfrac{1}{3}\delta_{ij}(v - u_0)^2) .
$$

This expression and expressions for $\rho(\delta)$, $u(\delta)$ and $P(\delta)$ together with the linearized version of eqs. (5.7) close eq. (5.5a).

Lastly, we evaluate $d_\varphi(f^*)$ (4.8) for f^* (5.4),

$$
d_\varphi(f^*) \approx (\mu_\varphi k_B T)^{-1} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij}\sigma_{ij} . \tag{5.8}
$$

The estimation of the left hand side of (4.8) depends essentially on φ. For the Maxwell molecules, supposing $g \approx f_0$, we obtain

$$
\sum_{(i)} |\lambda_{(i)}| a_{(i)}^2 \leqslant 4(\mu_M n P)^{-1} \sum_{i=1}^{3} \sum_{j=1}^{3} \sigma_{ij}\sigma_{ij} . \tag{5.9}
$$

Here $a_{(i)}$ represents the coefficients in expansion of δv into Hermits nonreducible tensor polynomials $H_{(i)}$, where (i) is the tensor multi-index, and $\lambda_{(i)}$ is the eigenvalue of linearized collision integral for the Maxwell molecules corresponding to the eigenfunction $H_{(i)}$ [1].

5.2. Example 2: the shock wave problem

Now we will consider the manifold which consists of the functions $f(a_-, a_+)$ (2.7) with the thermodynamic parameterization (2.9).

The functions $f_{\mp}$ are

$$f_{\mp} = n_{\mp} \varphi_{\mp} , \qquad \varphi_{\mp} = \left(\frac{2\pi k_B T_{\mp}}{m} \right)^{-3/2} \exp\left(-\frac{m(v - u_{\mp} i)^2}{2 k_B T_{\mp}} \right) .$$

Here i is the unit vector along the direction of the wave propagation, the rest of notations are standard.

We start with obtaining the functions $a_-(f)$ and $a_+(f)$. Exact equations which we should solve with respect to $a_{\mp}$ are

$$\int [f - f(a_-, a_+)] \ln f(a_-, a_+) \, d^3v = 0 ,$$

$$\int [f - f(a_-, a_+)] \, d^3v = 0 . \tag{5.10}$$

However, eqs. (5.10) are too complicated for direct solving. Therefore, we use the method of successive approximations (2.10) and (2.11).

According to (2.10), the zeroth approximation $a_{\mp}^{(0)}(f)$ is obtained from the equations

$$\int (f - a_-^{(0)} f_- - a_+^{(0)} f_+) \ln f \, d^3v = 0 ,$$

$$\int (f - a_-^{(0)} f_- - a_+^{(0)} f_+) \, d^3v = 0 . \tag{5.11}$$

The solution of (5.11) is easily found:

$$a_{\mp}^{(0)}(f) = \frac{\pm \int f \ln f \, d^3v \mp \langle \ln f \rangle_{\pm} \int f \, d^3v}{n_{\mp}(\langle \ln f \rangle_- - \langle \ln f \rangle_+)} . \tag{5.12}$$

The brackets $\langle \cdots \rangle_{\pm}$ mean averaging: $\langle \cdots \rangle_{\pm} = \int \cdots \varphi_{\pm} \, d^3v$.

The expression (5.12) determines the zeroth approximation of the function $f^*(a_-, a_+)$,

$$f_0^*(a_-(f), a_+(f)) = a_-^{(0)}(f) \, f_- + a_+^{(0)}(f) \, f_+ . \tag{5.13}$$

Next approximations $f_k^* = a_-^{(k)}(f) \, f_- + a_+^{(k)}(f) \, f_+$ are obtained according to (2.11) from the recurrent linear equations

$$\int (f - a_-^{(k)} f_- - a_+^{(k)} f_+) \ln f_{k-1}^* \, \mathrm{d}^3 v = 0 \, ,$$

$$\int (f - a_-^{(k)} f_- - a_+^{(k)} f_+) \, \mathrm{d}^3 v = 0 \, . \qquad (5.14)$$

The expression (5.12) contains the terms which are nonlinear with respect to the distribution f. Simplification occurs if we consider the "thin" neighborhood of the manifold. Then we represent the function f as

$$f = a_- f_- + a_+ f_+ + \Delta \qquad (5.15)$$

and suppose Δ to be small in some suitable sense. Within the accuracy of first-order terms we can write

$$a_-^{(k)}(f) = a_- + \delta a_-^{(k)}(a_-, a_+; \Delta) \, ,$$
$$a_+^{(k)}(f) = a_+ + \delta a_+^{(k)}(a_-, a_+; \Delta) \, . \qquad (5.16)$$

Here $\delta a_\pm^{(k)}(a_-, a_+; \Delta)$ are linear functionals with respect to Δ. The zeroth-order value in (5.16) yields

$$\delta a_\mp^{(0)} = \frac{\pm \int \Delta \ln(a_- f_- + a_+ f_+) \, \mathrm{d}^3 v \mp \langle \ln(a_- f_- + a_+ f_+) \rangle_\pm \int \Delta \, \mathrm{d}^3 v}{n_\mp [\langle \ln(a_- f_- + a_+ f_+) \rangle_- - \langle \ln(a_- f_- + a_+ f_+) \rangle_+]} \, . \qquad (5.17)$$

Easy calculations show that the zeroth approximation (5.17) gives the complete contribution within the accuracy of Δ, i.e. within this accuracy we have for all k

$$\delta a_\pm^{(k)}(a_-, a_+; \Delta) = \delta a_\mp^{(0)}(a_-, a_+; \Delta) \, .$$

Therefore, we can justify that the recurrent process (5.14) converges at least if f is close enough to the manifold $\{f(a_-, a_+)\}$. One can easily check that the function (5.13) with parameters (5.16) and (5.17) satisfies eq. (5.10) within the accuracy of Δ.

The quasi-equilibrium model which corresponds to the approximation (5.12) and (5.13) is

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial f}{\partial x_i} = -\tau^{-1}[f - a_-^{(0)}(f) f_- - a_+^{(0)}(f) f_+]$$
$$+ a_-^{(0)}(f) a_+^{(0)}(f) [Q(f_-, f_+) + Q(f_+, f_-)] \, . \qquad (5.18)$$

Here $a_-^{(0)}(f)$ and $a_+^{(0)}(f)$ are defined by the formula (5.13). The equations of

slow processes (3.4) are obtained from eqs. (2.8) by substituting the functions $a^{(0)}_-(f)$ and $a^{(0)}_+(f)$ (5.13).

The linearization (5.15), (5.16) and (5.17) yields instead of (5.18)

$$
f_-\left(\frac{\partial a_-}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial a_-}{\partial x_i}\right) + f_+\left(\frac{\partial a_+}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial a_+}{\partial x_i}\right) + \frac{\partial \Delta}{\partial t} + \sum_{i=1}^{3} v_i \frac{\partial \Delta}{\partial x_i}
$$
$$
= -\tau^{-1}[\Delta - \delta a^{(0)}_-(a_-, a_+; \Delta) f_- - \delta a^{(0)}_+(a_-, a_+; \Delta) f_+]
$$
$$
+ a_- a_+[Q(f_-, f_+) + Q(f_+, f_-)] + a_+ \delta a^{(0)}_-(a_-, a_+; \Delta) Q(f_-, f_+)
$$
$$
+ a_- \delta a^{(0)}_+(a_-, a_+; \Delta) Q(f_+, f_-) . \tag{5.19}
$$

Eq. (5.19) is linear with respect to the function Δ and therefore it is simpler than eq. (5.18). The closed set of equations with respect to the unknowns a_-, a_+ and Δ would be obtained when we will insert the functions $a_\mp(\Delta) = a_\mp + \delta a^{(0)}_\mp(a_-, a_+; \Delta)$ into eqs. (2.8) and expand these latter up to the linear terms. This procedure is quite simple and therefore the result is not presented here.

Lastly, we indicate that a significant simplification of the model occurs if we consider the small neighborhood of the equilibrium state (i.e. when we use the representation $f = F^0(1 + \delta)$, see the previous example).

The models (5.18) and (5.19) are suitable for investigation of the shock wave.

6. Conclusions

(1) The method of constructing the projector $M^*_{f(a)}(f)$ introduced in section 2 solves the problem of thermodynamic parameterization. The condition of the entropy growth during the rapid relaxation immediately results in the entropy balance equation for the slow process. One can prove that there is no other universal way to construct a thermodynamic parameterization of an arbitrary manifold. In particular, the parameterization (2.8) and eq. (2.7) solve the classical problem of ambiguousness of the Tamm–Mott–Smith approximation (see also ref. [8]). The recurrent process (2.10) and (2.11) gives the efficient method for explicitly constructing the planes of rapid motions.

(2) Quasi-equilibrium kinetic models of section 3 provide an extension of the arbitrary approximation. Their construction is based on the decomposition of motions in the neighborhood of the chosen approximation. The model collision integral (3.3) consists of two terms. The first of these terms describes the model rapid relaxation to the approximation $\{f(a)\}$ along the planes of rapid motions. The second term describes the slow motion in the neighborhood of $\{f(a)\}$. Both of these processes are described self-consistently.

(3) Due to the construction of the functionals $M^*_{f(a)}(f)$, the entropy increases in the model rapid process for any deviation from the slow manifold. On the contrary, the slow motion does not contradict the H-theorem only in the neighborhood of the slow manifold. The H-theorem of section 4 gives a constructive approach to evaluate this neighborhood.

(4) Examples considered in section 5 may be used for analytical and numerical investigations in various problems (e.g., sound propagation, shock waves, etc.; for more purposes of model equations see ref. [1]). Especially the linearized versions are probably most applicable. The problem of the validity of the H-theorem for the ES-model is solved.

(5) Although the model approach to the problems of kinetic theory is widespread in modern investigations, it cannot be considered as the most consequent. Other approaches to the problem of constructing a dynamic invariant reduced description can be found in refs. [9–14].

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