METHOD OF INVARIANT MANIFOLDS AND REGULARIZATION OF ACOUSTIC SPECTRA

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ABSTRACT

A new approach to the problem of reduced description for Boltzmann-type systems is developed. It involves a direct solution of two main problems: thermodynamicity dynamic invariance of reduced description. and Α universal construction is introduced, which gives а thermodynamic parameterization of an almost arbitrary approximation. Newton-type procedures of successive are developed which correct approximations dvnamic noninvariance. The method is applied to obtain corrections to the local Maxwell manifold using parametrics expansions instead of Taylor series into powers of Knudsen number. In particular, high the frequency acoustic spectra is obtained.

1. INTRODUCTION

In this paper we introduce a new method of successive approximations for solving the problem of reduced description for Boltzmann-type kinetic equations. The method is concordant with the *H*-theorem

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at each iteration. It is based on rapidly converging procedures of the Newton type. The method is free of any essential restrictions upon the choice of the initial approximation. In its basis it does not require any small parameters.

The method to be developed will be applicable to any dissipative system with a global convex Lyapunov function (e.g. the Boltzmann equation provided with suitable boundary conditions, chemical kinetic equations for closed systems, the Fokker-Planck equation, etc).

In this section we give a short survey of some difficulties of classical methods of the Boltzmann equation theory.

The main difficulty of the Chapman-Enskog method [1] are "nonphysical" properties of high-order approximations. This was stated by a number of authors and was discussed in detail in [2]. In particular, as it was noted in [3], the Burnett approximation results in a short-wave instability of the acoustic spectra. This fact contradicts the *H*-theorem (cf. in [3]).

The Hilbert expansion contains secular terms [2]. The latter contradicts the *H*-theorem. However, we are not sure this question was discussed in detail.

The other difficulties of both of these methods are: the restriction upon the choice of initial approximation (the local equilibrium approximation), the demand for a small parameter, and the usage of slowly converging Taylor expansions. These difficulties never allow a direct transfer of these methods on essentially nonequilibrium situations.

The main difficulty of the Grad method [4] is the uncontrollability of the chosen approximation. An extension of the list of moments can result in a certain success, but it can also give nothing. Difficulties of moment expansions in the problems of shock waves and

sound propagation can be seen in [2].

Many attempts were made to make these methods more . . perfect. For the Chapman-Enskog and Hilbert methods these attempts are based in general on some " good " rearrangement of expansions (e.g. neglecting high-order derivatives [2], reexpanding [2], Pade approximations and partial summing [5-7], etc.). This type of work with formal series is wide spread in physics. Sometimes the results are surprisingly good - from the renormalization theory in quantum fields to the Percus-Yevick equation and the ring-operator in statistical mechanics. However, one should realize that a success is not at a11 guaranteed. Moreover, rearrangements never remove the restriction upon the choice of the initial local equilibrium approximation.

Attempts to improve the Grad method are based on quasi-equilibrium approximations [8, 9]. It was found in [10] that Grad distributions are linearized versions of appropriate quasi-equilibrium approximations. A method which treats fluxes (e.g. moments with respect to collision integrals) as independent variables in а quasi-equilibrium description introduced in was [7, 11, 12].

An important feature of quasi-equilibrium approximations is that they are always thermodynamic, i.e. they with the *H*-theorem are concordant due to their construction. This question was discussed in detail in [13, 14]. However, quasi-equilibrium approximations do not remove the uncontrollability of the Grad method. Quasi-equilibrium approximations were criticized in [15]. This criticism holds also for the Grad method.

Finishing this short survey of classical methods, we pay attention to the fact that there exist some approximations which are assumed ad hoc, and which are

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not inserted into any successive procedure. The most famous of these approximations is the Tamm-Mott-Smith approximation in the shock wave problem [2].

τt. is convenient to formulate the problem of reduced description in a uniform way (a more precise formulation will be given in Section 2.1). Let an approximated reduced description is chosen. This means that a manifold (a "surface") is fixed in the space of distributions. Here we arrive at two general problems: 1. Thermodynamicity. We must define macroscopic dynamics on the manifold. In order to do this, we must project the Boltzmann equation onto some macroscopic parameters. The first problem is: how and onto which macroscopic parameters should one perform this projection? Which projector would make physical sense and will preserve thermodynamicity (the concordance with the the H-theorem) at the chosen macroscopic level?

Dynamic invariance. We understand that the chosen 2. manifold is not a dynamic invariant manifold of the equation. The notion "dynamic Boltzmann invariant appears in manifold" most of dynamic theories: а manifold is called dynamic invariant if the vector field of the dynamic system is tangent to this manifold in every point. Hence, we are willing to improve the chosen manifold in order to make it "more invariant". The second problem is: how to obtain these corrections in a general case (e.g. when there are no small parameters or other simplifications)? We hope that the solution of the problem would be method of second а successive approximations which would not require a too strong restriction upon the choice of the initial manifold.

The general problem of classical methods is that none of them gives a successive removal of dynamic noninvariance of reduced description with preservation of its thermodynamicity. The Grad method and its

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generalizations give thermodynamic approximations. if one takes the Grad distribution However. as an initial condition for the Boltzmann equation at the time t=0, then for t>0 the trajectory of the kinetic equation "takes off" from the initial manifold. One can neither obtain the corrections caused by this "take off", nor evaluate them. On the other even hand. the Chapman-Enskog and the Hilbert methods do not guarantee thermodynamicity. The question about the correction of noninvariance is also unclear for them.

In classical mechanics the problem of invariant manifolds was developed essentially by the famous Kolmogorov-Arnold-Moser theory (KAM) [16-18]. Two points of KAM methods are of prime importance: i) to construct directly an invariant manifold rather than a solution, and, ii) to use rapidly converging Newton method instead of Taylor expansions for this constructing.

we understand the problem of reduction for the of Boltzmann equation as a problem constructing а dynamic invariant manifold from given initial а manifold.

However, a direct application of the KAM methods faces many problems. The most essential of these problems is that at every iteration we should obtain approximations which are concordant with the H-theorem (the problem of thermodynamicity). If not, then the practical sense of these approximations is unclear.

In this paper we show how to solve this and some other problems and how to reduce the problem of reduction to solving linear problems. These linear problems are of one type in their essence.

In Section 2 we introduce a general method for constructing dynamic invariant manifolds for dissipative systems with a global convex Lyapunov function. In Section 3 we develop this method for the Boltzmann

equation. Section 3 serves for an intermediate between the general theory of Section 2 and Section 4 where we apply it to the problem of derivation of hydrodynamics from the Boltzmann equation. In Section 4 we apply the technique of pseudodifferential and Fourier integral operators to solve the equation of the first Newton-type iteration. In particular. ₩e consider а simple application of the method to the problem of acoustic spectra. As it was mentioned above, the short-wave instability is a typical problem of the Chapman-Enskog expansion. Usual methods of removing this phenomenon always require some ad hoc assumptions on the character of the improvement. All these methods are of a recipe character. A more general basis is required for making the regularization free of arbitrary assumptions. The method of invariant manifolds yields the improvement without any a priori assumption. Results are compared with the Burnett approximation and with a method of partial summing [5-7].

2. THE CONSTRUCTING OF DYNAMIC INVARIANT MANIFOLDS FOR DISSIPATIVE SYSTEMS

In this section we introduce a formal general scheme for constructing dynamic invariant manifolds for an abstract dissipative system. Basic notions we use are not rigorous in mathematical sense but they are sufficiently clear to understand the procedure, and to deal with its particular and more rigorous realizations.

2.1 Dynamic Invariance and Thermodynamicity

We denote as F a convex domain in a linear space E, and consider an equation in F:

$$\mathrm{d}f/\mathrm{d}t = J(f) \tag{2.1}$$

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Here $f \in F$, t is the time, and J(f) is the vector field (a smooth mapping $F \rightarrow E$: $f \mapsto J(f)$). Further, we call F the **phase space** of system (2.1). We assume that the domain Fis *positively invariant* with respect to equation (2.1): if f_t is a solution of eq. (2.1) and $f_0 \in F$, then $f_t \in F$ for all $t \ge 0$.

Equation (2.1) will be called the **dissipative** system, if a strictly convex functional H(f) is defined in *F*, for which the following inequality is valid:

$$dH(f)/dt \equiv D_f H(f) \cdot J(f) \leq 0$$
(2.2)

Here $D_f H(f)$ is the linear functional (the differential of the functional H(f) in the point f).

Denote as A a domain in a linear space B, and consider a smooth *immersion* $A \rightarrow F$: $a \mapsto f(a)$, where $a \in A$, and $f(a) \in F$. The set of points f(a), where a runs the domain A, will be called the **manifold with internal coordinates** a (or the **manifold** for short). The manifold will be denoted as $\{f(a)\}$ if we want to stress the coordinate dependence, or as \mathfrak{M} if we are not interested in this dependence. The elements of the manifold will be denoted either as f(a) or as $f_{\mathfrak{M}}$.

Thus, we can say that the immersion $a \mapsto f(a)$ equips the manifold \mathfrak{M} with the coordinate system. The coordinates *a* identify the points on the manifold.

For a given manifold \mathfrak{M} , we denote as $T_{f_{\mathfrak{M}}}$ the linear **tangent space** to \mathfrak{M} at the point $f_{\mathfrak{M}} \in \mathfrak{M}$. We always can identify $T_{f_{\mathfrak{M}}}$ with some linear subspace of the space E. Further, we will make no distinction between these two objects. The tangent space $T_{f(a)}$ is constructively defined as the image of the linear operator $D_a f(a)$, the latter is the differential of the immersion $A \rightarrow F$ at the point f(a). For the finite-dimensional case (i.e. when A is the domain in the finite-dimensional space B), the tangent space $T_{f(a)}$ is defined as the linear envelope of partial differentials $D_{a_i} f(a_1, \ldots, a_n)$, where $i=1, \ldots, n$, and $n=\dim B$.

Let the manifold \mathfrak{M} is given. The problem which always arises in applications is: how to determine the dynamics induced with the vector field J(f) on the manifold \mathfrak{M} ? In the Boltzmann equation (BE) theory, this problem appears when one deals with a manifold of distributions, and which approximates a solution of BE.

For example, the Tamm-Mott-Smith (TMS) approximation gives us the manifold $\{f(a_{-}, a_{+})\}$ which consists of distributions

$$f(a_{-}, a_{+}) = a_{-}f_{-} + a_{+}f_{+}$$
(2.3)

Here a_{\pm} and a_{\pm} (the coordinates on the manifold $\mathfrak{M}_{\mathrm{TMS}} = \{f(a_{\pm}, a_{\pm})\}$) are non-negative real functions of the position vector \vec{x} , and f_{\pm} and f_{\pm} are fixed Maxwellians. The problem of induced dynamics for $\mathfrak{M}_{\mathrm{TMS}}$ is as follows: considering a_{\pm} and a_{\pm} as values of the functions $a_{\pm}(\vec{x}, t)$ and $a_{\pm}(\vec{x}, t)$, to obtain dynamic equations for these functions induced with BE.

Next example is the manifold $\{f(n, \vec{u}, T)\}$ which consists of local Maxwellians (LM):

$$f(n, \vec{u}, T) = n \left(\frac{2\pi k_{\rm B}T}{m} \right)^{-3/2} \exp \left\{ -\frac{m(\vec{v} - \vec{u})^2}{2k_{\rm B}T} \right\}$$
(2.4)

The coordinates n, \vec{u} , and T are functions of \vec{x} . The problem of induced dynamics for the LM manifold \mathfrak{M}_{LM} is the same as for \mathfrak{M}_{TMS} : considering n, \vec{u} , and T as the values of the functions $n(\vec{x}, t)$, $\vec{u}(\vec{x}, t)$, and $T(\vec{x}, t)$, to obtain dynamic equations for these functions from BE.

<u>Remark</u>. When speaking about manifolds for BE, we usually deal with distributions which are labeled with a finite number of parameters for every spatial position vector \vec{x} . Distributions (2.3) and (2.4) illustrate this situation. Further, when speaking about such

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locally finite-dimensional manifolds, we will omit the term "local" (see remark (i) in Section 3).

The problem of induced dynamics is to construct vectors in the tangent spaces T_{f_m} induced with vectors $J(f_m)$ for every $f_m \in \mathbb{R}$. More precisely, for every $f_m \in \mathbb{R}$, we have to introduce a projector $P_{f_m}: E \to T_{f_m}$ which projects the vector $J(f_m)$ into the tangent space T_{f_m} :

$$P_{f_{\mathfrak{m}}}(J(f_{\mathfrak{m}})) \in T_{f_{\mathfrak{m}}}$$
(2.5)

The result of these projections for all $f_m \in \mathfrak{M}$ will give us a vector field of induced dynamics, and thus it will define the time evolution induced inside the manifold M. We may expect that the projectors P_{f_m} might be different for different points $f_m \in \mathfrak{M}$. Because of the immersion $A \rightarrow F$, we can identify the induced vector field in the tangent spaces with a certain vector field in the space Β. thus we can obtain the equation for and the coordinates a.

It should be stressed that the problem of induced dynamics itself is not a mathematical problem: one can any projector (2.5). Even monsters, choose such as $P_{f_{\mathfrak{m}}}(J(f_{\mathfrak{m}}))=0$ for all $f_{\mathfrak{m}}\in\mathfrak{M}$, do not contradict the mathematical viewpoint while they are absolutely senseless for solving a physical problem. On the other hand, the ambiguousness of the choice of P_{f_m} makes us to search for additional requirements upon the induced dynamics.

The only case, when no problems arise with the induced dynamics, occurs when the vectors $J(f_m)$ belong to the tangent spaces T_{f_m} for all $f_m \in \mathbb{R}$. The manifold \mathfrak{M} with this property will be called **the dynamic invariant** manifold of equation (2.1):

$$J(f_{\mathfrak{m}}) \in T_{f_{\mathfrak{m}}}$$
 for all $f_{\mathfrak{m}} \in \mathfrak{M}$ (2.6)

However, in the majority of cases, one deals with manifolds which lack the property of dynamic invariance (2.6). In applications, one usually solves the problem of induced dynamics by introducing the projectors $P_{f_{m}}$ based on a tradition and (or) physical motivation. For example, in the case of LM manifold, one usually defines the projector $P_{f_{m}}$ as: $f(n, \vec{u}, T)$

$$P_{f(n, \vec{u}, T)}(J) = f(n, \vec{u}, T) \left\{ \frac{1}{n^{1/2}} \lambda_0(J) + \frac{1$$

$$+\frac{m}{(2k_{\rm B}nT)^{1/2}}\sum_{i=1}^{3}(v_{i}-u_{i})\lambda_{i}(J)+\frac{1}{n^{1/2}}\left[\frac{m(v-u_{i})^{2}}{2k_{\rm B}T}-\frac{3}{2}\right]\lambda_{4}(J)\bigg\};$$

$$\lambda_{0}(J) = \frac{1}{n^{1/2}} \int 1 \cdot J d^{3}v; \quad \lambda_{\vec{i}}(J) = \frac{m}{(2k_{B}nT)^{1/2}} \int (v_{\vec{i}} - u_{\vec{i}}) J d^{3}v, \quad \vec{i} = 1, 2, 3$$
$$\lambda_{4}(J) = \frac{1}{n^{1/2}} \int \left(\frac{m(\vec{v} - \vec{u})^{2}}{2k_{B}T} - \frac{3}{2}\right) J d^{3}v \qquad (2.7)$$

For the TMS manifold, different types of projectors $P_{f(a_{-}, a_{+})}$ were considered in [2, 19, 20], and the choice of projector is the subject of an old discussion [2].

The example of LM manifold is remarkable: one can interpret the coordinates as the values of linear operators

$$M_{0}(f) = \int 1 \cdot J d^{3}v; \qquad M_{i}(f) = \frac{1}{n} \int v_{i} J d^{3}v; \qquad M_{4}(f) = \frac{m}{3k_{B}n} \int (\vec{v} - \vec{u})^{2} J d^{3}v.$$

The latter are defined in a neighborhood of $\mathfrak{M}_{\mathrm{LM}}$, and projector P is generated with the differentials f(n, u, T)of these operators. The values of operators $M_k(f)$, $k=0,\ldots,4$, are naturally interpreted as macroscopic parameters (i.e. the density, the flow velocity, and the temperature). This example brings us to a general way of constructing the projector P_{f_m} .

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For a given manifold M, we define the projector $P_{f_{\rm m}}$ in two steps.

<u>Step 1.</u> We introduce a parameterization with macroscopic parameters M for the manifold \mathfrak{M} . Denote as $U_{\mathfrak{M}}$ a neighborhood of the manifold \mathfrak{M} in F: $\mathfrak{M} \subset U_{\mathfrak{M}} \subset F$. Let $M(\cdot)$ be a smooth mapping $M: U_{\mathfrak{M}} \longrightarrow \widetilde{M}$, where \widetilde{M} is a linear space. We assume that $M(\cdot)$ has two properties:

(i)
$$M(U_{\mathfrak{m}}) = M(\mathfrak{M})$$
(2.8a)

i.e. the image of the neighborhood $U_{\rm m}$ coincides with the image of the manifold M, and

(ii) The restriction of $M(\cdot)$ to \mathfrak{M} , $M \mid_{\mathfrak{M}}$, has a smooth reverse mapping $M(\mathfrak{M}) \rightarrow \mathfrak{M}$ which maps M(f) into $f(M) \leq \mathfrak{M}$:

$$M \mapsto f(M) \in \mathfrak{M} \tag{2.8b}$$

The mapping $M(\cdot)$ with these two properties will be called the macroscopic mapping.

In order to stress the parameterization of the manifold \mathfrak{M} with macroscopic parameters M, we write it as $\{f(M)\}$. Note that, due to the properties (i) and (ii), the mapping $M(\cdot)$ gives a (nonlinear) projection of the neighborhood $U_{\mathfrak{M}}$ into \mathfrak{M} according to the rule:

$$U_{\mathfrak{m}} \xrightarrow{\longrightarrow} M(\mathfrak{M}) \xrightarrow{\longrightarrow} \mathfrak{M}$$

$$f \longmapsto M(f) \longmapsto f(M)$$

$$(2.9)$$

<u>Step 2.</u> Given a manifold $\{f(M)\}$, we define the projector $P_{f(M)}$ as

$$P_{f(M)}(J) = D_{M}f(M) \circ D_{f}M(f) \Big|_{f=f(M)} \cdot J$$
 (2.10)

Here $D_M f(M)$ is the differential of the immersion $M(\mathfrak{M}) \rightarrow F$ in the point f(M), and $D_f M(f) \Big|_{f=f(M)}$ is the differential of the mapping M(f) in the point f(M). Obviously, $P_{f(M)}^2(J) = P_{f(M)}(J)$ because f(M(f)) = f if $f \in \mathfrak{M}$. Projector (2.10) gives us the vector field of induced dynamics:

$$P_{f(M)}(J(f(M)))$$
 (2.11)

Operator $P_{f(M)}$ projects the vector J(f(M)) into the tangent space $T_{f(M)}$, the latter being the image of the operator $D_M f(M)$. Definition (2.11) yields the equation of induced dynamics in terms of macroscopic parameters M

$$\frac{\mathrm{d}M}{\mathrm{d}t} = D_f M(f) \Big|_{f=f(M)} \cdot J(f(M))$$
(2.12)

If we have fixed a manifold $\{f(a)\}$ using some immersion $A \rightarrow F$, then the introduction of parameterization with macroscopic parameters M assumes the smooth isomorphism $M(\{f(a)\} \leftrightarrow A$ established with the relation $a \mapsto M(f(a)) = M(a)$. In this case we say that M(f) equips the manifold $\{f(a)\}$ with a new coordinate system M(a), and we write it as $\{f(M(a))\}$. Then formula (2.12) is rewritten as follows:

$$\frac{\mathrm{d}M(a)}{\mathrm{d}t} = D_f M(f) \begin{vmatrix} \cdot J(f(M(a))) \\ f = f(M(a)) \end{vmatrix}$$
(2.12a)

The latter equation can be considered as the induced equation for the coordinates a on the manifold $\{f(a)\}$, created with macroscopic mapping M(f). Due to the smooth isomorphism $a \vdash \neg M(a)$ assumed, we can rewrite it as:

$$\left[\frac{DM(a)}{Da}\right] \circ \frac{\mathrm{d}a}{\mathrm{d}t} = D_f M(f) \left| \begin{array}{c} \cdot J(f(M(a))) \\ f = f(M(a)) \end{array} \right|$$
(2.12b)

Here $\left[\frac{DM(a)}{Da}\right]$ is the derivative of the isomorphism $a \mapsto M(a)$.

The notion "macroscopic parameters" used reflects the situation with BE: the values of operator M(f) can be interpreted as observable physical quantities. It is necessary to distinguish the parameterization of \mathfrak{M} with macroscopic parameters from that with the coordinates *a*.

In the latter case we do not undertake a consideration of the neighborhood $U_{\rm m}$. For example, natural coordinates of the LM manifold are macroscopic parameters, while the coordinates $a_{\rm m}$ and $a_{\rm m}$ of the TMS manifold are not (i.e. they are not defined as the values of some macroscopic mapping with properties (2.8a) and (2.8b)).

Further we consider only the approach to obtain the induced dynamics via macroscopic parameterization. It should be stressed here that this approach does not yet solves the problem of ambiguousness in the choice of projector P_{f_m} We have only reformulated this ambiguousness by replacing it into the choice of the macroscopic mapping M(f). Hence, we have to search for additional restrictions upon the choice of M(f) for a given manifold \mathfrak{M} .

Up to now, all considerations were appropriate to any equation (2.1), regardless of whether it is the dissipative system or not. The main feature of dissipative systems is the inequality (2.2) (this is the *H*-theorem for BE).

Hence, it is natural to introduce the principle of **conservation of the type of dynamics** in the induced dynamics. For dissipative systems, this principle states that the vector field of induced dynamics should preserve the inequality (2.2).

For a given manifold \mathfrak{M} and for its macroscopic parameterization $\{f(M)\}$, we denote as H(M) the function H(f(M)), and we assume that H(M) is smooth for all $M \in M(\mathfrak{M})$. Parameterization $\{f(M)\}$ of the manifold \mathfrak{M} will be called **thermodynamic** (for short, manifold $\{f(M)\}$ will be called thermodynamic as well), if the following inequality is valid for all $M \in M(\mathfrak{M})$:

$$\frac{\mathrm{d}H(M)}{\mathrm{d}t} = D_M H(M) \circ D_f M(f) \Big|_{f=f(M)} \cdot J(f(M)) \leq 0 \qquad (2.13)$$

Here $D_{\mu}H(M)$ is the differential of the functional H(M). In other words, the principle of conservation of type of dynamics for dissipative systems is the expressed with inequality (2.13) as a request upon the choice of macroscopic mapping M(f) in the neighborhood of the given manifold m. we stress here that the request on thermodynamicity is directed to the mapping $M(\cdot)$ (i.e. to the choice of induced dynamics) rather than to the manifold m itself. Of course, not any manifold m is suitable for creating the thermodynamic parameterization, but the restriction upon the choice of suitable m is incomparably weaker than that of the thermodynamic parameterization (see next section). Obviously, not every choice of M(f) for given \mathfrak{M} satisfies inequality (2.13), and thus the request on thermodynamicity of parameterization is not trivial. Thermodynamicity of parameterization will be stressed with the asterisks : $\{f^{*}(M)\}\$ for the manifold, and $M^{*}(\cdot)$ for macroscopic mapping. Dynamic invariant manifold of dissipative system is obviously thermodynamic for any choice of M(f)in its neighborhood.

The request on conservation of the type of dynamics is very important. For example, if we consider Hamiltonian systems instead of dissipative ones, then this request means that the induced vector field should have the Hamiltonian structure.

we consider the request on thermodynamicity as the prime restriction upon the choice of projectors $P_{f_{m}}$. Other (additional) restrictions depend on the particular type of the dissipative system under consideration. For BE, these additional restrictions may respond, for example, to usual conservation laws (i. e. to conservation of the number of particles, of momentum, and of energy).

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A specific family of approximations for dissipative systems consists of quasi-equilibrium manifolds. Let U be an open convex domain in F. Consider a smooth mapping M(·): U→M, where M is a linear space. We assume that
1) For every M∈M(U), there exists an unique solution f^{*}(M)∈U of the variational problem:

$$H(f) \rightarrow \min \quad \text{for } M(f) = M \quad (2.14)$$

2) There exists a smooth reverse mapping $M \mapsto f^*(M)$ for

every $M \in M(U)$, and this is a smooth immersion $M(U) \rightarrow F$. The manifold $\{f(M)\}$, which consists of solutions of the variational problem (2.14), is called the quasiequilibrium manifold. It is easy to see that the mapping $M(\cdot)$, for which assumptions 1) and 2) are valid, holds at a time the properties (2.8a) and (2.8b). Vector field of induced dynamics for quasi-equilibrium manifold $\{f(M)\}$ is determined with projector (2.10).(M)Quasi-equilibrium manifolds are thermodynamic due to elsewhere, their construction (see for example However, usually in applications. [8, 9, 13, 14]). quasi-equilibrium manifolds are not dynamic invariant.

The general problem is to construct a dynamic invariant manifold, starting with a given initial dynamic noninvariant manifold. For dissipative systems this problem consists of two main parts:

Problem 1. For a given manifold \mathfrak{M} , one has to determine the thermodynamic parameterization $\{f^*(M)\}$.

Problem 2. For a given manifold $\{f^{(M)}\}\)$, one has to obtain a correction which decreases its deviation from a dynamic invariant manifold (i.e. to make the initial manifold "more invariant").

These two problems are interconnected. On the one hand, the search for thermodynamic parameterization gives us the projector P_{*} and thus defines the $f^{*}(M)$ defect caused with noninvariance. On the other hand, a

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correction of dynamic noninvariance gives us a new manifold, and we have to determine the induced dynamics for this new manifold.

It is convenient to rewrite the condition (2.6) in other form, utilizing the projector $P_{f(M)}$:

$$\Delta(f(M)) \equiv P_{f(M)}(J(f(M)) - J(f(M))) = 0 \qquad (2.15a)$$

or, in detail notation:

$$\Delta(f(M)) \equiv D_{M}f(M) \circ D_{f}M(f) \Big|_{f=f(M)} \cdot J(f(M)) - J(f(M)) = 0 \quad (2.15b)$$

According to Problem 2, we consider expression (2.15a) as the nonlinear equation (the invariance equation) which we have to solve starting with a given initial manifold \mathfrak{M}_0 . Thus, we have to develop a method of successive approximations to solve equation (2.15a). According to Problem 1, we have to create thermodynamic parameterization for each of these approximations, including the initial approximation \mathfrak{M}_0 .

Thus, the **problem of reduced description** for dissipative systems consists of Problems 1 and 2.

In next section we solve Problem 1 (the problem of thermodynamic parameterization) for an almost arbitrary manifold \mathfrak{M} , for dissipative systems of the general type. In section 2.3 we develop Newton-type methods to solve equation (2.15a), and this methods will be combined with the method of thermodynamic parameterization.

2. 2 Thermodynamic Parameterization

In this section we introduce a universal construction which gives the thermodynamic parameterization $\{f^*(M)\}$ for the manifold \mathfrak{M} . This construction is based on a specific choice of the thermodynamic macroscopic mapping $M^*(f)$ in the neighborhood $U_{\mathfrak{m}} \subset F$. The

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mostly important features of our construction are:

1) This construction depends only on H(f) but not on J(f) (i.e. it is *universal* for all dissipative systems (2.1) with given H(f)).

2) This construction is *the only* universal one (i.e. this is the unique construction with property 1).

In order to fulfill this program, we firstly introduce a method of constructing the macroscopic mapping M(f) with the properties (2.8a) and (2.8b). Macroscopic mapping M(f) will be constructed in two steps:

Step 1. For every $f \in U_m$, using linear in f equations, we search for the point $f_m \in \mathfrak{M}$ which satisfies the condition

$$M(f) = M(f_m)$$

Step 2. For every $f_{\mathfrak{m}} \in \mathfrak{M}$, we define parameters $M(f_{\mathfrak{m}})$ so that smooth reverse mapping $M(\mathfrak{M}) \to \mathfrak{M}$ should exist, and it should be a smooth immersion $M(\mathfrak{M}) \to F$.

In other words, in Step 1, we define a projection of the neighborhood $U_{\rm m}$ onto the manifold \mathfrak{M} (see also (2.9)). In Step 2 we create a coordinate system on the manifold \mathfrak{M} and, in accordance with Step 1, this will be the parameterization with macroscopic parameters.

In Step 1, for every $f_{m} \in \mathfrak{M}$, we define linear transforms $M_{f_{m}}(f)$ which depend smoothly on f_{m} , and we take:

$$M(f) = M(f_{\rm m}), \text{ if } M_{f_{\rm m}}(f - f_{\rm m}) = 0$$
 (2.16)

Here $f \in U_m$. In other words, we give the value $M(f_m)$ to $f \in U_m$ if $f - f_m$ belongs to the kernel of $M_{f_m}(f)$:

$$M(f) = M(f_{m}), \text{ if } f - f_{m} \in \ker M_{f_{m}}$$
(2.16a)

The sufficient condition for the univalent solvability of linear equations $M_{f_m}(f-f_m)=0$ in U_m (we can choose a sufficiently small U_m) is the

transversality condition:

$$\ker M_{f_{\mathfrak{m}}} + T_{f_{\mathfrak{m}}} = E, \qquad \ker M_{f_{\mathfrak{m}}} \cap T_{f_{\mathfrak{m}}} = \{0\}$$

The essence of the method proposed for constructing macroscopic mapping M(f) is a description of ker M_{f_m} in (2.16). Step 1 has the principal meaning because for a given \mathfrak{M} one can introduce many different transforms $M_{f_m}(f)$. Step 2 is usually straightforward after $M_{f_m}(f)$ was chosen. Usually in applications, in Step 2, we are able to identify $M_{f_m}(f)$ with M(f) (i.e. we can create the coordinate system on \mathfrak{M} using the values $M_{f_m}(f_m)$). In this case we can take:

$$M(f_{\rm m}) = M_{f_{\rm m}}(f_{\rm m}), \qquad M(f) = M_{f_{\rm m}}(f) \Big|_{M_{f_{\rm m}}(f - f_{\rm m}) = 0}$$
(2.17)

For example, in the case of LM manifold, we take $M_{f_{\mathfrak{m}}}(f)$ as the direct sum of five linear mappings:

$$M_{f(n, \vec{u}, T)}(f) = \left\{ \int 1 \cdot f d^{3}v; \quad \int v_{i} f d^{3}v, \quad i = 1, 2, 3; \quad \int v^{2} f d^{3}v \right\}$$

These do not depend on $f(n, \vec{u}, T) \in \mathfrak{M}_{LM}$, and the kernels ker*M* are the same for all $f(n, \vec{u}, T) \in \mathfrak{M}_{LM}$. $f(n, \vec{u}, T)$ Physically, condition *M* $(f-f(n, \vec{u}, T))=0$ gives $f(n, \vec{u}, T)$ those distributions *f* which have the density, the flow velocity, and the temperature equal to corresponding parameters *n*, \vec{u} , and *T* of the local Maxwellian $f(n, \vec{u}, T)$.

For the given manifold \mathfrak{M} , the derivation of the *thermodynamic* macroscopic mapping $M^{*}(f)$ in accordance with the procedure proposed requires a specific choice of linear transforms $M_{f_{\mathfrak{M}}}^{*}(f)$ in $U_{\mathfrak{M}}$. We will now introduce a condition under which the transforms $M_{f_{\mathfrak{M}}}(f)$ will be thermodynamic. Next we will discuss the sufficiency and the necessity of this condition.

Denote as μ_f the dual variable:

$$\mu_f = D_f H(f) \tag{2.18}$$

Here $D_f H(f)$ is the linear functional: the differential of the functional H(f) in the point f. Due to the strict convexity of H(f), there exists a one-into-one relation $\mu \leftrightarrow f$.

Macroscopic mapping M(f) will be thermodynamic if, for all $f_m \in \mathfrak{M}$, the equalities

$$M(f) = M(f_m)$$

imply

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$$f - f_{\mathfrak{m}} \in \ker \mu_{f_{\mathfrak{m}}}$$
 (i.e. $\mu_{f_{\mathfrak{m}}} \cdot (f - f_{\mathfrak{m}}) = 0$),

where

$$\left\| \mu_{f_{\mathfrak{m}}} = D_{f}^{H(f)} \right\|_{f=f_{\mathfrak{m}}}$$

Thus, the condition of thermodynamicity is:

$$M(f) = M(f_m) \Rightarrow f - f_m \in \ker \mu_{f_m}$$
 (2.19)

Here $f \in U_{\mathfrak{m}}$. In other words, the linear transform $M_{f_{\mathfrak{m}}}(f)$ in (2.16) will be thermodynamic, if

$$\ker M_{f_{\mathfrak{m}}}(f) \subseteq \ker \mu_{f_{\mathfrak{m}}}$$
(2.20)

Equations $\mu_{f_{\mathfrak{m}}} \cdot (f - f_{\mathfrak{m}}) = 0$ are solvable with respect to $f_{\mathfrak{m}}$, for every f from some neighborhood of \mathfrak{m} , only if the manifold \mathfrak{m} is not tangent to the level of the functional H(f) in any point $f_{\mathfrak{m}}$. This *transversality condition* is the only principal constraint on the choice of \mathfrak{m} .

Further, we assume this transversality condition is satisfied.

Condition (2.19) (or (2.20)) initializes the construction of $M_{f_m}(f)$ in (2.16) for the a priori given manifold MR. The standard description of $\ker \mu_{f_m}$ is given

by functionals $M_{f_m}^*(f)$:

$$M_{f_{\mathfrak{m}}}^{*}(f) = \mu_{f_{\mathfrak{m}}} \cdot f$$
 (2.21)

Here $f \in U_m$. Linear transform $M_{f_m}(f)$ will give thermodynamicity if ker $M_{f_m}(f) < \ker M_{f_m}^*(f)$. Obviously, if we take ker $M_{f_m}(f) = \ker M_{f_m}^*(f) \cap \ker M_{f_m}'(f)$, where $M_{f_m}'(f)$ is an arbitrary linear mapping, then implication (2.19) remains valid for $M_{f_m}(f)$. This makes possible to complete step 2, and to construct the thermodynamic macroscopic mapping $M^*(f)$ in the manner of (2.17). Usually in applications, the following strategy of constructing of thermodynamic ker $M_{f_m}(f)$ is convenient: one takes ker $M_{f_m}^*(f)$ and intersects it with a sufficient number of kerL, where kerL are kernels of some linear mappings L(f), so that (2.17) gives a coordinate system on \mathfrak{M} . Linearity plays no key role.

we will now consider the sufficiency and the necessity of condition (2.19).

Condition (2.19) is sufficient for thermodynamicity of $M^*(f)$ because of the following duality principle: $f_{\rm m}$ is the unique solution of the variational problem:

$$H(f) \rightarrow \min \quad \text{for} \quad f \in U_{\mathfrak{m}} \cap (\ker \mu_{f_{\mathfrak{m}}} + f_{\mathfrak{m}})$$
 (2.23)

This is so because:

i) H(f) is the strictly convex functional, and

ii) $K_{f_{\mathfrak{m}}} = U_{\mathfrak{m}} \cap (\ker \mu_{f_{\mathfrak{m}}} + f_{\mathfrak{m}})$, is the convex neighborhood of $f_{\mathfrak{m}}$ in $(\ker \mu_{f_{\mathfrak{m}}} + f_{\mathfrak{m}})$ (if necessary, one can always take for $U_{\mathfrak{m}}$ a smaller neighborhood of \mathfrak{m}).

In other words, $f_{\mathfrak{m}}$ gives the only minima of H(f) in the convex domain $K_{f_{\mathfrak{m}}}$ which belongs to the hyperplane $\Gamma_{f_{\mathfrak{m}}}$:

$$\Gamma_{f_{m}} = \left\{ f \in E \, \middle| \, M_{f_{m}}^{*}(f - f_{m}) = 0 \right\}$$
(2.24)

Taking into account (2.19) and (2.23), we see that $f_{\rm m}$ is also the unique solution of the variational problem:

$$H(f) \longrightarrow \min \quad \text{for} \quad M^*(f) = M^*(f_{\mathfrak{m}}) \tag{2.25}$$

Here $f \in U_{\mathfrak{m}}$. This is so because, due to (2.20), $K_{f_{\mathfrak{m}}}$ is wider than $U_{\mathfrak{m}} \cap (\ker M_{f_{\mathfrak{m}}} + f_{\mathfrak{m}})$, and according to (2.23) $f_{\mathfrak{m}}$ gives the only minima to H(f) in $K_{f_{\mathfrak{m}}}$.

Finally, as we have defined $f_{\rm m}$ as the solution of variational problem (2.25), the thermodynamicity of $M^*(f)$ can be proved straightforwardly in the same manner as for quasi-equilibrium manifolds $\{f^*(M)\}$ (2.14) (see elsewhere, for example [8, 9, 13, 14]).

An important particular case is that when the manifold \mathfrak{M} is a quasi-equilibrium manifold $\{f^*(M)\}\$ (2.14). Then no new macroscopic mapping is required. Quasi-equilibrium manifold $\{f^*(M)\}\$ is thermodynamic due to its construction because

$$\operatorname{ker} D_{f}^{M(f)} \Big|_{f=f^{*}(M)}^{f \operatorname{ker} \mu} f^{*}(M)$$

Due to the duality principle (2.23), one can consider an arbitrary manifold \mathfrak{M} as if it was a quasi-equilibrium manifold after the appropriate parameterization.

It is remarkable that condition (2.19) accounts only the Lyapunov functional *H* but not the vector field of dissipative systems. Now we will demonstrate the necessity of this condition. In order to do this, we have to turn to a consideration of a whole family of dissipative systems with a given functional *H*.

Denote as $\mathbf{3}_H$ the family of vector fields $J(\cdot)$ which define dissipative systems (2.1) with the given Lyapunov

functional *H*. Due to inequality (2.2), vector $J \in E$ can represent a vector J(f) for some $J(\cdot) \in \mathfrak{Z}_{H}$ if it belongs to the allowed half-space E_{f}^{th} :

 $E_f^{\text{th}} = \left\{ J \in E \middle| \ \mu_f \cdot J \leq 0 \right\}$

The interior of E_f^{th} will be called the *strictly allowed* half-space E_f^{-} :

 $E_{f}^{-} \left\{ J \in E \left| \begin{array}{c} \mu_{f} \cdot J < 0 \end{array} \right\}$

Condition $\mu_f \cdot J=0$ defines a partition of E into two half-spaces, $E=E_f^{\text{th}}\cup E_f^+$, where E_f^+ is the strictly forbidden half-space:

$$E_f^+ = \left\{ J \in E \left| \begin{array}{c} \mu_f \cdot J > 0 \end{array} \right\}$$

None of vectors from E_f^+ can represent a vector J(f) for any $J(\cdot) \in \mathfrak{Z}_{H'}$

Dealing with the whole family \Im_{H} , it is convenient to reformulate the request on thermodynamicity of induced dynamics. Same as for the space *E*, we define the allowed, the strictly allowed, and the strictly forbidden half-subspaces of $T_{f_{-}}$:

$$T_{f_{\mathfrak{m}}}^{\mathfrak{th}} = \left\{ J \in T_{f_{\mathfrak{m}}} \middle| \begin{array}{l} \mu_{f_{\mathfrak{m}}} \cdot J \leq 0 \end{array} \right\} = E_{f_{\mathfrak{m}}}^{\mathfrak{th}} \cap T_{f_{\mathfrak{m}}}$$

$$T_{f_{\mathfrak{m}}}^{-} = \left\{ J \in T_{f_{\mathfrak{m}}} \middle| \begin{array}{l} \mu_{f_{\mathfrak{m}}} \cdot J < 0 \end{array} \right\} = E_{f_{\mathfrak{m}}}^{-} \cap T_{f_{\mathfrak{m}}}$$

$$T_{f_{\mathfrak{m}}}^{+} = \left\{ J \in T_{f_{\mathfrak{m}}} \middle| \begin{array}{l} \mu_{f_{\mathfrak{m}}} \cdot J > 0 \end{array} \right\} = E_{f_{\mathfrak{m}}}^{+} \cap T_{f_{\mathfrak{m}}}$$

Projector $P_{f_{\mathfrak{m}}}$ will be called *uniformly thermodynamic* if $P_{f_{\mathfrak{m}}}(E_{f_{\mathfrak{m}}}^{\mathfrak{th}}) \subseteq T_{f_{\mathfrak{m}}}^{\mathfrak{th}}$ (2.26)

Note that, due to the *transversality condition* formulated above, the latter inclusion is an equality:

$$P_{f_{\mathfrak{m}}}(E_{f_{\mathfrak{m}}}^{\mathfrak{th}})=T_{f_{\mathfrak{m}}}^{\mathfrak{th}}$$

and that two similar equalities also take place:

$$P_{f_{\mathfrak{m}}}(E_{f_{\mathfrak{m}}}^{\pm}) = T_{f_{\mathfrak{m}}}^{\pm}$$

In other words, the uniformly thermodynamic projectors transform all "physically allowed microscopic vectors" $E_{f_{\rm m}}^{\rm th}$ into "physically allowed macroscopic vectors" $T_{f_{\rm m}}^{\rm th}$ and thus they give thermodynamic induced dynamics for all representatives of the family \mathfrak{Z}_{μ} .

Consider the family \mathfrak{I}_{H} and a manifold \mathfrak{M} . Condition (2.19) is **necessary** for thermodynamic parameterization in the following sense: this is the unique condition in Step 1 which defines the thermodynamic parameterization of \mathfrak{M} for all dissipative vector fields \mathfrak{I}_{H} . In other words, projector defined by condition (2.19) is the only uniformly thermodynamic projector.

In fact, let us consider a parameterization of \mathfrak{M} defined with some macroscopic mapping $N(\cdot)$, different from $M^{*}(\cdot)$ defined via condition (2.19). It means that

$$\mathrm{ker}^{\mathcal{V}}_{f_{\mathfrak{m}}} \neq \mathrm{ker}^{\mu}_{f_{\mathfrak{m}}}$$

for some $f_{\rm m} \in \mathfrak{M}$. Here $\mathcal{V}_{f_{\rm m}} = D_f N(f) |_{f=f_{\rm m}}$. Then there exists $J_0 \in E_{f_{\rm m}}^-$, for which $J_0 \in \ker \mathcal{V}_{f_{\rm m}}$, and $J_0 \notin \ker \mu_{f_{\rm m}}$. Let $U_{J_0} \subset E_{f_{\rm m}}^-$ be a neighborhood of J_0 . Denoting as $\mathcal{P}_{\mathcal{V}}$ the projector $\mathcal{U}_{f_{\rm m}}$ defined by the macroscopic mapping $N(\cdot)$, we see that the image $\mathcal{P}_{\mathcal{V}} (U_{J_0}) \subset T_{f_{\rm m}}$ is a neighborhood of zero in $T_{f_{\rm m}}^-$, and, hence,

$$P_{\mathcal{V}_{f_{\mathfrak{m}}}(U_{J_{0}})\cap T_{f_{\mathfrak{m}}}^{+}\neq\emptyset}$$

In other words, there exist strictly allowed vectors $J(f_m)$ that transform into strictly forbidden vectors

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 $T_{f_{\rm m}}^+$ under the action of projector $P_{\mathcal{V}_{f_{\rm m}}}$. On contrary, a $T_{f_{\rm m}}^+$ strictly allowed neighborhood U_{J_0} always transforms into a strictly allowed neighborhood under a projection which satisfies condition (2.19).

The uniform character of condition (2.19) might be illustrated with the following example. Consider all kinetic equations with the Boltzmann H-function (i.e. all BE with all possible collision integrals including rigid spheres, Lennard-Johnes, BGK, etc) and a fixed manifold (say, the TMS manifold). Then, if we derive the induced dynamics for $\mathfrak{M}_{\mathsf{TMS}}$ using only linear mappings (such as $\int v_x^2 f d^3 v$, $\int v_x^3 f d^3 v$, etc; see [2]), then, for some $f_{m} \in \mathfrak{M}_{TMS}$, there exist collision integrals for which the induced dynamics will not satisfy the thermodynamicity condition in the point $f_{\rm m}$ (see in this connection the [21]).The only condition which will give paper thermodynamic induced dynamics for all ΒE is the realization of condition (2.19) for \mathfrak{M}_{TMS} [20].

Thus, in this section, we have introduced a method for constructing the thermodynamic parameterization in the general case, and thus we have solved the Problem 1 of Section 2.1. In the next section we will consider an approach to correct dynamic noninvariance.

2. 3 Iterative Methods for Invariance Equation

In this section we introduce Newton-type procedures for a search of corrections to a dynamic noninvariant manifold \mathfrak{M} . We consider the case when the manifold is parameterized with macroscopic parameters M: $\mathfrak{M}=\{f(M)\}$. In the preceding section we have learned to construct thermodynamic macroscopic parameterization. Thus, when we are developing procedures of corrections, we are free

to pay no attention to whether $\{f(M)\}$ is thermodynamic or not: thermodynamicity can be always arranged in the end of calculations. The invariance equation (2.15a) is completely geometric, it contains no explicit time dependence. The latter appears only when we derive the induced dynamics, and only at this step we have to apply the principle of thermodynamic parameterization.

We start with the invariance equation (2.15b). Let the manifold $\{f_0(M)\}$ is given. Its dynamic noninvariance means that the defect $\Delta(f_0(M))$ is not identical to zero.

In order to correct the manifold $\{f_0(M)\}$, we search for a new manifold $\{f_1(M)\}$, representing $f_1(M)$ as

$$f_{1}(M) = f_{0}(M) + \delta f_{1}(M)$$
 (2.27)

This search should give a one-into-one relation $f_1(M) \leftrightarrow f_0(M)$. In order to arrange this relation, we require

$$\delta f_1(M) \in \ker P_{f_0(M)}$$
(2.28)

In other words, we search for the new point $f_1(M)$ labeled with the same value M as the point $f_0(M)$.

We are going to obtain the correction to $\{f_0(M)\}\$ via a method of successive approximations. We want that this method would not require neither any strong restriction upon the choice of $\{f_0(M)\}\$, nor small parameters, etc. We represent two methods of this type.

Method 1. Substituting expression (2.27) into (2.15b) instead of f(M), and next preserving linear in $\delta f_1(M)$ terms, we obtain a formal linear in $\delta f_1(M)$ equation:

$$\begin{split} & D_{M} \delta f_{1}(M) \circ D_{f} M(f) \Big|_{f = f_{0}(M)} \cdot J(f_{0}(M)) + \\ & + D_{M} f_{0}(M) \circ D_{f}^{2} M(f) \Big|_{f = f_{0}(M)} \cdot (\delta f_{1}(M), J(f_{0}(M)) - \\ \end{split}$$

$$-\left[1 - D_{M}f_{0}(M) \circ D_{f}M(f) \middle|_{f=f_{0}(M)} \cdot \right] D_{f}J(f) \middle|_{f=f_{0}(M)} (\delta f_{1}(M)) + \Delta (f_{0}(M)) = 0$$

$$(2.29)$$

Here $D_f^2 M(f) \Big|_{f=f_0(M)}$ is a bilinear operator (the second differential of M(f)), and $D_f J(f) \Big|_{f=f_0(M)}$ is the linear operator (the differential of the mapping $J(f): E \rightarrow E$).

Equation (2.29) is the first iteration of the Newton method [22] as applied to equation (2.15b). Constraint (2.28) is the additional condition for unambiguous solvability of equation (2.29). Equation (2.28) initializes the method of successive approximations for solving the invariance equation (2.15b).

It is clear that the first and the second terms in (2.29) give the linear variation of the projector: the first term gives the variation of the image of the projector, while the second term gives the variation of its kernel. The rest of the terms in (2.29) give the variation of the vector field.

Method 2. We search for a new manifold $\{f_1(M)\}\$ where the vector field $J(f_1(M))$ is parallel to the tangent space $T_{f_0(M)}$. In linear approximation, we obtain an equation for the first correction $\delta f_1(M)$ (2.27) as:

$$\left[P_{f_0(M)}(\cdot)-1\right](J(f_0(M)+D_f^{J(f)}|_{f=f_0(M)}(\delta f_1(M)))=0 \quad (2.30)$$

Additional condition for this equation is again the constraint (2.28).

In order to demonstrate the sense of the two methods proposed, we will consider the case of linear manifolds for linear dissipative systems.

Consider real Hilbert space G with the scalar product (f, g), and a linear dissipative system

 $df/dt = Af \tag{2.31}$

with the functional H(f)

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$$H(f) = \frac{1}{2}(f, f)$$
 (2.32)

In (2.31), A is a linear, negatively defined, bounded, and selfadjoint operator, $A: G \rightarrow G$. We assume that the spectra of A consists of non-degenerated eigentvalues $\lambda_{(m)}$, $m=0, 1, \ldots$

The dual variable μ_f (2.18) is

$$\mu_{f} = f; \qquad \mu_{f} \cdot g = (f, g) \tag{2.33}$$

Consider linear manifolds $\mathfrak{M}_e = ae$, where (e, e) = 1, and $a \in \mathbb{R}$ (i.e. \mathfrak{M}_e is a line in *G*, defined with the unit vector *e*).

Invariance equation (2.15b) for \mathfrak{M}_{ρ} is:

$$e(e, Ae) - Ae = 0 \tag{2.34}$$

Normalized solutions of equation (2.34) are unit vectors $e_{(m)}$ which define the eigentspaces $m_{e_{(m)}} = ae_{(m)}$ of operator *A*, corresponding to eigentvalues $\lambda_{(m)}$.

Assume that we have chosen the linear manifold $\mathfrak{M}_{e_0} = ae_0$, and e_0 is not the eigentvector of operator A. We have to correct the initial manifold \mathfrak{M}_{e_0} in order to make it closer to a solution of equation (2.34).

we search for a new linear manifold $\mathfrak{M}_{e_1} = ae_1$. It is sufficient to find any vector $x_1 \in \mathfrak{M}_{e_1}$, then $\mathfrak{M}_{e_1} = a(x_1 / \|x_1\|)$. We search for x_1 in the form (2.27):

$$x_1 = e_0 + \delta x_1 \tag{2.35}$$

Additional condition (2.28) yields:

$$(\delta_{x_1}, e_0) = 0$$
 (2.36)

Method 1 (formula (2.29)) gives: $(A - (e_0, Ae_0) \operatorname{Id})(e_0 + \delta x_1) = 2e_0(\delta x_1, (A - (e_0, Ae_0) \operatorname{Id})e_0)$ (2.37)

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Here Id is the identy operator. Using additional condition (2.36), we obtain the unique solution of equation (2.37):

$$e_{0} + \delta x_{1} = \frac{1}{(e_{0}, (A - (e_{0}, Ae_{0}) \operatorname{Id})^{-1} e_{0})} (A - (e_{0}, Ae_{0}) \operatorname{Id})^{-1} e_{0} (2.38)$$

Being rewritten in the basis $e_{(m)}$, expression (2.38) gives:

$$e_0 + \delta x_1 \propto \sum_{(m)} e_{(m)} - \frac{(e_{(m)}, e_0)}{\lambda_{(m)} - (e_0, Ae_0)}$$
 (2.39)

We see that the leading term of the series (2.39) corresponds to the number m^* which gives the minima to the function $z(m) = |\lambda_{(m)}^{-}(e_0, Ae_0)|$. In other words, the leading term corresponds to the eigentspace $m_{e_m^*}$ which is the "nearest neighbor" of the linear manifold $m_{e_0^*}$. Thus, Method 1 gives a search of the eigentvector e_m^* . (m)

Method 2 (formula (2.30) gives:

$$(\mathrm{Id} - e_0(e_0, \cdot))A(e_0 + \delta x_1) = 0$$
 (2.40)

Taking into account the additional condition (2.36), we obtain the unique solution of equation (2.40):

$$e_0 + \delta x_1 = \frac{1}{(e_0, A^{-1}e_0)} A^{-1} e_0$$
 (2.41)

In the basis $e_{(m)}$ we obtain:

$$e_0 + \delta x_1 \propto \sum_{(m)} e_{(m)} \frac{(e_{(m)}, e_0)}{\lambda_{(m)}}$$
 (2.42)

The leading term of the expansion (2.42) corresponds to the number m_* which labels the eigentvalue with the minimal module. Thus, Method 2 results in a search for the eigentvector $e_{(m_*)}$ which is the direction of the "slowest relaxation" to the equilibrium point x=0.

The example of linear manifolds for linear dissipative systems considered shows the difference

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between the two methods for obtaining corrections. The choice of a method in particular applications depends on the physical sense of the problem. In particular, Method is preferable when one searches for invariant 2 manifolds with slowest relaxation properties, and it used in Section 4 for will be derivation of hydrodynamics from the Boltzmann equation..

Thus, we have introduced the two main objectives constructing dynamic invariant manifolds for for dissipative systems: the method of thermodynamic parameterization (Section 2.2) and Newton-type procedures to the dynamic successive correct noninvariance (Section 2.3). In the next section we will combine these two procedures into the algorithm of constructing dynamic invariant manifolds for dissipative systems (the method of invariant manifold).

2. 4 Description of the Method of Invariant Manifold

The algorithm starts with the choice of an initial manifold \mathfrak{M}_0 . This choice depends on the particular physical problem, and we are not able to consider this question in general. However, the rest of the algorithm does not essentially depend on this choice. Here we assume only that \mathfrak{M}_0 satisfies the transversality condition of Section 2.2.

- step 1. Choose the initial manifold mo.
- <u>Step 2</u>. Construct the thermodynamic parameterization $\{f_0^*(M)\}\$ for the manifold \mathfrak{M}_0 in accordance with the algorithm of Section 2.2.
- <u>Step 3</u>. Calculate the defect $\Delta(f_0^*(M))$ (2.15a). If $\Delta(f_0^*(M)) \equiv 0$, then \mathfrak{M}_0 is a dynamic invariant manifold. If $\Delta(f_0^*(M)) \neq 0$, then search for a mew manifold \mathfrak{M}_1 in accordance with Method 1 or Method 2 of Section 2.3.
- <u>Step 4</u>. Construct the thermodynamic parameterization

 $\{f_1^*(M)\}$ for the manifold \mathfrak{M}_1 in accordance with the algorithm of Section 2.2.

Then the procedure is continued (go to Step 3).

In the next section we will discuss physical ideas behind the method of invariant manifold.

2. 5 Physical and Geometrical Interpretation

The method introduced in Section 2.4 is based on two points: 1) thermodynamic parameterization (Section 2.2) and, 2) successive corrections of the dynamic noninvariance (Section 2.3). These points reflect the Problem 1 and the Problem 2 outlined in Section 2.1, and they give the immediate formalization to the two general assumptions of macroscopic kinetics:

 The choice of any approximated reduced description (i.e. of any manifold) always involves an implicit assumption on decomposition of times of relaxation.
 A dynamic invariant manifold of slow motions is located in a neighborhood of the chosen approximation.

when obtaining the thermodynamic parameterization for the initial manifold \mathfrak{M} , we act as if a times hierarchy hypotheses corresponded to the choice. This means that we act as if a "rapid" relaxation to the states $f_m \in \mathfrak{m}$ occurs in some neighborhood of the manifold M, and then a "slow" motion along M takes place. During relaxation, the Lyapunov functional H(f) decreases, and at the end of rapid processes it reaches a minimum on manifolds of rapid motions. The gradient of the Liapunov functional is *normal* to these manifolds of rapid motions points. Therefore, at the minima in linear approximation, equation $\mu_{f_{\mathfrak{m}}} \cdot f = \mu_{f_{\mathfrak{m}}} \cdot f_{\mathfrak{m}}$ is valid for those points f which relax to the point $f_{\rm m}$ in rapid processes. linear approximation, Τn other words, in rapid relaxation occurs on hyperplanes of rapid motions $\Gamma_{f_{\rm m}}$

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(2.24), the latter are linear approximations to the manifolds of rapid motions.

Duality principle (2.23) states that the point $f_{\rm m}$ is the only point of minima of the functional on the hyperplane of rapid motions $\Gamma_{f_{\rm m}}$. In general, the hyperplanes of rapid motions $\Gamma_{f_{\rm m}}$ are *nonparallel* for different points $f_{\rm m} \in \mathfrak{M}$.

In order to create a coordinate system on \mathfrak{M} , we simply have to *add* some macroparameters M(f). This addition is almost arbitrary, one should only supply the independence and completeness of the set $\{M_{f_{\mathfrak{M}}}^{*}(f), M(f)\}$ in the neighborhood of \mathfrak{M} . Then the manifold \mathfrak{M} will be parameterized with the set $\{M_{f_{\mathfrak{M}}}^{*}(f_{\mathfrak{M}}), M(f_{\mathfrak{M}})\}$.

The choice of the set $\{M_{f_{\mathfrak{M}}}^{*}(f), M(f)\}\}$ yields the following picture of rapid relaxation in the neighborhood of the manifold \mathfrak{M} : the system relaxes towards \mathfrak{M} along the planes of rapid motions $R_{f_{\mathfrak{M}}}$. The plane of rapid motions $R_{f_{\mathfrak{M}}}$ which includes the point $f_{\mathfrak{M}}$ is the cross-section of the hyperplane of rapid motions $\Gamma_{f_{\mathfrak{M}}}$ with the planes $\{f \mid D_{f}M(f) \mid f=f_{\mathfrak{M}} \cdot (f-f_{\mathfrak{M}})=0\}$:

$$R_{f_{m}} = \left\{ f \left| M_{f_{m}}^{*} (f - f_{m}) = 0; D_{f}^{M}(f) \right|_{f = f_{m}} \cdot (f - f_{m}) = 0 \right\}$$

The simplest case occurs when M(f) is a set of linear functionals.

The hyperplane of rapid motions $\Gamma_{f_{\mathfrak{m}}}$ is the only hyperplane where the levels of the functional H(f)"surround" the point $f_{\mathfrak{m}}$. This illustrates the duality principle (2.23).

Thus, in Step 2 of Section 2.4, we take (for a while) that the initially chosen manifold is already a "good" manifold of slow motions, and this alone yields

the proper induced dynamics. Naturally, we understand that the decomposition of motions assumed might be only approximate. Hence, in Step 2, which immediately follows Step 1, we *reject* this picture of relaxation, and we approximately correct the dynamic noninvariance. Then, in Step 4, we again *act as if* the corrected manifold is a manifold of slow motions, etc.

The problem of dynamic invariant manifolds has a very specific sound for dissipative kinetics. Namely, one should expect that these manifolds are manifolds of slow motion. This is rather a fine point, and we give some additional explanations.

Usually when one talks about decomposition of motions (i.e. about the times hierarchy), then one keeps in mind the existence of a small parameter. This small parameter should express the ratio of the time of rapid relaxation to the time of macroscopic observation. One may expect that the rapid relaxation results in a "sufficiently good" manifold of slow motions (i.e. in a "sufficiently invariant" manifold).

However, this situation is far from being simple. There is always a place to doubt on whether the chosen parameter is sufficiently small. Even for finitedimensional dissipative systems (e.g. chemical kinetics) the steady-state manifolds might not always be referred as to good approximations (see a precise study "The Steady-State Approximations, Fact or Fiction?" by E. Farrow and D. Edelson [23], and also [24]).

On the other hand, there are no small parameters in the general case, but still one can construct a "good" approximation which approximately describes the evolution at a considerable period. For example, the TMS approximation illustrates this situation: a small parameter lacks in the strong shock wave problem but, nevertheless, one can consider the TMS approximation as

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a suitable approximation for this problem. Hence, we should take that the two assumptions mentioned above are appropriate to the TMS approximation (at least approximately).

For a chosen approximated reduced description, one can not say beforehand whether the decomposition of motions indeed corresponds to the choice. Nevertheless, we act as if the chosen manifold is already a "good" manifold of slow motions. This immediately leads to the definition of hyperplanes of rapid motions via the principle of decrease of the Lyapunov functional in rapid relaxation as described above in Section 2.2. τt. is important that the method of invariant manifold avoids a search for small parameters for constructing the manifolds of rapid motions. We obtain thermodynamic parameterization for the initial manifold. At the same time we remember that the chosen approximation is not a dynamic invariant manifold. We are able to measure the error $\Delta(f_m)$ caused by noninvariance, and we are able to approximately correct this error by solving the linear equation of the first Newton-type iteration. Then we again act as if the corrected manifold is a good manifold of slow motions, etc.

In the next section we apply the method of invariant manifold to the Boltzmann equation.

3. THE CONSTRUCTING OF DYNAMIC INVARIANT MANIFOLDS FOR THE BOLTZMANN EQUATION

In this section we apply the method of invariant manifold to the Boltzmann equation (BE). Firstly, we will interpret the key notions of Section 2 for BE.

The phase space F (Section 2.1) consists of distribution functions $f(\vec{v}, \vec{x})$ which depend on the spatial variable \vec{x} and on velocity variable \vec{v} . The

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variable \vec{x} spans an open domain $\Omega_{\chi} \subseteq \mathbb{R}^{3}_{\chi}$, and the variable \vec{v} spans the space \mathbb{R}^{3}_{V} . We require that $f(\vec{v}, \vec{x}) \in F$ are nonnegative functions, and also that the following integrals are finite for every $\vec{x} \in \Omega_{\chi}$ (the existence of moments and of the entropy):

$$I_{\vec{x}}^{(i_1i_2i_3)}(f) = \int v_1^{i_1} v_2^{i_2} v_3^{i_3} f(\vec{v}, \vec{x}) d^3 v, \quad i_1 \ge 0, \quad i_2 \ge 0, \quad i_3 \ge 0; \quad (3.1a)$$

$$H_{\overrightarrow{x}}(f) = \int f(\overrightarrow{v}, \overrightarrow{x}) (\ln f(\overrightarrow{v}, \overrightarrow{x}) - 1) d^3v, \quad H(f) = \int H_{\overrightarrow{x}}(f) d^3x \quad (3.1b)$$

Here and below integration in \vec{v} is made over \mathbb{R}^3_{v} , and it is made over Ω_x in \vec{x} . For every fixed $\vec{x} \in \Omega_x$, I, and $H_{\vec{x}}$ might be treated as functionals defined in F.

we write BE in the form of (2.1) using standard notations [2]:

$$\frac{\partial f}{\partial t} = J(f), \qquad J(f) = -v_{S} \frac{\partial f}{\partial x_{S}} + Q(f, f) \qquad (3.2)$$

Here and further a summation in two repeated indices is assumed, and Q(f, f) stands for the Boltzmann collision integral [1]. The latter represents the dissipative part of the vector field J(f) (3.2).

In this paper we consider the case when boundary conditions for equation (3.2) are relevant to the local with respect to \vec{x} form of the H-theorem.

For every fixed \vec{x} , we denote as $H^0_{\vec{x}}(f)$ the space of linear functionals

$$\sum_{i=0}^{4} a_{i}(\vec{x}) \int \psi_{i}(\vec{v}) f(\vec{v}, \vec{x}) d^{3}v,$$

where $\psi_{i}(\vec{v})$ represent summational invariants of a collision [1, 2] $(\psi_{0}=1, \psi_{i}=v_{i}, i=1, 2, 3, \psi_{4}=v^{2})$. We write $(\mod H^{0}_{,i}(f))$ if an expression is valid within the accuracy of adding a functional from $H^{0}_{,i}(f)$. The local *H*-theorem states: for any functional

$$H_{\vec{x}}(f) = \int f(\vec{v}, \vec{x}) (\ln f(\vec{v}, \vec{x}) - 1) d^{3}v \pmod{H_{\vec{x}}^{0}(f)}$$
(3.3)

the following inequality is valid:

$$\frac{dH}{\dot{x}}(f)/dt \equiv \int Q(f,f) \left| f = f(\vec{v},\vec{x}) \right| \ln f(\vec{v},\vec{x}) d^3v \leq 0$$
(3.4)

Expression (3.4) is equal to zero if and only if $\ln f = \sum_{i=0}^{4} a_{i}(\vec{x}) \psi_{i}(\vec{v}).$

Although all functionals (3.3) are equivalent in the sense of the *H*-theorem, it is convenient to deal with the functional $H_{\vec{v}}(f) = \int f(\vec{v}, \vec{x}) (\ln f(\vec{v}, \vec{x}) - 1) d^3 v$.

All what was said in Section 2 can be applied to BE (3.2) with no significant changes. Now we will discuss some specific points.

i) Local manifolds. Although the general description of manifolds $\mathfrak{M} \subset F$ (Section 2.1) holds as well for BE, a specific class of manifolds might be defined due to the different character of spatial and of velocity dependencies in BE vector field (3.2). These manifolds will be called **local manifolds**, and they are constructed as follows. Denote as F_{loc} the set of functions $f(\vec{v})$ with finite integrals

a)
$$I^{(i_1i_2i_3)}_{1}(f) = \int v_1^{i_1} v_2^{i_2} v_3^{i_3} f(\vec{v}) d^3 v, \quad i_1 \ge 0, \, i_2 \ge 0, \, i_3 \ge 0;$$

b) $H(f) = \int f(\vec{v}) \ln f(\vec{v}) d^3 v$
(3.5)

In order to construct a local manifold in F, we, firstly, consider a manifold in F_{1oc} . Namely, we define a domain $A \subseteq B$, where B is a linear space, and consider a smooth immersion $A \rightarrow F_{1oc}: a \mapsto f(a, \vec{v})$. The set of functions $f(a, \vec{v}) \in F_{1oc}$, where a spans the domain A, is a manifold in F_{1oc} . Secondly, we consider all bounded and sufficiently smooth functions $a(\vec{x}): \Omega_X \rightarrow A$, and we define the local manifold in F as the set of functions $f(a(\vec{x}), \vec{v})$. Roughly speaking, the local manifold is a set of functions which are parameterized with \vec{x} -dependent functions $a(\vec{x})$. A local manifold will be called a **locally finite-dimensional** manifold if *B* is a finite-dimensional linear space.

Locally finite-dimensional manifolds are a natural initial approximations for constructing source of dynamic invariant manifolds in BE theory. For example, the TMS manifold (2.3) and the LM manifold (2.4) are finite-dimensional manifolds. locally They are parameterized with finite sets of \vec{x} -dependent functions. The LM manifold is parameterized with five macroscopic parameters (i.e. with five hydrodynamic moments), the TMS manifold is parameterized with two coordinates, $a_{\perp}(\vec{x})$ and $a_{\perp}(\vec{x})$. Further, all expressions corresponding to the function $f(a(\vec{x}), \vec{v})$ will be labeled with $a(\vec{x})$. ii) Thermodynamic parameterization. The specificity of thermodynamic parameterization for manifolds in BE theory is due to the type of the Boltzmann H-function. Namely, the functionals $H_{\rightarrow}(f)$ (3.3) are homogeneous: for any λ , where $0 < \lambda < \infty$, we have:

$$H_{\stackrel{}{\xrightarrow{}}}(\lambda f) = \lambda H_{\stackrel{}{\xrightarrow{}}}(f) \pmod{H_{\stackrel{}{\xrightarrow{}}}(f)}$$
(3.6)

The dual variable μ_f (2.18) is:

$$\begin{aligned} \mu_{f} \Big|_{f=f(\vec{x},\vec{v})} &= D_{f}^{H(f)} \Big|_{f=f(\vec{x},\vec{v})} &= D_{f}^{H}_{\vec{x}}(f) \Big|_{f=f(\vec{x},\vec{v})} &= \\ &= \ln f(\vec{v},\vec{x}) \end{aligned}$$
(3.7)

Consider the local form of M_f^* (f) (2.21):

$$M_{\vec{x}, f_{\mathfrak{M}}}^{*}(f) = \int f(\vec{v}, \vec{x}) \ln f_{\mathfrak{M}}(\vec{v}, \vec{x}) d^{3}v \qquad (3.8)$$

The value of the functional $M_{\tilde{x}, f_{\tilde{m}}}^{*}$ in the point $f_{\tilde{m}} \in \mathfrak{m}$ is

equal to:

$$M_{\vec{x}, f_{\mathfrak{M}}}^{*}(f_{\mathfrak{M}}) = \int f_{\mathfrak{M}}(\vec{v}, \vec{x}) \ln f_{\mathfrak{M}}(\vec{v}, \vec{x}) d^{3}v \equiv H_{\vec{x}}(f_{\mathfrak{M}}) \pmod{H_{\vec{x}}^{0}(f_{\mathfrak{M}})}$$
(3.9)
Thus, equation (2.12) for the macroscopic parameter
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 $M_{\vec{x}, f_{\mathfrak{M}}}^{*}(f_{\mathfrak{M}})$ is the entropy balance equation.

It is necessary to stress here that, in spite of external simplicity of this result (the entropy balance is indeed "natural"), equation the idea to use functionals (3.8) for constructing the thermodynamic projector is not evident. Indeed, functionals (3.8) are neither usual moment functionals (3.1a) nor the entropy (3.1b) in the neighborhood of the manifold M. According to the physical interpretation (Section 2.5), the entropy balance equation appears immediately from the idea of decomposition of motions in the neighborhood of the manifold m.

Let $\{f(a(\vec{x}), \vec{v})\}$ be a locally *r*-dimensional manifold, where $a(\vec{x}) = (a_1(\vec{x}), \dots, a_r(\vec{x}))$. We now give explicit expressions for thermodynamic parameterization of $\{f(a(\vec{x}), \vec{v})\}$ in the important particular case when one adds *r*-1 independent linear functionals $L_{\vec{x}, \vec{i}}$ functionals $M_{\vec{x}, \vec{f}_{\mathfrak{M}}}^{*}$ (f) (3.8): $\vec{x}, \vec{f}_{\mathfrak{M}}$

$$L_{\vec{x}, \vec{i}}(f) = \int I_{\vec{i}}(\vec{v}) f(\vec{x}, \vec{v}) d^{3}v, \quad i = 1, \dots, r-1 \quad (3. 10)$$

The natural source of these linear functionals are, for example, the moment functionals (3.1a).

For every fixed \vec{x} , we can consider $\{f(a(\vec{x}), \vec{v})\}$ as a finite-dimensional manifold.

The thermodynamic macroscopic mapping $M_{\dot{x}}^{*}(f)$ is defined as:

 $M_{\vec{x}}^{*}(f) = (3.11a)$ = $(\int f(\vec{x}, \vec{v}) \ln f(a(\vec{x}), \vec{v}) d^{3}v, \int I_{\vec{i}}(\vec{v}) f(\vec{x}, \vec{v}) d^{3}v, \quad \vec{i}=1, \dots, r-1)$

This mapping equips the manifold $\{f(a(\vec{x}), \vec{v})\}$ with a new coordinate system:

$$H(a(\vec{x})) = \int f(a(\vec{x}), \vec{v}) \ln f(a(\vec{x}), \vec{v}) d^3v,$$

$$L_{i}(a(\vec{x})) = \int I_{i}(\vec{v}) f(a(\vec{x}), \vec{v}) d^{3}v, \quad i=1, \dots, r-1 \quad (3.11b)$$

Thus, in detail notation, we can write

$$\{f^{*}(H(a(\vec{x})), L_{1}(a(\vec{x})), \dots, L_{r-1}(a(\vec{x})), \vec{v})\}\$$

for the manifold $\{f(a(\vec{x}), \vec{v})\}$ parameterized with macroscopic parameters (3.11b).

Thermodynamic projector $P^*_{a(\vec{x})}(J)$ is defined as: $P^*_{a(\vec{x})}(J) = (3.11c)$

$$=\frac{\partial f^{*}(H(a(\vec{x})), L_{1}(a(\vec{x})), \dots, L_{r-1}(a(\vec{x})), \vec{v})}{\partial H(a(\vec{x}))} \int \ln f(a(\vec{x}), \vec{v}) J d^{3}v +$$

$$+\sum_{i=1}^{r-1} \frac{\partial f^{*}(\mathcal{H}(a(\vec{x})), L_{1}(a(\vec{x})), \dots, L_{r-1}(a(\vec{x})), \vec{v})}{\partial L_{i}(a(\vec{x}))} \int I_{i}(\vec{v}) J d^{3}v$$

Dynamic equations for macroscopic parameters (3.11b) induced with the BE vector field (3.2) via thermodynamic projector (3.11c) are:

$$\frac{\partial H(a(\vec{x}))}{\partial t} + \operatorname{div}_{H}^{j}(a(\vec{x})) = \sigma(a(\vec{x}));$$

$$\frac{\partial L_{i}(a(\vec{x}))}{\partial t} + \operatorname{div}_{L_{i}}^{j}(a(\vec{x})) = R_{i}(a(\vec{x})); \qquad (3.11d)$$

$$\vec{j}_{H}(a(\vec{x})) = \int \vec{v} f(a(\vec{x}), \vec{v}) \ln f(a(\vec{x}), \vec{v}) d^{3}v;$$

$$\vec{j}_{L_{i}}(a(\vec{x})) = \int \vec{v} I_{i}(\vec{v}) f(a(\vec{x}), \vec{v}) d^{3}v;$$

$$\sigma(a(\vec{x})) = \int \ln f(a(\vec{x}), \vec{v}) Q(f(a(\vec{x}), \vec{v}), f(a(\vec{x}), \vec{v})) d^{3}v;$$

$$r_{i}(a(\vec{x}), \vec{v}) = \int \ln f(a(\vec{x}), \vec{v}) Q(f(a(\vec{x}), \vec{v}), f(a(\vec{x}), \vec{v})) d^{3}v;$$

$$R_{i}(a(\vec{x})) = \int I_{i}(\vec{v})Q(f(a(\vec{x}), \vec{v}), f(a(\vec{x}), \vec{v}))d^{3}v \qquad (3. 11e)$$

Equations (3.11d) might be also treated as r dynamic equations for unknowns a_1, \ldots, a_r .

iii) <u>Dynamic invariance</u>. All considerations of Section 2 concerning construction of dynamic invariant manifolds are completely applicable to BE vector field (3.2). We

represent only an equation for the first correction to the locally *r*-dimensional manifold $\mathfrak{M}_0 = \{f_0(a(\vec{x}), \vec{v})\}.$

we search for a first correction in the form of (2.27):

$$f_{1}(a(\vec{x}), \vec{v}) = f_{0}(a(\vec{x}), \vec{v}) + \delta f_{1}(a(\vec{x}), \vec{v})$$
(3.12a)

Considering the thermodynamic parameterization of \mathfrak{M}_0 given with expressions (3.11), we obtain an equation (Method 2 of Section 2.3)):

$$(P_{a(\vec{x})}^{0*}(\cdot)-1)J_{lin, a(\vec{x})}^{0}(\delta f_{1}(a(\vec{x}), \vec{v})) + \Delta(f_{0}(a(\vec{x}), \vec{v})) = 0;$$

$$J^{0}\underset{\text{lin, }a(\vec{x})}{(g)} = -v_{S} \frac{\partial g}{\partial x_{S}} + L_{f_{0}}(a(\vec{x}), \vec{v})(g);$$

$$\Delta(f_0(a(\vec{x}), \vec{v})) = (P^*_{a(\vec{x})}(\cdot) - 1)J(f_0(a(\vec{x}), \vec{v}))$$
(3.12b)

Here L stands for the Boltzmann collision $f_0(a(\vec{x}), \vec{v})$ integral, linearized in the point $f_0(a(\vec{x}), \vec{v})$, and projector P^* , is defined according to (3.11c).

Additional conditions (2.28) for equation (3.12b) are:

$$\int \ln f(a(\vec{x}), \vec{v}) \delta f_{1}(a(\vec{x}), \vec{v}) d^{3}v = 0,$$

$$\int I_{i}(\vec{v}) \delta f_{1}(a(\vec{x}), \vec{v}) d^{3}v = 0, \quad i = 1, ..., r = 1 \quad (3.12c)$$

According to the iterative scheme of section 2.4, after solving equation (3.12b), we have to introduce new thermodynamic parameterization, and next we can make the second iteration, etc. In some cases, we can use linearizations of vector field different from that in equation (3.12b). For example, instead of the pure Newton scheme, we can use its Kantorovich's modification [22] (i.e. linearization of operator J(f) in a fixed point at every iteration).

iv) Invariance equation in a moving reference system.

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In some cases, it is convenient to consider BE vector field in a reference system which moves with the flow velocity. In this reference system, we define the BE vector field as:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = J_{u}(f), \qquad \frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + u_{\overrightarrow{x}, S}(f) \frac{\partial f}{\partial x_{S}};$$

$$J_{u}(f) = -(v_{S} - u_{\overrightarrow{x}, S}(f)) - \frac{\partial f}{\partial x_{S}} + Q(f, f) \qquad (3.13)$$

Here u_{\downarrow} (f) stands for the s-th component of the flow x, s velocity:

$$u_{\overrightarrow{x},S}(f) = n_{\overrightarrow{x}}^{-1}(f) \int v_{S} f(\overrightarrow{v},\overrightarrow{x}) d^{3}v; \quad n_{\overrightarrow{x}}(f) = \int f(\overrightarrow{v},\overrightarrow{x}) d^{3}v \quad (3.14)$$

In particular, this form of BE vector field is convenient when the initial manifold \mathfrak{M}_0 consists of functions $f_{\mathfrak{M}_0}$ which depend explicitly on $(\vec{v}-\vec{u}_{\vec{x}}(f))$ (i.e., if functions $f_{\mathfrak{M}_0} \in \mathfrak{M}_0$ do not change under velocity shifts: $\vec{v} \rightarrow \vec{v} + \vec{c}$, where \vec{c} is a constant vector).

Substituting $J_u(f)$ (3.13) instead of J(f) (3.2) into all expressions which depend on the BE vector field, we transfer all procedures developed above into the moving reference system. In particular, we obtain the following analog of the invariance equation of the first iteration (3.12b):

 $(P^{0*}_{a(\vec{x})}(\cdot)^{-1})J^{0}_{u, \min, a(\vec{x})}(\delta f_{1}(a(\vec{x}), \vec{v})) + \Delta(f_{0}(a(\vec{x}), \vec{v})) = 0;$ $J^{0}_{u, \min, a(\vec{x})}(g) = \{n^{-1}_{\vec{x}}(f_{0}(a(\vec{x})))) \int v_{s}gd^{3}v + \frac{1}{x} + u_{\vec{x}, s}(f_{0}(a(\vec{x})))n^{-1}_{\vec{x}}(f_{0}(a(\vec{x})))) \int gd^{3}v\} \frac{\partial f_{0}(a(\vec{x}), \vec{v})}{\partial x_{s}} - \frac{1}{x} + u_{\vec{x}, s}(f_{0}(a(\vec{x})))) \frac{\partial g}{\partial x_{s}} + L_{f_{0}}(a(\vec{x}), \vec{v})$

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$$\Delta(f_0(a(\vec{x}), \vec{v})) = (P^*_{a(\vec{x})}(\cdot) - 1)J_u(f_0(a(\vec{x}), \vec{v}))$$
(3.15)

Additional conditions (3.12c) do not depend on the vector field, and thus they remain valid for equation (3.15).

v) <u>Positivity and normalization</u>. When searching for a correction, we should be ready to face two problems that are typical for any method of successive approximations in BE theory. Namely, the first of this problems is that the correction

$$f_{\mathfrak{M}_{k+1}} = f_{\mathfrak{M}_k} + \delta f_{\mathfrak{M}_{k+1}}$$

obtained from the linearized invariance equation of the k+1-th iteration may be not a non-negatively defined function and thus it can not be used directly to define the thermodynamic projector for the k+1-th approximation. In order to overcome this difficulty, we can treat the procedure as a process of correcting the dual variable μ_f (3.9) rather than the process of immediate correcting the distribution functions. Then, at the k+1-th iteration, we search for new dual variables $\mu_f |_{\mathfrak{M}_{k+1}}$:

$$\mu_{f} |_{\mathfrak{M}_{k+1}} = \mu_{f} |_{\mathfrak{M}_{k}} + \delta \mu_{f} |_{\mathfrak{M}_{k+1}}$$
(3.16)

Due to the relationship $\mu_f \leftrightarrow f$ (3.9), we have:

$$\delta \mu_{f} |_{\mathfrak{M}_{k+1}} = \varphi_{\mathfrak{M}_{k+1}} + O(\delta f_{\mathfrak{M}_{k+1}}^{2}), \quad \varphi_{\mathfrak{M}_{k+1}} = f_{\mathfrak{M}_{k}} \delta f_{\mathfrak{M}_{k+1}}$$
(3.17)

Thus, solving the linear invariance equation of the k-th iteration with respect to the unknown function $\delta f_{\mathfrak{M}_{k+1}}$, we find a correction to the dual variable $\varphi_{\mathfrak{M}_{k+1}}$ (3.17), and we derive the corrected distributions $f_{\mathfrak{M}_{k+1}}$ as k+1

$$f_{\mathfrak{M}_{k+1}} = \exp(\mu_f |_{\mathfrak{M}_k} + \varphi_{\mathfrak{M}_{k+1}}) = f_{\mathfrak{M}_k} \exp(\varphi_{\mathfrak{M}_{k+1}})$$
(3.18)

Functions (3.18) are positive, and they satisfy the

invariance equation and the additional conditions of the type (3.12c) within the accuracy of $\varphi_{\mathfrak{M}_{k+1}}$.

However, the second difficulty which might occur is that functions (3.18) might have no finite integrals (3.1). In particular, this difficulty can be a result of some approximations used in solving equations (3.12b) or Hence, we have to "regularize" the functions (3.15).Α sketch of an approach to make this (3.18). $f_{\mathfrak{M}_{k+1}}$ regularization might be as follows: instead of (3.18), we consider functions:

$$f_{\mathfrak{M}_{k+1}}^{(\beta)} = f_{\mathfrak{M}_{k}} \exp(\varphi_{\mathfrak{M}_{k+1}} + \varphi^{\operatorname{reg}}(\beta))$$
(3.19)

Here $\varphi^{\text{reg}}(\beta)$ is a function labeled with $\beta \in B$, and B is a linear space. We assume that integrals (3.1a) and (3.1b) are finite for all values β in (3.19). Then we deriver β_* from the condition of coincidence of macroscopic parameters

$$M_{k}(f_{\mathfrak{M}_{k+1}}^{(\beta)}) = M_{k}(f_{\mathfrak{M}_{k}})$$
(3.20)

macroscopic mapping Here M is the of the *k*-th approximation. Further consideration of this procedure remains out of frames of this paper. In particular, (₽́*) regularization $f_{\mathfrak{M}}$ is required for the first time only at Step 4 of Section 2.4 (i.e. for obtaining thermodynamic equations for the first correction). The two difficulties mentioned here are not specific for the approximate method developed. For example, corrections to the LM distribution in the Chapman-Enskog method [1] and the thirteen-moment Grad approximation [4] are not non-negatively defined functions, while the thirteenmoment quasi-equilibrium approximation [10] has no finite integrals (3. 1a) and (3. 1b).

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4. CORRECTIONS TO THE LOCAL MAXWELL MANIFOLD

In this section we apply the method of invariant manifold to a particular situation when the initial manifold consists of local Maxwellians (2.4) (the LM manifold). This manifold and its corrections play the role the problem of derivation central in of hydrodynamics from BE. Hence, any method of approximate investigation of BE should be tested with the LM manifold. Classical methods (Chapman-Enskog and Hilbert methods) use Taylor-type expansions into powers of a small parameter (Knudsen number expansions). However, as the method of invariant mentioned above, we have manifold, generally speaking, assumes no small parameters, at least in its formal where part convergency properties are not discussed. will ₩e appropriate technique to consider develop an the invariance equation of the first iteration in Section 4.2. This involves ideas of parametrics expansions of the theory of pseudodifferential and Fourier integral operators [25, 26]. This approach will make it possible to reject the restriction of using small parameters.

4.1 Equation of First Iteration

The LM manifold consists of distributions f_0 which are labeled with parameters n, \vec{u} , and T:

$$f_{0}(n, \vec{u}, T) = n \left[\frac{2\pi k_{B}T}{m} \right]^{-3/2} \exp \left\{ -\frac{m(\vec{v} - \vec{u})^{2}}{2k_{B}T} \right\}$$
(4.1)

Parameters n, \vec{u} , and T in (4.1) are functions depending on \vec{x} . In this section we will not indicate this dependency explicitly.

Distribution $f_0(n, \vec{u}, T)$ is the unique solution of the variational problem:

$$H(f) = \int f \ln f d^{3} v \longrightarrow \min \quad \text{for} \quad M_{0}(f) = \int 1 \cdot f d^{3} v = n;$$

$$M_{i}(f) = \int v_{i} f d^{3} v = n u_{i}, \quad i = 1, 2, 3; \quad M_{4}(f) = \int v^{2} f d^{3} v = \frac{3nk_{B}T}{m} + n u^{2}$$
(4.2)

Hence, the LM manifold is a quasi-equilibrium manifold. Considering n, \vec{u} , and T as five scalar parameters (see the remark on locality in Section 3), we see that LM manifold is parameterized with the values of $M_S(f)$, $S=0,\ldots,4$, which are defined in the neighborhood of LM manifold. It is sometimes convenient to consider the variables $M_S(f_0)$, $S=0,\ldots,4$, as new coordinates on LM manifold. The relationship between the sets $\{M_S(f_0)\}$ and $\{n, \vec{u}, T\}$ is:

$$m = M_0; \qquad u_i = M_0^{-1} M_i, \quad i = 1, 2, 3; \qquad T = \frac{m}{3k_B} M_0^{-1} (M_4 - M_0^{-1} M_i M_i)$$
(4.3)

According to (4.2), the parameterization with $M_0(f_0), \ldots, M_4(f_0)$ (or, which is the same, with n, \vec{u} , and T) is thermodynamic.

Thermodynamic projector P (J) onto the $f_0(n, \vec{u}, T)$ tangent space T is defined as: $f_0(n, \vec{u}, T)$

$$P_{f_0(n, \vec{u}, T)}(J) = \sum_{S=0}^{4} \frac{\partial f_0(n, \vec{u}, T)}{\partial M_S} \int \psi_S J d^3 v$$
(4.4)

Here we have assumed that n, \vec{u} , and T are functions of M_0, \ldots, M_4 (see relationship (4.3)), and

$$\psi_0 = 1, \quad \psi_i = v_i, \quad i = 1, 2, 3, \quad \psi_4 = v^2$$
 (4.5)

Calculating derivatives in (4.4), and next returning to variables n, \vec{u} , and T, we obtain:

$$P_{f_{0}(n, \vec{u}, T)}(J) = f_{0}(n, \vec{u}, T) \left\{ \left[\frac{1}{n} - \frac{mu_{i}}{nk_{B}T}(v_{i} - u_{i}) + \left(\frac{mu^{2}}{3nk_{B}} - \frac{T}{n} \right) \left(\frac{m(\vec{v} - \vec{u})}{2k_{B}T^{2}} - \frac{3}{2T} \right) \right] \int 1 \cdot J d^{3}v + \left[\frac{m}{nk_{B}T}(v_{i} - u_{i}) - \frac{2mu_{i}}{3nk_{B}} \left(\frac{m(\vec{v} - \vec{u})}{2k_{B}T^{2}} - \frac{3}{2T} \right) \right] \int v_{i}J d^{3}v + \left[\frac{m}{nk_{B}T}(v_{i} - u_{i}) - \frac{2mu_{i}}{3nk_{B}} \left(\frac{m(\vec{v} - \vec{u})}{2k_{B}T^{2}} - \frac{3}{2T} \right) \right] \int v_{i}J d^{3}v + \left[\frac{m}{nk_{B}T}(v_{i} - u_{i}) - \frac{2mu_{i}}{3nk_{B}} \left(\frac{m(\vec{v} - \vec{u})}{2k_{B}T^{2}} - \frac{3}{2T} \right) \right] \int v_{i}J d^{3}v + \frac{m}{nk_{B}T}(v_{i} - u_{i}) - \frac{mu_{i}}{3nk_{B}} \left[\frac{m(\vec{v} - \vec{u})}{2k_{B}T^{2}} - \frac{3}{2T} \right] \left[\int v_{i}J d^{3}v + \frac{m}{nk_{B}T} \left(\frac{m}{nk_{B}T} \right) \right] \right]$$

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$$+ \frac{m}{3nk_{\rm B}} \left[\frac{m(\vec{v} - \vec{u})^{2}}{2k_{\rm B}T^{2}} - \frac{3}{2T} \right] \int v^{2}J d^{3}v \right\}$$
(4. 6a)
It is sometimes convenient to rewrite (4. 6a) as:

$$P_{f_{0}}(n, \vec{u}, T)^{(J)=f_{0}}(n, \vec{u}, T) \int_{s=0}^{4} \psi^{(S)} \int \psi^{(S)}(n, \vec{u}, T)^{J} d^{3}v (4. 6b)$$
Here

$$\psi^{(0)}_{f_{0}}(n, \vec{u}, T) = n^{-1/2}, \quad \psi^{(i)}_{f_{0}}(n, \vec{u}, T) = (\frac{2}{n})^{1/2}c_{i}, \quad i=1, 2, 3,$$

$$\psi^{(4)}_{f_{0}}(n, \vec{u}, T) = (\frac{2}{3n})^{1/2}(c^{2} - \frac{3}{2}); \quad c_{i} = (m/2k_{\rm B}T)^{1/2}(v_{i} - u_{i}) \quad (4. 7)$$
It is easy to check that

$$\int f_{0}(n, \vec{u}, T) \psi^{(k)}_{f_{0}}(n, \vec{u}, T) \int_{0}^{0}(n, \vec{u}, T) d^{3}v = \delta_{kI} \quad (4. 8)$$

Here δ_{kI} is the Kronecker delta.

The defect of the LM manifold at the point $f_0(n, \vec{u}, T)$ is:

$$\Delta(f_{0}(n,\vec{u},T)) = P_{f_{0}(n,\vec{u},T)} \left[-(v_{s}-u_{s}) \frac{\partial f_{0}(n,\vec{u},T)}{\partial x_{s}} + Q(f_{0}(n,\vec{u},T)) \right] - \left[-(v_{s}-u_{s}) \frac{\partial f_{0}(n,\vec{u},T)}{\partial x_{s}} + Q(f_{0}(n,\vec{u},T)) \right] =$$

$$= P_{f_{0}(n,\vec{u},T)} \left[-(v_{s}-u_{s}) \frac{\partial f_{0}(n,\vec{u},T)}{\partial x_{s}} \right] + (v_{s}-u_{s}) \frac{\partial f_{0}(n,\vec{u},T)}{\partial x_{s}} \quad (4.9)$$

Substituting (4.6a) into (4.9), we obtain:

$$\Delta (f_0(n, \vec{u}, T)) = f_0(n, \vec{u}, T) \left\{ \left[\frac{m(\vec{v} - \vec{u})^2}{2k_B T} - \frac{5}{2} \right] (v_j - u_j) \frac{\partial \ln T}{\partial x_j} + \frac{m}{k_B T} (((v_j - u_j))(v_s - u_s) - \frac{1}{3} \delta_{js} (\vec{v} - \vec{u})^2) \frac{\partial u_s}{\partial x_j} \right\}$$

$$(4. 10)$$

The LM manifold is not a dynamic invariant manifold of the Boltzmann equation (the defect (4.10) is not identical to zero). we search for a correction to the LM manifold as:

$$f_{1}(n, \vec{u}, T) = f_{0}(n, \vec{u}, T) + \delta f_{1}(n, \vec{u}, T)$$
(4.11)

In this paper we will use the Method 2 (see section 2.3) for obtaining the correction $\delta f_1(n, \vec{u}, T)$ because we search for a manifold of slow (hydrodynamic) motions. We introduce the representation:

$$\delta f_{1}(n, \vec{u}, T) = f_{0}(n, \vec{u}, T) \varphi(n, \vec{u}, T)$$
(4.12)

Then the equation of the first iteration in the form of (3.17) for the correction $\varphi(n, \vec{u}, T)$ is:

$$\begin{cases} P_{f_0(n,\vec{u},T)}(\cdot) -1 \} (-(v_s - u_s) \frac{\partial f_0(n,\vec{u},T)}{\partial x_s} + \\ +f_0(n,\vec{u},T) L_{f_0(n,\vec{u},T)}(\phi) - (v_s - u_s) \frac{\partial (f_0(n,u,T)\phi)}{\partial x_s} - \\ -n^{-1} (f_0(n,\vec{u},T)) [\int v_s f_0(n,\vec{u},T) \phi d^3 v + \\ +u_s (f_s(n,\vec{u},T)) [\int (n,\vec{u},T) \phi d^3 v + \\ +u_s (f_s(n,\vec{u},T)) [f_s(n,\vec{u},T) \phi d^3 v] \frac{\partial f_0(n,\vec{u},T)}{\partial x_s} = 0 \end{cases}$$

$$(A = 13a)$$

$$+u_{S}(f_{0}(n, u, T)) \downarrow f_{0}(n, u, T) \varphi d^{s}v] \xrightarrow{\circ} \partial x_{S}$$
Here $f_{0}(n, u, T) \downarrow I_{0}(n, u, T) \varphi d^{s}v$ (4. 13a)

Here $f_0(n, \dot{u}, T)L$ (ϕ) is the linearized Boltzmann $f_0(n, \dot{u}, T)$ collision integral:

$$L_{f_{0}(n, \vec{u}, T)}(\phi) = \int W(\vec{v}', \vec{v}_{1}' | \vec{v}, \vec{v}_{1}) f_{10}(n, \vec{u}, T) \times (\phi' + \phi'_{1} - \phi_{1} - \phi_{1}$$

and $w(\vec{v}', \vec{v}'_1 | \vec{v}, \vec{v}'_1)$ is the kernel of the Boltzmann collision integral, standard notations label the velocities before and after a collision.

Additional condition (3.14c) for equation (4.13a) has the form:

$$P_{f_0(n, \vec{u}, T)}(f_0(n, \vec{u}, T)\phi) = 0$$
(4.15)

In detail notation:

 $\int \mathbf{1} \cdot f_0(n, \vec{u}, T) \varphi d^3 v = 0, \quad \int v_i f_0(n, \vec{u}, T) \varphi d^3 v = 0, \quad i = 1, 2, 3,$

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$$\int v^2 f_0(n, \vec{u}, T) \phi d^3 v = 0$$
 (4.16)

Eliminating in (4.13a) the terms containing $\int v_s f_0(n, \vec{u}, T) \varphi d^3 v$ and $\int f_0(n, \vec{u}, T) \varphi d^3 v$ with the aid of (4.16), we obtain the following form of equation (4.13a):

$$\left\{P_{f_0(n,\vec{u},T)}(\cdot)^{-1}\right\}(-(v_s^{-u_s})\frac{\partial f_0(n,\vec{u},T)}{\partial x_s} + \right.$$

 $+f_{0}(n, \vec{u}, T)L (\varphi) - (v_{s}-u_{s})\frac{\partial(f_{0}(n, \vec{u}, T)\phi)}{\partial x_{s}} = 0 \quad (4. 13b)$

In order to consider the properties of equation (4.13b), it is useful to introduce real Hilbert spaces G with scalar products: $f_0(n, \vec{u}, T)$

$$(\Psi, \Psi) = \int f_0(n, \vec{u}, T) \Phi \psi d^3 v$$
 (4.17)

Each Hilbert space is associated with the corresponding LM distribution $f_0(n, \vec{u}, T)$.

The projector P (4.6b) is associated with a $f_0(n, \vec{u}, T)$

projector Π which acts in the space G : $f_0(n, \vec{u}, T)$

$$\Pi_{f_0(n, \vec{u}, T)}(\phi) = f_0^{-1}(n, \vec{u}, T)P_{f_0(n, \vec{u}, T)}(f_0(n, \vec{u}, T)\phi)$$
(4.18)

It is an orthogonal projector because

$$\Pi_{f_0(n, \vec{u}, T)} (\phi) = \sum_{s=0}^{4} \phi(s) (\phi(s)) (\phi(s))$$

Here $\psi^{(s)}_{f_0(n, \vec{u}, T)}$ are given by the expression (4.7).

we can rewrite the equation of the first iteration (4.13b) in the form:

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$$L_{f_0(n, \vec{u}, T)}^{(\psi) + K} f_0(n, \vec{u}, T)^{(\psi)} = D_{f_0(n, \vec{u}, T)}^{(4.20)}$$

Notations used here are:

$$D_{f_{0}(n,\vec{u},T)} = f_{0}^{-1}(n,\vec{u},T) \Delta(f_{0}(n,\vec{u},T)); \qquad K_{f_{0}(n,\vec{u},T)}(\phi) = f_{0}^{-1}(n,\vec{u},T) \Delta(f_{0}(n,\vec{u},T)); \qquad K_{f_{0}(n,\vec{u},T)}(\phi) = f_{0}^{-1}(n,\vec{u},T) (v_{s}-u_{s}) \frac{\partial(f_{0}(n,\vec{u},T)\phi)}{\partial x_{s}} (4.21)$$

The additional condition for equation (4.20) is:

$$(\psi^{(S)}_{0}, \vec{u}, \vec{T}), \psi^{(S)}_{0}, \vec{u}, \vec{T}) = 0, \quad S = 0, \dots, 4$$
 (4.22)

Now we will list the properties of the equation (4.20) for usual models of a collision [1]: a) The linear integral operator $\int_{0}^{L} (n, \vec{u}, T)$ is selfadjoint in the scalar product $(\cdot, \cdot)_{f_0(n, \vec{u}, T)}$, and the quadric form $(\varphi, L, (\varphi))$ is negatively defined $f_{\varphi}(n, \vec{u}, T)$ in ImL $f_0(n, \vec{u}, T)$ b) The kernel of L does not depend on $f_0(n, \vec{u}, T)$, $f_0(n, \vec{u}, T)$ and it is the linear envelope of the polynomials $\psi_0=1$, $\psi_{i} = v_{i}, \quad i = 1, 2, 3, \text{ and } \psi_{4} = v^{2}.$ c) The RHS D is orthogonal to kerL in $f_0(n, \vec{u}, T)$ is orthogonal to kerL in $f_0(n, \vec{u}, T)$ the sense of the scalar product $(\cdot, \cdot)_{f_0(n, \vec{u}, T)}$. d) The projecting operator Π $f_0(n, \vec{u}, T)$ is the selfadjoint projector onto kerL $f_0(n, \vec{u}, T)$ $\Pi_{f_0(n, \vec{u}, T)} (\phi) \in \ker L_{f_0(n, \vec{u}, T)}$ (4.23)

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projects orthogonally. Projector II $f_0(\vec{n}, \vec{u}, T)$ is orthogonal to $f_0(n, \vec{u}, T)$ e) The image of the operator K $\ker L f_0(n, \vec{u}, T)$

f) Additional condition (4.22) require the solution of equation (4.20) to be orthogonal to kerL $f_0(n, \vec{u}, T)$

These properties result in the necessity condition solving the equation (4.20) with the additional for constraint (4.22). This means the following: equation (4.20), provided with constraint (4.22), satisfies the necessary condition for to have an unique solution in ImL

 $f_0(n, \vec{u}, T)$

<u>Remark</u>. Because of the *differential* part of the operator are not able to apply the Fredholm ₩e $f_0(n, \vec{u}, T)$

alternative to obtain the necessary and sufficient conditions for solvability of equation (4.22). Thus, the condition mentioned here is, rigorously speaking, only the necessity condition. Nevertheless, we will still develop a formal procedure for solving the equation (4.20).

To this end, we paid no attention to the dependency of all functions, spaces, operators, etc, on \vec{x} . It is useful to rewrite once again the equation (4.20) in order to separate the local in \vec{x} operators from those differential. Furthermore, we will replace the subscript $f_0(n, \vec{u}, T)$ with the subscript \vec{x} in all expressions. We represent (4.20) as:

$$A_{\text{loc}}(\vec{x}, \vec{v}) \Phi - A_{\text{diff}}(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v}) \Phi = -D(\vec{x}, \vec{v});$$
$$A_{\text{loc}}(\vec{x}, \vec{v}) \Phi = -\{L_{\vec{x}}(\vec{v}) \Phi + (\prod_{\vec{x}} (\vec{v}) - 1)\Gamma_{\vec{x}} \Phi\};$$

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$$\begin{split} &A_{\text{diff}}(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v}) \Phi = (\prod_{\vec{x}} (\cdot)^{-1}) ((v_{s}^{-}u_{s}^{-}) \frac{\partial}{\partial x_{s}} \Phi); \\ &\Pi_{\vec{x}}(\vec{v}) \quad g = \sum_{s=0}^{4} \psi_{\vec{x}}^{(s)}(\psi_{\vec{x}}^{(s)}, g); \\ &\psi_{\vec{x}}^{(0)} = n^{-1/2}, \quad \psi_{\vec{x}}^{(s)} = (\frac{2}{n})^{1/2} c_{\vec{x}}(\vec{x}, \vec{v}), \quad s = 1, 2, 3, \\ &\psi_{\vec{x}}^{(4)} = (\frac{2}{3n})^{1/2} (c_{\vec{x}}^{(\vec{x},\vec{v})} - \frac{3}{2}); \quad c_{\vec{x}}(\vec{x}, \vec{v}) = (m/2k_{B}T(\vec{x}))^{1/2} (v_{\vec{x}}^{-}u_{\vec{x}}(\vec{x})) \\ &r_{\vec{x}}^{=} (v_{s}^{-}u_{s}) \left(\frac{\partial \ln n}{\partial x_{s}} + \frac{m}{k_{B}T} (v_{\vec{x}}^{-}u_{\vec{x}}) \frac{\partial u_{\vec{x}}}{\partial x_{s}} + \left(\frac{m(\vec{v} - \vec{u})^{2}}{2k_{B}T}^{2} - \frac{3}{2} \right) \frac{\partial \ln T}{\partial x_{s}} \right]; \\ &D(\vec{x}, \vec{v}) = \left\{ \left(\frac{m(\vec{v} - \vec{u})^{2}}{2k_{B}T} - \frac{5}{2} \right) (v_{\vec{x}}^{-}u_{\vec{x}}) \frac{\partial \ln T}{\partial x_{\vec{x}}} + \frac{m}{k_{B}T} (((v_{\vec{x}}^{-}u_{\vec{x}}))^{-\frac{1}{3}} \delta_{\vec{x}s}(\vec{v} - \vec{u})^{2}) \frac{\partial u_{s}}{\partial x_{\vec{x}}} \right\}$$

$$(4. 24)$$

Here we have omitted the dependence on \vec{x} in the functions $n(\vec{x})$, $u_{\vec{x}}(\vec{x})$, and $T(\vec{x})$. Further, if no discrepancy might occur, we will always assume this dependence, and we will not indicate it explicitly.

The additional condition for this equation is:

 $\prod_{X} (\varphi) = 0$

Equation (4.24) is linear in φ . However, the main difficulty in solving this equation is caused with the differential in \vec{x} operator A_{diff} which does not commutate with the local in \vec{x} operator A_{loc} .

4. 2 Parametrics Expansion

section we introduce a procedure In this to construct approximate solutions of equation (4.23). This procedure involves an expansion similar to the parametrics in the theory of expansion pseudodifferential (PDO) and Fourier integral operators (FIO).

Considering $\varphi \in ImL_{x}$, we write a formal solution of x

equation (4.24) as:

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$$\varphi(\vec{x}, \vec{v}) = (A_{10C}(\vec{x}, \vec{v}) - A_{diff}(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v}))^{-1}(-D(\vec{x}, \vec{v})) \qquad (4.25)$$

It is useful to extract the differential operator $\frac{\partial}{\partial \vec{x}}$ from out the operator $A_{\text{diff}}(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v})$:

$$\varphi(\vec{x}, \vec{v}) = (1 - B_S(\vec{x}, \vec{v}) \frac{\partial}{\partial x_S})^{-1} \varphi_{1oc}(\vec{x}, \vec{v})$$
(4.26)

Notations used here are:

$$\begin{split} \varphi_{1 \text{ oc}}(\vec{x}, \vec{v}) &= A_{1 \text{ oc}}^{-1}(\vec{x}, \vec{v}) (-D(\vec{x}, \vec{v})) = \\ &= [-L_{\vec{x}}(\vec{v}) - (\Pi_{\vec{x}}(\vec{v}) - 1)\Gamma_{\vec{x}}]^{-1} (-D(\vec{x}, \vec{v})); \\ B_{S}(\vec{x}, \vec{v}) &= A_{1 \text{ oc}}^{-1}(\vec{x}, \vec{v}) (\Pi_{\vec{x}}(\vec{v}) - 1) (v_{S} - u_{S}) = \\ &= [-L_{\vec{x}}(\vec{v}) - (\Pi_{\vec{x}}(\vec{v}) - 1)\Gamma_{\vec{x}}]^{-1} (\Pi_{\vec{x}}(\vec{v}) - 1) (v_{S} - u_{S}) \\ \end{split}$$
(4. 27)

We will now discuss in more detail the character of expressions in (4.27).

For every \vec{x} , the function $\varphi_{loc}(\vec{x}, \vec{v})$, considered as a function of \vec{v} , is an element of the Hilbert space $G_{\vec{x}}$. It gives a solution to the integral equation:

$$-L_{\vec{x}}(\vec{v})\phi_{1\text{oc}} - (\prod_{\vec{x}}(\vec{v}) - 1)(\Gamma_{\vec{x}}\phi_{1\text{oc}}) = (-D(\vec{x}, \vec{v}))$$
(4.28)

This latter linear integral equation has an unique solution in $imL_{\downarrow}(\vec{v})$. Indeed,

$$\ker A_{1 \text{ oc}}^{+}(\vec{x}, \vec{v}) = \ker (L_{\vec{x}}(\vec{v}) + (\Pi_{\vec{x}}(\vec{v}) - 1)r_{\vec{x}})^{+} = \\ = \ker (L_{\vec{x}}(\vec{v}))^{+} \cap \ker (r_{\vec{x}}(\Pi_{\vec{x}}(\vec{v}) - 1)), \text{ and } G_{\vec{x}} \cap \Pi_{\vec{x}}(\vec{v})G_{\vec{x}} = \{0\}.$$

Thus, the existence of the unique solution of equation (4.28) follows from the Fredholm alternative.

Consider the operator $R(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v})$:

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$$R(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v}) = (1 - B_{S}(\vec{x}, \vec{v}) \frac{\partial}{\partial x_{S}})^{-1}$$
(4.29)

One can represent it as a formal series:

$$R(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v}) = \sum_{m=0}^{\omega} \left[B_{S}(\vec{x}, \vec{v}) \frac{\partial}{\partial x_{S}} \right]^{m}$$
(4.30)

Here

$$[B_{S}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S}}]^{m} = B_{S_{1}}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S_{1}}} \dots B_{S_{m}}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S_{m}}}$$
(4.31)

Every term of the type (4.31) can be represented as a finite sum of operators which are superpositions of the following two operations: of the integral in \vec{v} operations with kernels depending on \vec{x} , and of differential in \vec{x} operations.

Our goal is to obtain an explicit representation of the operator $R(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v})$ (4.29) as an integral operator. If the operator $B_S(\vec{x}, \vec{v})$ would not depend on \vec{x} (i.e. if no dependence on spatial variables would occur in kernels of integral operators, in $B_S(\vec{x}, \vec{v})$), then we could reach our goal via usual Fourier transformation. However, operators $B_S(\vec{x}, \vec{v})$ and $\frac{\partial}{\partial x_k}$ do not commutate, and thus this elementary approach does not work. We will develop a method to obtain the required explicit representation using the ideas of PDO and IOF technique.

We start with the representation (4.30). Our strategy is to transform every summand (4.31) in order to place integral in \vec{v} operators $B_S(\vec{x}, \vec{v})$ left to differential operators $\frac{\partial}{\partial x_k}$. The transposition of every pair $\frac{\partial}{\partial x_k} B_S(\vec{x}, \vec{v})$ yields an elementary transform:

$$\frac{\partial}{\partial x_k} B_{\mathcal{S}}(\vec{x}, \vec{v}) \rightarrow B_{\mathcal{S}}(\vec{x}, \vec{v}) \frac{\partial}{\partial x_k} - [B_{\mathcal{S}}(\vec{x}, \vec{v}), \frac{\partial}{\partial x_k}] \quad (4.32)$$

Here [M, N] = MN - NM denotes the commutator of operators M and N. We can represent (4.31) as:

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$$[B_{S}(\vec{x}, \vec{v}) \frac{\partial}{\partial x_{S}}]^{II} = B_{S_{1}}(\vec{x}, \vec{v}) \dots B_{S_{II}}(\vec{x}, \vec{v}) \frac{\partial}{\partial x_{S_{1}}} \dots \frac{\partial}{\partial x_{S_{II}}} + \\ + O([B_{S_{I}}(\vec{x}, \vec{v}), \frac{\partial}{\partial x_{S_{II}}}])$$
(4.33)

Here $O([B_{s_{j}}(\vec{x},\vec{v}),\frac{\partial}{\partial x_{s_{k}}}])$ denotes the terms which contain one or more pairs of brackets $[\cdot, \cdot]$. The first term in (4.33) contains no these brackets. We can continue this process of selection and extract the first-order in the number of pairs of brackets terms, the second-order terms, etc. Thus, we arrive at the **expansion into powers** of commutator of the expressions (4.31).

In this paper we will consider explicitly the zeroth-order term of this commutator expansion. Neglecting all terms with brackets in (4.33), we write:

$$[B_{S}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S}}]^{m}_{0} = B_{S_{1}}(\vec{x},\vec{v})\dots B_{S_{m}}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S_{1}}}\dots \frac{\partial}{\partial x_{S_{m}}} (4.33a)$$

Here the subscript zero indicates the zeroth order with respect to the number of brackets.

We now substitute expressions $[B_{S}(\vec{x}, \vec{v})\frac{\partial}{\partial x_{S}}]^{m}_{0}$ (4.33a) instead of expressions $[B_{S}(\vec{x}, \vec{v})\frac{\partial}{\partial x_{S}}]^{m}$ (4.31) into the series (4.30):

$$R_{0}(\vec{x}, \frac{\partial}{\partial \vec{x}}, \vec{v}) = \sum_{m=0}^{\infty} \left[B_{S}(\vec{x}, \vec{v}) \frac{\partial}{\partial x_{S}} \right]^{m}$$
(4.30a)

The action of every summand (4.33a) might be defined via the Fourier transform with respect to spatial variables.

Denote as F the direct Fourier transform of a function $g(\vec{x}, \vec{v})$:

$$Fg(\vec{x}, \vec{v}) \equiv \hat{g}(\vec{k}, \vec{v}) = \int g(\vec{x}, \vec{v}) \exp(-ik_S x_S) d^{p}x \qquad (4.34a)$$

Here p is the spatial dimension. Then the inverse Fourier transform is:

$$g(\vec{x}, \vec{v}) \equiv F^{-1}\hat{g}(\vec{k}, \vec{v}) = (2\pi)^{-p} \int \hat{g}(\vec{k}, \vec{v}) \exp(ik_{s}x_{s}) d^{p}k \qquad (4.34b)$$

The action of the operator (4.33a) on a function $g(\vec{x}, \vec{v})$ is defined as:

$$[B_{S}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S}}]^{m}_{0}g(\vec{x},\vec{v}) =$$

$$=(B_{S_{1}}(\vec{x},\vec{v})\dots B_{S_{m}}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S_{1}}}\dots \frac{\partial}{\partial x_{S_{m}}})(2\pi)^{-p}\hat{g}(\vec{k},\vec{v})e^{ik}s^{x}sd^{p}k =$$

$$=B_{S_{1}}(\vec{x},\vec{v})\dots B_{S_{m}}(\vec{x},\vec{v})\frac{\partial}{\partial x_{S_{1}}}\dots \frac{\partial}{\partial x_{S_{m}}})(2\pi)^{-p}\hat{g}(\vec{k},\vec{v})e^{ik}s^{x}sd^{p}k =$$

$$= (2\pi)^{-p} \int \exp(ik_{s}x_{s}) [ik_{l}B_{l}(\vec{x},\vec{v})]^{m} g(\vec{k},\vec{v}) d^{p}k \qquad (4.35)$$
The account of (4.35) in the formula (4.30a) yields the

The account of (4.35) in the formula (4.30a) yields the following definition of the operator R_0 :

$$R_{0}g(\vec{x},\vec{v}) = (2\pi)^{-p} \int e^{ik} s^{x} s(1-ik_{l}B_{l}(\vec{x},\vec{v}))^{-1} \hat{g}(\vec{k},\vec{v}) d^{p}k \qquad (4.36)$$

This is the Fourier integral operator (note that the kernel of this integral operator depends on \vec{k} and on \vec{x}). The commutator expansion introduced above is a version of the parametrics expansion [25, 26], while expression (4.36) is the leading term of this expansion. The kernel $(1-ik_{I}B_{I}(\vec{x},\vec{v}))^{-1}$ is called the main symbol of the parametrics.

The account of (4.36) in the formula (4.26) yields the zeroth-order term of parametrics expansion $\varphi_0(\vec{x}, \vec{v})$:

$$\varphi_{0}(\vec{x}, \vec{v}) = F^{-1} (1 - ik_{I}B_{I}(\vec{x}, \vec{v}))^{-1}F\varphi_{1}oc \qquad (4.37)$$

In detail notation:

$$\varphi_{0}(\vec{x},\vec{v}) = (2\pi)^{-p} \int \exp(ik_{S}(x_{S}-y_{S}))^{\times} \\ \times (1-ik_{S}[-L_{\vec{x}}(\vec{v}) - (\Pi_{\vec{x}}(\vec{v}) - 1)r_{\vec{x}}]^{-1} (\Pi_{\vec{x}}(\vec{v}) - 1)(v_{S}-u_{S}(\vec{x})))^{-1} \\ \times [-L_{\vec{x}}(\vec{v}) - (\Pi_{\vec{y}}(\vec{v}) - 1)r_{\vec{y}}]^{-1} (-D(\vec{y},\vec{v}))d^{p}yd^{p}k$$

$$(4.38)$$

we now will list the steps to calculate the function $\varphi_0(\vec{x}, \vec{v})$ (4.38).

Step 1. Solve the linear integral equation

$$\begin{bmatrix} -L_{\vec{x}}(\vec{v}) - (\prod_{\vec{x}}(\vec{v}) - 1)r_{\vec{x}}] \phi_{1oc}(\vec{x}, \vec{v}) = -D(\vec{x}, \vec{v})$$
(4.39a)

and obtain the function $\varphi_{loc}(\vec{x}, \vec{v})$. <u>Step 2</u>. Calculate the Fourier transform $\hat{\varphi}_{loc}(\vec{k}, \vec{v})$:

$$\hat{\varphi}_{\text{loc}}(\vec{k},\vec{v}) = \int \varphi_{\text{loc}}(\vec{y},\vec{v}) \exp(-ik_{s}y_{s}) d^{p}y \qquad (4.39b)$$

<u>Step 3</u>. Solve the linear integral equation

$$\begin{bmatrix} -L_{\vec{x}}(\vec{v}) - (\prod_{\vec{x}}(\vec{v}) - 1)(r_{\vec{x}} + ik_{s}(v_{s} - u_{s}(\vec{x}))) \hat{\psi}_{0}(\vec{x}, \vec{k}, \vec{v}) = -\hat{D}(\vec{x}, \vec{k}, \vec{v});$$

$$-\hat{D}(\vec{x}, \vec{k}, \vec{v}) = [-L_{\vec{x}}(\vec{v}) - (\prod_{\vec{x}}(\vec{v}) - 1)r_{\vec{x}}]\hat{\Psi}_{loc}(\vec{k}, \vec{v})$$
(4.39c)

and obtain the function $\hat{\varphi}_0(\vec{x}, \vec{k}, \vec{v})$. <u>Step 4</u>. Calculate the inverse Fourier transform $\varphi_0(\vec{x}, \vec{v})$:

$$\varphi_0(\vec{x}, \vec{v}) = (2\pi)^{-p} \int \hat{\varphi}_0(\vec{x}, \vec{k}, \vec{v}) \exp(ik_s x_s) d^p k \qquad (4.39d)$$

Completing these four steps, we obtain an explicit expression for the zeroth-order term of parametrics expansion $\varphi_0(\vec{x}, \vec{v})$ (4.37).

As we have already mentioned above, equation (4.39a) of Step 1 has an unique solution in $imL_{\vec{x}}(\vec{v})$. Equation (4.39c) of Step 3 has the same property. Indeed, for every \vec{k} , the RHS $-\hat{D}(\vec{x}, \vec{k}, \vec{v})$ is orthogonal to $im\Pi_{\vec{x}}(\vec{v})$, and thus the existence and the uniqueness of formal solution $\hat{\varphi}_0(\vec{x}, \vec{k}, \vec{v})$ follows again from the Fredholm alternative.

Thus, in Step 3, we obtain the unique solution $\hat{\Psi}_0(\vec{x}, \vec{k}, \vec{v})$. For every \vec{k} , this is a function which belongs to $\operatorname{im} L_{\vec{x}}(\vec{v})$. Accounting that $f_0(\vec{x}, \vec{v}) = f_0(n(\vec{x}), \vec{u}(\vec{x}), T(\vec{x}), \vec{v})$ expose no explicit dependency on \vec{x} , we see that the inverse Fourier transform of Step 4 gives $\Psi_0(\vec{x}, \vec{v}) \in \operatorname{im} L_{\vec{x}}(\vec{v})$.

Equations (4.39a)-(4.39d) provide us with the scheme of constructing the zeroth-order term of parametrics expansion. Finishing this section, we will outline briefly the way to calculate the first-order term of this expansion. Consider a formal operator $R=(1-AB)^{-1}$. Operator R is defined by a formal series:

$$R = \sum_{m=0}^{\infty} (AB)^{m} \qquad (4.40)$$

In every term of this series, we want to place operators A left to operators B. In order to do this, we have to commutate B with A from left to right. The commutation of every pair BA yields the elementary transform

$$BA \xrightarrow{\cdot} AB - [A, B]$$

where [A, B] = AB - BA. Extracting the terms with no commutators [A, B] and with a single commutator [A, B], we arrive at the following representation:

 $R=R_0+R_1+(\text{terms with more than two brackets})$ (4.41a) Here

$$R_0 = \sum_{m=0}^{\infty} A^m B^m; \qquad (4.41b)$$

$$R_{1} = -\sum_{m=2}^{\infty} \sum_{i=2}^{m} i A^{m-i} [A, B] A^{i-1} B^{i-1} B^{m-i}$$
(4.41c)

Operator R_0 (4.41b) is the zeroth-order term of parametrics expansion derived above. Operator R_1 (the **first-order term of parametrics expansion**) can be represented as follows:

$$R_{1} = -\sum_{m=1}^{\infty} m A^{m} [A, B] \left(\sum_{i=0}^{\infty} A^{i} B^{i} \right) B^{m} = -\sum_{m=1}^{\infty} m A^{m} C B^{m}, \quad C = [A, B] R_{0} \quad (4. 41d)$$

This expression can be considered as an *ansatz* for the formal series (4.40), and it gives the most convenient way to calculate R_1 . Its structure is similar to that of R_0 . Continuing in this manner, we can derive the second-order term R_2 , etc. We will not discuss these questions in this paper.

In the next section we will consider in a more detail the first-order term of parametrics expansion.

4.3 Finite-Dimensional Approximations to Integral Equations

Dealing further only with the zeroth-order term of parametrics expansion (4.38), we have to solve two linear integral equations, (4.39a) and (4.39c). These equations satisfy the Fredholm alternative, and thus they have unique solutions. The problem we face here is exactly of the same level of complexity as that of the Chapman-Enskog method [1]. The usual approach is to replace integral operators with some appropriate finite-dimensional operators.

First we will recall standard objectives of finitedimensional approximations, considering equation (4.39a). Let $p_i(\vec{x}, \vec{v})$, where i=1, 2, ..., be a basis in $\operatorname{im} L_{\vec{x}}(\vec{v})$. Every function $\phi(\vec{x}, \vec{v}) \in \operatorname{im} L_{\vec{x}}(\vec{v})$ might be represented in this basis as:

$$\varphi(\vec{x}, \vec{v}) = \sum_{i=1}^{\infty} a_i(\vec{x}) p_i(\vec{x}, \vec{v}); \quad a_i(\vec{x}) = (\varphi(\vec{x}, \vec{v}), p_i(\vec{x}, \vec{v}))_{\vec{x}} \quad (4.42)$$

Equation (4.39a) is equivalent to an infinite set of linear algebraic equations with respect to unknowns $a_{i}(\vec{x})$:

$$\sum_{i=1}^{\infty} m_{ki}(\vec{x}) a_{i}(\vec{x}) = d_{k}(\vec{x}), \quad k=1, 2, \dots$$
(4.43)

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$$m_{ki}(\vec{x}) = (p_k(\vec{x}, \vec{v}), A_{10c}(\vec{x}, \vec{v}) p_i(\vec{x}, \vec{v}))_{\vec{x}};$$

$$d_k(\vec{x}) = -(p_k(\vec{x}, \vec{v}), D(\vec{x}, \vec{v}))_{\vec{x}}$$
(4.44)

For a finite-dimensional approximation of equation (4.43) we use a projection onto a finite number of basis elements $p_{i}(\vec{x}, \vec{v}), \quad i=i_{1}, \ldots, i_{n}$. Then, instead of (4.42), we search for the function φ_{fin} :

$$\varphi_{\text{fin}}(\vec{x}, \vec{v}) = \sum_{S=1}^{H} a_{i_{S}}(\vec{x}) p_{i_{S}}(\vec{x}, \vec{v})$$
(4.45a)

Infinite set of equations (4.43) is replaced with a

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finite set of linear algebraic equations with respect to $a_{i_{s}}(\vec{x})$, where $s=1, \ldots, n$:

$$\sum_{l=1}^{n} m_{i_{s}} i_{l} (\vec{x}) a_{i_{l}} (\vec{x}) = d_{i_{s}} (\vec{x}), \quad s = 1, \dots, n \quad (4.45b)$$

There are no a priori restrictions upon the choice of the basis, as well as upon the choice of its finite-dimensional approximations. In this paper we use the standard basis of unreducible Hermit tensors (see, for example, [2, 4]). The simplest appropriate version of a finite-dimensional approximation occurs if the finite set of Hermit tensors is chosen as:

$$p_{k}(\vec{x}, \vec{v}) = c_{k}(\vec{x}, \vec{v}) (c^{2}(\vec{x}, \vec{v}) - \frac{5}{2}), \quad k = 1, 2, 3;$$

$$p_{i,j}(\vec{x}, \vec{v}) = c_{i}(\vec{x}, \vec{v}) c_{j}(\vec{x}, \vec{v}) - \frac{1}{3} \delta_{i,j} c^{2}(\vec{x}, \vec{v}), \quad i, j = 1, 2, 3;$$

$$c_{i}(\vec{x}, \vec{v}) = v_{T}^{-1}(\vec{x}) (v_{i} - u_{i}(\vec{x})), \quad v_{T}(\vec{x}) = (2k_{B}T(\vec{x})/m)^{1/2} \quad (4.46)$$

It is important to stress here that "good" properties of orthogonality of Hermit tensors, as well as of other similar polynomial systems in BE theory, have the local in \vec{x} character, i. e. when these functions are treated as polynomials in $\vec{c}(\vec{x}, \vec{v})$ rather than polynomials in \vec{v} . For example, functions $p_k(\vec{x}, \vec{v})$ and $p_{jj}(\vec{x}, \vec{v})$ (4.46) are orthogonal in the sense of the scalar product $(\cdot, \cdot)_{,:}$

 $(p_k(\vec{x}, \vec{v}), p_{ij}(\vec{x}, \vec{v}))_{\vec{x}} \propto e^{-c^2(\vec{x}, \vec{v})} p_k(\vec{x}, \vec{v}) p_{ij}(\vec{x}, \vec{v}) d^3 c(\vec{x}, \vec{v}) = 0$ On contrary, functions $p_k(\vec{y}, \vec{v})$ and $p_{ij}(\vec{x}, \vec{v})$ are not orthogonal neither in the sense of the scalar product $(\cdot, \cdot)_{\vec{y}}$, nor in the sense of the scalar product $(\cdot, \cdot)_{\vec{y}}$, if $\vec{y} \neq \vec{x}$. This distinction is important for constructing the parametrics expansion. Further, we will omit the dependencies on \vec{x} and \vec{v} in the dimensionless velocity $c_j(\vec{x}, \vec{v})$ (4. 46) if no misunderstanding might occur.

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In this paper we will consider the case of one-dimensional in \vec{x} equations. We assume that:

$$u_1(\vec{x}) = u(x_1), \quad u_2 = u_3 = 0, \quad T(\vec{x}) = T(x_1), \quad n(\vec{x}) = n(x_1)$$
(4.47)

We write x instead of x_1 below. Finite-dimensional approximation (4.46) requires only two functions:

$$p_{3}(x, \vec{v}) = c_{1}^{2}(x, \vec{v}) - \frac{1}{3}c^{2}(x, \vec{v}), \quad p_{4}(x, \vec{v}) = c_{1}(x, \vec{v})(c^{2}(x, \vec{v}) - \frac{5}{2}),$$

$$c_{1}(x, \vec{v}) = v_{T}^{-1}(x)(v_{1} - u(x)), \quad c_{2, 3}(x, \vec{v}) = v_{T}^{-1}(x)v_{2, 3} \quad (4.48)$$

we now will make a step-by-step calculation of the zeroth-order term of parametrics expansion, in the case, for the finite-dimensional one-dimensional approximation (4.48).

<u>Step 1</u>. Calculation of $\varphi_{loc}(x, \vec{v})$ from equation (4.39a). we search for the function $\varphi_{loc}(x, \vec{v})$ in the

approximation (4.48) as:

$$\varphi_{1oc}(x, \vec{v}) = a_{1oc}(x) \left(c_1^2 - \frac{1}{3}c^2 \right) + b_{1oc}(x) c_1 \left(c^2 - \frac{5}{2} \right)$$
(4.49)

Finite-dimensional approximation (4.45b) of integral equation (4.39a) in the basis (4.48) yields;

$$m_{33}(x)a_{1oc}(x)+m_{34}(x)b_{1oc}(x)=\alpha_{1oc}(x);$$

$$m_{43}(x)a_{10c}(x) + m_{44}(x)b_{10c}(x) = \beta_{10c}(x); \qquad (4.50)$$

Notations used are:

$$\begin{split} m_{33}(x) &= n(x)\lambda_{3}(x) + \frac{11}{9} \frac{\partial u}{\partial x}; \qquad m_{44}(x) = n(x)\lambda_{4}(x) + \frac{27}{4} \frac{\partial u}{\partial x}; \\ m_{34}(x) &= m_{43}(x) = \frac{v_{T}(x)}{3} \left[\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right]; \\ \lambda_{3, 4}(x) &= -\frac{1}{\pi^{3/2}} \int e^{-c^{2}(\vec{x}, \vec{v})} p_{3, 4}(x, \vec{v}) L_{\vec{x}}(\vec{v}) p_{3, 4}(\vec{x}, \vec{v}) d^{3}c(\vec{x}, \vec{v}) > 0 \\ \alpha_{1oc}(x) &= -\frac{2}{3} \frac{\partial u}{\partial x}; \quad \beta_{1oc}(x) = -\frac{5}{4} v_{T}(x) \frac{\partial \ln T}{\partial x} \qquad (4.51) \\ \text{Parameters } \lambda_{3}(x) \text{ and } \lambda_{4}(x) \text{ are easily expressed via} \end{split}$$

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Enskog integral brackets, and they are calculated in [1] for a wide class of molecular models.

Solving equation (4.50), we obtain coefficients $a_{1oc}(x)$ and $b_{1oc}(x)$ in the expression (4.49): $a_{1oc} = \frac{A_{1oc}(x)}{Z(x,0)}; \quad b_{1oc} = \frac{B_{1oc}(x)}{Z(x,0)}; \quad Z(x,0) = m_{33}(x)m_{44}(x) - m_{34}^2(x);$ $A_{1oc}(x) = \alpha_{1oc}(x)m_{44}(x) - \beta_{1oc}(x)m_{34}(x);$ $B_{1oc}(x) = \beta_{1oc}(x)m_{33}(x) - \alpha_{1oc}(x)m_{34}(x);$ $a_{1oc} = \frac{-\frac{2}{3} \frac{\partial u}{\partial x} \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) + \frac{5}{12}v_T^2 \frac{\partial \ln T}{\partial x} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2}{\left(n\lambda_4 + \frac{27}{4} \frac{\partial u}{\partial x} \right) - \frac{v_T^2}{9} \left(\frac{\partial \ln n}{\partial x} + \frac{11}{2} \frac{\partial \ln T}{\partial x} \right)^2} \right)$

These expressions complete Step 1.

<u>Step 2</u>. Calculation of Fourier transform of $\varphi_{loc}(x, \vec{v})$ and its expression in the local basis.

In this step we make two operations:

i) The Fourier transformation of the function
$$\varphi_{\text{loc}}(x, \vec{v})$$
:
 $\hat{\varphi}_{\text{loc}}(x, \vec{v}) = \int_{-\infty}^{+\infty} \exp(-iky)\varphi_{\text{loc}}(y, \vec{v})dy$ (4.53)

ii) The representation of $\hat{\varphi}_{1oc}(\vec{k}, \vec{v})$ in the local basis $\{p_0(\vec{x}, \vec{v}), \dots, p_4(\vec{x}, \vec{v})\}$:

$$p_{0}(x, \vec{v}) = 1, \quad p_{1}(x, \vec{v}) = c_{1}(x, \vec{v}), \quad p_{2}(x, \vec{v}) = c^{2}(x, \vec{v}) - \frac{3}{2}, \quad (4.54)$$

$$p_{3}(x, \vec{v}) = c_{1}^{2}(x, \vec{v}) - \frac{1}{3}c^{2}(x, \vec{v}), \quad p_{4}(x, \vec{v}) = c_{1}(x, \vec{v})(c^{2}(x, \vec{v}) - \frac{5}{2})$$

Operation (ii) is necessary for completing Step 3 because there we deal with *x*-dependent operators. Obviously, the function $\hat{\phi}_{loc}(k,\vec{v})$ (4.53) is a finite-order polynomial in \vec{v} , and thus the operation (ii) is exact.

We obtain in (ii):

$$\hat{\varphi}_{1\text{oc}}(x, k, \vec{v}) \equiv \hat{\varphi}_{1\text{oc}}(x, k, \vec{c}(x, \vec{v})) = \sum_{i=0}^{4} \hat{h}_{i}(x, k) p_{i}(x, \vec{v}) \quad (4.55)$$

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$$\hat{h}_{i}(x, k) = (p_{i}(x, \vec{v}), p_{i}(x, \vec{v}))_{x}^{-2} (\hat{\varphi}_{loc}(k, \vec{v}), p_{i}(x, \vec{v}))_{x} \quad (4.56)$$

Introduce notations:

$$\vartheta = \vartheta(x, y) = (T(x)/T(y))^{1/2}, \quad \gamma = \gamma(x, y) = \frac{u(x) - u(y)}{v_T(y)}$$
(4.57)

Coefficients $\hat{h}_{i}(x, k)$ (4.56) have the following explicit form:

$$\hat{h}_{i}(x, k) = \int_{-\infty}^{+\infty} \exp(-iky) h_{i}(x, y) dy; \quad h_{i}(x, y) = Z^{-1}(y, 0) g_{i}(x, y)$$

$$g_{0}(x, y) = B_{10c}(y) (\gamma^{3} + \frac{5}{2}\gamma(\vartheta^{2} - 1)) + \frac{2}{3}A_{10c}(y)\gamma^{2};$$

$$g_{1}(x, y) = B_{10c}(y) (3\vartheta\gamma^{2} + \frac{5}{2}\vartheta(\vartheta^{2} - 1)) + \frac{4}{3}A_{10c}(y)\vartheta\gamma;$$

$$g_{2}(x, y) = \frac{5}{3}B_{10c}(y)\vartheta^{2}\gamma;$$

$$g_{3}(x, y) = B_{10c}(y)2\vartheta\gamma + A_{10c}(y)\vartheta^{2};$$

$$g_{4}(x, y) = B_{10c}(y)\vartheta^{3} \qquad (4.58)$$

$$\text{Here } Z(y, 0), \quad B_{10c}(y) \text{ and } A_{10c}(y) \text{ are functions defined }$$

$$\text{in } (4.52) \qquad \text{Step 3. Calculation of the function } \hat{\psi}_{0}(x, k, \vec{v}) \text{ from }$$

$$equation (4.39c).$$

Linear integral equation (4.39c) has character similar to that of equation (4.39a). We search for the function $\hat{\varphi}_{0}(x, k, \vec{v})$ in the basis (4.48) as:

$$\hat{\varphi}_{0}(x, k, \vec{v}) = \hat{a}_{0}(x, k) p_{3}(x, \vec{v}) + \hat{b}_{0}(x, k) p_{4}(x, \vec{v})$$
(4.59)

Finite-dimensional approximation of the integral equation (4.39c) in the basis (4.48) yields the following equations for unknowns $\hat{a}_0(x, k)$ and $\hat{b}_0(x, k)$

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Solving equations (4.60), we obtain functions $a_0(x, k)$ and $\hat{b}_0(x, k)$ in (4.59):

$$\hat{a}_{0}(x, k) = \frac{\hat{\alpha}_{0}(x, k)m_{44}(x) - \hat{\beta}_{0}(x, k)(m_{34}(x) + \frac{1}{3}ikv_{T}(x))}{Z(x, \frac{1}{3}ikv_{T}(x))};$$

$$\hat{b}_{0}(x, k) = \frac{\hat{\beta}_{0}(x, k)m_{33}(x) - \hat{\alpha}_{0}(x, k)(m_{34}(x) + \frac{1}{3}ikv_{T}(x))}{Z(x, \frac{1}{3}ikv_{T}(x))}$$
(4. 62)

Here

$$Z(x, \frac{1}{3}ikv_{T}(x)) = Z(x, 0) + \frac{k^{2}v_{T}^{2}(x)}{9} + \frac{2}{3}ikv_{T}(x)m_{34}(x) = \left[n\lambda_{3} + \frac{11}{9}\frac{\partial u}{\partial x}\right] \left[n\lambda_{4} + \frac{27}{4}\frac{\partial u}{\partial x}\right] - \frac{v_{T}^{2}(x)}{9} \left[\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right]^{2} + \frac{k^{2}v_{T}^{2}(x)}{9} + \frac{2}{9}ikv_{T}^{2}(x) \left[\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right]$$
(4.63)

<u>Step 4</u>. Calculation of the inverse Fourier transform of the function $\hat{\Psi}_0(x, k, \vec{v})$.

The inverse Fourier transform of the function $\hat{\varphi}_0(x, k, \vec{v})$ (4.59) yields:

$$\Phi_0(x, \vec{v}) = a_0(x) p_3(x, \vec{v}) + b_0(x) p_4(x, \vec{v})$$
(4.64)

Here

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$$a_{0}(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(ikx)\hat{a}_{0}(x, k) dk,$$

$$b_{0}(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \exp(ikx)\hat{b}_{0}(x, k) dk \qquad (4.65)$$

Taking into account expressions (4.52), (4.61)-(4.63), and (4.58), we obtain the explicit expression for the finite-dimensional approximation of the zeroth-order term of parametrics expansion (4.64):

$$a_{0}(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dk \exp(ik(x-y))Z^{-1}(x, \frac{1}{3}ikv_{T}(x))^{\times} \\ \times \left\{ Z(x, 0)h_{3}(x, y) + [S_{\alpha}(x, y)m_{44}(x) - S_{\beta}(x, y)m_{34}(x)] - \right. \\ \left. -\frac{1}{3}ikv_{T}(x)[m_{34}(x)h_{3}(x, y) + m_{44}(x)h_{4}(x, y) + S_{\beta}(x, y)] \right\}; \\ b_{0}(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dk \exp(ik(x-y))Z^{-1}(x, \frac{1}{3}ikv_{T}(x))^{\times} \\ \times \left\{ Z(x, 0)h_{4}(x, y) + [S_{\beta}(x, y)m_{33}(x) - S_{\alpha}(x, y)m_{34}(x)] - \right. \\ \left. -\frac{1}{3}ikv_{T}(x)[m_{34}(x)h_{4}(x, y) + m_{33}(x)h_{3}(x, y) + S_{\alpha}(x, y)] \right\}$$
(4.66)

4. 4 Hydrodynamic Equations

Now we will discuss briefly the utility of results obtained in Section 4.3 for hydrodynamics.

The correction to LM functions $f_0(n, \vec{u}, T)$ (4.1) obtained has the form:

$$f_{1}(n, \vec{u}, T) = f_{0}(n, \vec{u}, T)(1 + \phi_{0}(n, \vec{u}, T))$$
(4.67)

Here the function $\varphi_0(n, \vec{u}, T)$ is given explicitly with expressions (4.64)-(4.66).

The usual form of closed hydrodynamic equations for n, \vec{u} , and T, where the traceless tension tensor σ_{ik} and the heat flux vector q_i are expressed via hydrodynamic variables, will be obtained if we substitute the function (4.67) into balance equations of the density, momentum, and of the of the energy. For LM approximation, these balance equations result in Euler equation of the nonviscid liquid (i.e. $\sigma_{ik}(f_0)=0$, and $q_i(f_0) \equiv 0$). For the correction f_1 (4.67), we obtain the following expressions of $\sigma = \sigma_{xx}(f_1)$ and $q = q_x(f_1)$ (all other components are equal to zero in the onedimensional situation under consideration):

$$\sigma = \frac{1}{3}na_0, \qquad q = \frac{5}{4}nb_0 \tag{4.68}$$

Here a_0 and b_0 are given by expression (4.66).

From the geometrical viewpoint of Section 2, hydrodynamic equations with the tension tensor and the heat flux vector (4.68) have the following interpretation: we take the corrected manifold \mathfrak{M}_1 which consists of functions f_1 (4.67), and we project the BE vectors $J_u(f_1)$ onto tangent spaces T_{f_1} using the LM projector P_{f_0} (4.6a).

Although a detailed investigation of these hydrodynamic equations is a subject of a special study and it is not the goal of this paper, some points should be mentioned.

<u>Nonlocality</u>. Expressions (4.66) expose a nonlocal spatial dependency, and, hence, the corresponding hydrodynamic equations are nonlocal. This nonlocality appears through two contributions. The first of these contributions might be called a *frequency-response* contribution, and it comes through explicit non-polynomial k-dependency of integrands in (4.66). This latter dependency has the form:

 $\int_{-\infty}^{+\infty} \frac{A(x, y) + ikB(x, y)}{C(x, y) + ikD(x, y) + k^2 E(x, y)} \exp(ik(x-y)) dk \quad (4.69)$

Integration over k in (4.69) can be completed via axillary functions.

The second nonlocal contribution might be called *correlative*, and it is due to relationships via (u(x)-u(y)) (the difference of flow velocities in points x and y) and via T(x)/T(y) (the ratio of temperatures in points x and y).

<u>Acoustic spectra</u>. The purely frequency-response contribution to hydrodynamic equations is relevant to small perturbations of equilibria. The tension tensor σ and the heat flux q (4.68) are:

$$\sigma = -(2/3)\pi_0 T_0 R \left[2\varepsilon \frac{\partial u'}{\partial \xi} - 3\varepsilon^2 \frac{\partial^2 T'}{\partial \xi^2} \right];$$

$$q = -(5/4)T_0^{3/2}\pi_0 R \left[3\varepsilon \frac{\partial T'}{\partial \xi} - (8/5)\varepsilon^2 \frac{\partial^2 u'}{\partial \xi^2} \right]$$
(4.70)

Here

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$$R = \left[1 - (2/5)\varepsilon^2 \frac{\partial^2}{\partial \xi^2}\right]^{-1}$$
 (4.71)

In (4.70), we have expressed parameters λ_3 and λ_4 via the viscosity coefficient μ of the Chapman-Enskog method [1] (it is easy to see from (4.51) that $\lambda_3 = \lambda_4 \propto \mu^{-1}$ for spherically symmetric models of a collision), and we have used the following notations: T_0 and n_0 are the equilibrium temperature and density, $\xi = (\eta T_0^{1/2})^{-1} n_0 x$ is the dimensionless coordinate, $\eta = \mu(T_0)/T_0$, $u' = T_0^{-1/2} \delta u$, $T' = \delta T/T_0$, $n' = \delta n/n_0$, and δu , δT , δn are the deviations of the flux velocity, of the temperature and of the density from their equilibrium values u=0, $T=T_0$ and $n=n_0$. We also use the system of units with $k_{\rm B}=m=1$.

In the linear case, the parametrics expansion degenerates, and its zeroth-order term (4.39d) gives the solution of equation (4.24).



FIG. 1

The dispersion relationship for the approximation (4.70) is:

$$\omega^{3} + (23k^{2}/6D)\omega^{2} + \{k^{2} + (2k^{4}/D^{2}) + (8k^{6}/5D^{2})\}\omega + (5k^{4}/2D) = 0;$$

$$D = 1 + (4/5)k^{2}$$
Here k is the wave vector. Acoustic dispersion curves

 $\omega(k)$ for approximation (4.70) are depicted in FIG.1 (solid line). They are compared with the second (the Burnett) approximation of the Chapman-Enskog expansion

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[3] (dashed line) and with the regularization of the Burnett approximation via partial summing of the Chapman-Enskog expansion [5, 7] (punctuated dashed line). Arrows indicate an increase of k^2 .

Acoustic spectra given by dispersion relationship (4.72) contains no nonphysical short-wave instability characteristic to the Burnett approximation. The regularization of the Burnett approximation [5,7] has the same feature. Both of these approximations predict a limit of the decrement $Re\omega$ for short waves.

<u>Nonlinearity</u>. Nonlinear dependency on $\frac{\partial u}{\partial x}$, on $\frac{\partial \ln T}{\partial x}$, and on $\frac{\partial \ln n}{\partial x}$ appears already in the local approximation φ_{loc} (4.52). In order to outline some peculiarities of this nonlinearity, we represent the zeroth-order term of the expansion of a_{loc} (4.52) into powers of $\frac{\partial \ln T}{\partial x}$ and $\frac{\partial \ln n}{\partial x}$.

$$a_{10c} = -\frac{2}{3} \frac{\partial u}{\partial x} \left(n\lambda_3 + \frac{11}{9} \frac{\partial u}{\partial x} \right)^{-1} + O\left(\frac{\partial \ln T}{\partial x}, \frac{\partial \ln n}{\partial x} \right)$$
(4.73a)

This expression describes the asymptotic of the "purely nonlinear" contribution to the tension tensor σ (4.68) for a strong divergency of a flow. The account of nonlocality yields instead of (4.70a):

$$a_{0}(x) = -\frac{1}{2\pi} \int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} dk \exp(ik(x-y)) \frac{2}{3} \frac{\partial u}{\partial y} \left[n\lambda_{3} + \frac{11}{9} \frac{\partial u}{\partial y} \right]^{-1} \times \left[\left(n\lambda_{3} + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_{4} + \frac{27}{4} \frac{\partial u}{\partial x} \right) + \frac{k^{2}v_{T}^{2}}{9} \right]^{-1} \left[\left(n\lambda_{3} + \frac{11}{9} \frac{\partial u}{\partial x} \right) \left(n\lambda_{4} + \frac{27}{4} \frac{\partial u}{\partial x} \right) + \frac{4}{9} \left[n\lambda_{4} + \frac{27}{4} \frac{\partial u}{\partial y} \right] \frac{\partial u}{\partial x} v_{T}^{-2} \left(u(x) - u(y) \right)^{2} - \frac{2}{3} ik \frac{\partial u}{\partial x} \left(u(x) - u(y) \right) \right] + \left(\frac{\partial \ln \pi}{\partial x}, \frac{\partial \ln \pi}{\partial x} \right)$$

$$(4.74b)$$

Both expressions, (4.74a) and (4.74b) become singular when

$$\frac{\partial u}{\partial y} \rightarrow \frac{\partial u}{\partial y}^* = -\frac{9n\lambda_3}{11}$$
 (4.75)

Hence, the tension tensor (4.69) becomes infinite if $\frac{\partial u}{\partial v}$

tends to $\frac{\partial u}{\partial y}^*$ in any point y. In other words, the flow becomes infinitely viscid when $\frac{\partial u}{\partial y}$ approaches the negative value $-\frac{9n\lambda_3}{11}$. This infinite viscosity threshold prevents a transfer of the flow into nonphysical region of negative viscosity if $\frac{\partial u}{\partial y} > \frac{\partial u}{\partial y}^*$ because of the infinitely strong dumping at $\frac{\partial u}{\partial y}^*$. This peculiarity was detected in [6,7] as a result of partial summing of the Chapman-Enskog expansion. In particular, partial summing for the simplest nonlinear situation [6] yields the following expression for the tension tensor σ :

$$\sigma_{\mathrm{IR}} = \sigma_{\mathrm{IR}} + \sigma_{\mathrm{IR}}; \quad \sigma_{\mathrm{IR}} = -\frac{4}{3} \left(1 - \frac{5}{3} \varepsilon^2 \frac{\partial^2}{\partial \xi^2} \right)^{-1} \left(\varepsilon \frac{\partial u}{\partial \xi} + \varepsilon^2 \frac{\partial^2 \theta}{\partial \xi^2} \right); \quad \theta' = T' + n';$$

$$\sigma_{\mathrm{IIR}} = \frac{28}{9} \left(1 + \frac{7}{3} \varepsilon \frac{\partial u}{\partial \xi} \right)^{-1} \frac{\partial^2 u}{\partial \xi^2} \quad (4.76)$$

Notations here follow (4.70) and (4.71). Expression (4.76) might be considered as a "rough draft" of the "full" tension tensor defined by a_0 (4.66). It accounts both the frequency-response and the nonlinear contributions (σ_{IR} and σ_{IIR} , respectively) in a simple form of a sum. However, the superposition of these contributions in (4.66) is more complicated. Moreover, the explicit correlative nonlocality of expression (4.66) was never detected neither in [6], nor in numerous examples of partial summing [7].

Nevertheless, approximation (4.76) contains the peculiarity of viscosity similar to that in (4.73a) and (4.73b). In dimensionless variables and $\mathcal{E}=1$, expression (4.76) predicts the infinite threshold at velocity divergency equal to -(3/7), rather than -(9/11) in (4.73a) and (4.73b). Viscosity tends to zero as the divergency tends to positive infinity in both approximations. Physical interpretation of these phenomena was given in [6]: large *positive* values of $\frac{\partial u}{\partial x}$ means that the

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FIG. 2

gas diverges rapidly, and the flow becomes nonviscid because the particles retard to exchange their momentum. On contrary, its *negative* values (such as -(3/7) for (4.76) and -(9/11) for (4.73a) and (4.73b)) describe a strong compression of the flow. Strong deceleration results in "solid fluid" limit with an infinite viscosity.

FIG. 2 compares the qualitative character of dimensionless viscosities D/D_{NS} , where D_{NS} is the

Navier-Stokes viscosity, for approximation (4.73a) (solid line), for partial summing (4.76) (punctuated dashed line), and for the Burnett approximation [6] (dashed line). The latter changes the sign at a regular point and, hence, nothing prevents the flow to transfer into the nonphysical region.

Thus, hydrodynamic equations for approximation (4.67) are both nonlinear and nonlocal. This result is not surprising, accounting the integro-differential character of equation (4.24).

It is important that no small parameters were used neither when we were deriving equation (4.24) nor when we were obtaining the correction (4.67).

We stress once again that the problem of reduced description (such as derivation of hydrodynamics) can be posed and investigated without using small parameters. This question was already discussed in Section 2.5. Here we will make some additional clarifications.

It seems "natural" to introduce the usual parameter ε^{-1} , where ε is Knudsen number, in front of the collision integral in equation (4.20), and to develop a Taylor-type perturbation technique for this equation. Representing φ in (4.20) as a formal series

$$\varphi = \sum_{m=0}^{\infty} \varepsilon^{m+1} \varphi^{(m)}$$
(4.77)

one can easily obtain a set of linear integral equations with respect to unknown functions $\varphi^{(m)}$:

$$\begin{array}{c} L \\ f_{0}(n, \vec{u}, T) \end{array} (\begin{array}{c} (m) \\ f_{0}(n, \vec{u}, T) \end{array}) = D^{(m)} \\ f_{0}(n, \vec{u}, T) \end{array} ; \qquad \begin{array}{c} D^{(0)} \\ f_{0}(n, \vec{u}, T) \end{array} = D \\ f_{0}(n, \vec{u}, T) \end{array} f_{0}(n, \vec{u}, T) \end{array} ,$$

$$D_{0}^{(m)} = -K_{0}^{(m-1)}, \quad m \ge 1$$

$$f_{0}^{(m, \vec{u}, T)} = f_{0}^{(m, \vec{u}, T)}, \quad m \ge 1$$

$$(4.78)$$

Function D and operator K are defined $f_0(n, \vec{u}, T)$ $f_0(n, \vec{u}, T)$ in (4.21).

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The system (4.78) is recurrently solvable. In particular, the correction $\varphi^{(0)}$ coincides with the first correction of the Chapman-Enskog method [1]. The higher order terms in expansion (4.78) also have the form similar to that of the Chapman-Enskog method, i.e. they have *polynomial* dependency on spatial derivatives of n, \vec{u} , and *T*. However, it is preferable to avoid this approach because of at least two reasons:

i) A truncation of the formal series (4.77) at any $m \ge 1$ is not reliable. Even though the corrections $\varphi^{(m)}$ do not completely coincide with the corresponding terms of the Chapman-Enskog expansion, the experience of dealing with the Burnett and the super-Burnett approximations shows that they are "bad" when used directly. In particular, the Burnett and the super-Burnett corrections result in a short-wave instability of equilibria [3] and in "negative viscosity" regimes under high gradients.

ii) Examples given above show a certain similarity between results obtained via Newton-type method of solving the invariance equation and parametrics expansion, and those obtained via partial summing of Taylor-type expansions (i. e. a method which treats the series (4.77) as a whole), especially in the highly nonequilibrium regions. This similarity of a properly chosen method of partial summing to the method of invariant manifold is not random (see, for instance, [18] in the case of KAMtheory). However, it is rather difficult to define the notion "the proper choice", and thus "successful methods of partial summing" are always of an ad hoc character.

5. CONCLUSIONS

we have considered the two main problems of reduced description for dissipative systems: the problem of thermodynamicity (Problem 1 of Section 2.1) and the problem of dynamic invariance (Problem 2 of Section 2.1). Main results in this direction are:

i) Problem 1 is solved completely in Section 2.2. There is no other universal way (i.e. independent of the particular choice of collision integral) to construct thermodynamic parameterization for an arbitrary manifold.

ii) Iterative Newton-type methods to correct the dynamic noninvariance are developed in Section 2.3 in order to solve Problem 2.

These two results are combined into the method of invariant manifold. The method developed requires no special choice of initial approximation, as well as small parameters. Thus, it provides a common approach to different problems as the obtaining hydrosuch of dynamics, shock waves, initial layers, etc. Specificity of each problem is to be accounted via a relevant choice of initial manifold, while the procedure of thermodynamic parameterization and of obtaining corrections is uniform in its essence.

As applied to the problem of derivation of hydrodynamics from the Boltzmann equation (Section 4), the method of invariant manifold, together with the parametrics expansion, eliminates the necessity of using Knudsen number expansions. New nonlocal and nonlinear hydrodynamic equations derived in Sections 4.3 and 4.4 contain no short-wave instability and negative viscosity characteristic to the Chapman-Enskog method.

The question about the convergency of successive approximations is not difficult for finite-dimensional dissipative systems. For the Boltzmann equation this question remains open. The complexity of this problem is stressed by the fact that the global existence and uniqueness of the solution is a particular case of this problem.

REFERENCES

1.	S. Chapman and T. Cowling, "Mathematical Theory of
	Non-uniform Gases", Univ. Press, Cambridge, (1958).
2.	C. Cercignani, "Theory and Applications of the
	Boltzmann Equation", Scottish Acad. Press, Edinburg,
	(1975).
3.	À. V. Bobylev, Dokl. Acad. Nauk USSR, 262, 71(1982).
4.	H. Grad, Comm. Pure and Appl. Math., 2, 331(1949).
5.	A. N. Gorban and I. V. Karlin, TTSP, 21 , 101(1992);
<i>6</i> .	I. V. Karlin, TTSP, 21 , 291(1992);
0. 7.	A. N. Gorban and I. V. Karlin, in: "Modelling in
7.	Biology and Chemistry. New Approaches", ed. R. G.
	Khlebopros, Nauka, Novosibirsk, P. 69–117(1992).
0	
8.	A. M. Kogan, L. I. Rozonoer, Dokl. Acad. Nauk USSR,
0	158 , 566(1964).
9.	L. I. Rozonoer, in: "Thermodynamics and Kinetics of
	Biological Processes", ed. A. I. Zotin, Nauka,
	Moscow, (1980)
10.	A. M. Kogan, Pricl. Math. Mech., 29, 122(1965).
11.	I. V. Karlin, in: "Mathematical Problems of Chemical Kinetics", eds. K. I. Zamaraev and G. S. Yablonski,
	Kinetics", eds. K. I. Zamaraev and G. S. Yablonski,
	Nauka, Novosibirsk, P. 7-42(1989).
12.	I. V. Karlin, Modelling, Measurement & Control, C,
	AMSE Press, 34, No. 4, 1(1993).
13.	A. N. Gorban, "Equilibrium Encircling", Nauka,
	Novosibirsk, (1984).
14.	A. N. Gorban, V. I. Bykov and G. S. Yablonskii,
	"Essays on Chemical Relaxation", Nauka, Novosibirsk,
	(1986).
15.	
	(1967).
16.	
	(1954).
17.	V. I. Arnold, Uspekhi Math. Nauk, 18, 91(1963).
	J. Moser, Math. Ann., 169 , 136(1967).
19.	M. Lampis, Meccanica, 12 , 171(1977).
	A. N. Gorban and I. V. Karlin, Physica A,
	190, 393 (1992).
21.	I. Hosokawa and S. Inage, J. Phys. Jap., 55,
	3402(1986).
22.	L. V. Kantorovich and G. P. Akilov, "Functional
	Analysis", Nauka, Moscow, (1977).
23.	E. Farrow and D. Edelson, Int. J. Chem. Kinet., 6, 787
	(1974).
24.	G. S. Yablonskii, V. I. Bykov, A. N. Gorban, V. I.
	Elokhin, "Kinetic Models of Catalytic Reactions"
	(Comprehensive Chemical Kinetics, V. 32), Elsevier,
	Amsterdam, (1991).
25.	F. Treves, "Introduction to Pseudodifferential and
	Fourier Integral Operators", Plenum, NY, (1982).

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26. M. A. Shubin, "Pseudodifferential Operators and Spectral Theory", Nauka, Moscow, (1978).

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