TWO-STEP APPROXIMATION OF SPACE-INDEPENDENT RELAXATION

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ABSTRACT

An express method to approximate trajectories of space-independent kinetic equations is developed. It involves a two-step treatment of relaxation through a quasi-equilibria located on a line emerging from the initial state in the direction prescribed by the kinetic equation. A test for the Boltzmann equation shows the validity of the method.

1. INTRODUCTION

In this paper we introduce a new method of constructing approximate trajectories for space-independent kinetic equations confirming to the second law of thermodynamics. Classical examples are the space-independent Boltzmann equation and chemical kinetics equations for closed homogeneous systems. This family of kinetic equations is characterized by the following general properties:

(i). There exists a set of functions which remain constant on a solution (these are density, momentum and energy in context of the Boltzmann equation).

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(ii). There exists a convex function which mono-
tonically decreases along any solution from its value in
the initial state to an absolute minima in the final
equilibrium state (this is the H-theorem for the Boltz-
mann equation).

Usually we do know only the initial and the final
(equilibrium) states, and the kinetic equation neither
can be solved exactly, nor contains small parameters to
develop a reliable perturbation theory. Still, we would
like to get (perhaps a rather rough but a simple) appro-
ximation of the relaxation trajectory.

To be certain, we will speak about the Boltzmann
equation. Denote as $f(\mathbf{v}, t)$ a one-body distribution func-
tion, where $\mathbf{v}$ is velocity of a particle, and t is the
time. The dynamics of $f(\mathbf{v}, t)$ is governed by the space-
independent Boltzmann equation

$$\frac{\partial f(\mathbf{v}, t)}{\partial t} = Q(f) \qquad (1.1)$$

Here $Q(f)$ is the Boltzmann collision integral [1]. In-
dependently of a specific choice of operator $Q(f)$, equa-
tion (1.1) has the following properties reflecting fea-
tures (i) and (ii):

(i). For any a, $\mathbf{b}$, and c, and for any f providing
existence of integrals, we have (conservation laws):

$$\int (a+\mathbf{b}\cdot\mathbf{v}+cv^2)Q(f)\,\mathrm{d}^3v = 0 \qquad (1.2)$$

(ii). Denote as $H_0(f)$ the space of linear
functionals $\int (a+\mathbf{b}\cdot\mathbf{v}+cv^2)f\,\mathrm{d}^3v$. Symbol $(\mathrm{mod}H_0(f))$ will
indicate that an expression is valid within the accuracy
of adding a functional from $H_0(f)$. For any functional
$H(f)$,

$$H(f) = \int f\ln f\,\mathrm{d}^3v \quad (\mathrm{mod}H_0(f)) \qquad (1.3)$$

the following inequality takes place (the H-theorem):

$$\sigma(f)=\int Q(f)\ln f\,d^3v \leq 0 \qquad (1.4)$$

Expression $\sigma(f)$ (1.4) is called the H-function production in the state f, and it is equal to zero only for $f \propto A\exp\{cv^2+\mathbf{b}\cdot\mathbf{v}\}$ $(c<0)$.

Initial condition to equation (1.1) will be denoted as $f_0(\mathbf{v})$, i.e. $f(\mathbf{v},0)=f_0(\mathbf{v})$. Further we sometimes omit the dependence on $\mathbf{v}$. With no restriction, we assume that the initial state satisfies the conditions:

$$\int f_0 d^3v=1, \quad \int f_0 \mathbf{v}\,d^3v=0, \quad \int f_0 v^2 d^3v=3 \qquad (1.5)$$

Conservation laws (1.2) and the H-theorem (1.4) result in the following properties of solutions:

(i). At each time $t \geq 0$, solution $f(\mathbf{v},t)$ which comes from out the initial state f_0, satisfies the equalities:

$$\int f(\mathbf{v},t)d^3v=1, \qquad \int f(\mathbf{v},t)\mathbf{v}\,d^3v=\mathbf{0}, \qquad \int f(\mathbf{v},t)v^2 d^3v=3$$

(ii). For $t \to \infty$, solution $f(\mathbf{v},t)$ tends to the equilibrium state which is the Maxwell distribution f_B^0:

$$f_B^0=(2\pi)^{-3/2}\,\exp\left(-\frac{1}{2}v^2\right) \qquad (1.6)$$

This tendency is accompanied with a monotonic decrease of values of the H-function $H(f)\big|_{f=f(\mathbf{v},t)}$:

$$\frac{dH}{dt}=\sigma(f)\Big|_{f=f(\mathbf{v},t)} \leqslant 0,$$

and $\frac{dH}{dt}=0$ only for f_B^0 (1.6).

A set of states f which the solution $f(\mathbf{v},t)$ spans as t runs from zero to infinity, will be called the

trajectory. In this paper we will consider the trajectories as geometrical objects, regardless of at what time the solution comes to the states on the trajectory. Let us consider a more convenient standard representation.

A continuous immersion of the segment $0 \leq a \leq 1$ into the phase space, $a \mapsto f(\mathbf{v}, a)$, will be called a *thermodynamically admissible path from* f_0 *to* f_B^0 (*TAP*) [2] if the following conditions are satisfied:

$$f(\mathbf{v}, a)\Big|_{a=0} = f_0 \tag{1.7}$$

$$f(\mathbf{v}, a)\Big|_{a=1} = f_B^0 \tag{1.8}$$

$$\int f(\mathbf{v}, a)\left\{1, \mathbf{v}, v^2\right\} d^3 v = \left\{1, \mathbf{0}, 3\right\} \tag{1.9}$$

$$H(f(a')) > H(f(a'')), \quad \text{if } a' < a'' \tag{1.10}$$

Roughly speaking, TAP is a "string" in the phase space joining the states f_0 and f_B^0. The initial tip of TAP ($a=0$) is the distribution f_0, the final tip ($a=1$) is the Maxwell function f_B^0. Condition (1.9) expresses the conservation of the first five moments along this string. Condition (1.10) conforms to the second law of thermodynamics: the motion along the TAP from the initial tip to its final tip should be accompanied with the decay of the H-function.

One of the TAPs represents the trajectory of solution to equation (1.1) with the initial condition f_0, and any approximation of the trajectory should be a TAP.

Our goal is to construct the simplest approximation of a trajectory conforming with requests (1.7)-(1.10),

and using only the function $Q(f_0)$. We will follow the two objectives:

1. Within some time after $t=0$, there occurs a relaxation directed essentially along the vector $Q(f_0)$. In the end of this process the system comes to an intermediate state f^*, such that $f^*-f_0 \propto Q(f_0)$, and

2. Next there occurs a rectilinear relaxation from the state f^* towards the equilibria f_B^0.

In other words, we imply a two-step picture of relaxation. The first step is a relaxation from the initial state f_0 into an intermediate state f^* along the straight line emerging from f_0 and directed along $Q(f_0)$. The second step is a relaxation along the straight line which connects the state f^* with the Boltzmann equilibria f_B^0. The second step represents a trajectory of the Bhatnagar-Gross-Krook (BGK) model kinetic equation [3] with f^* for the initial condition. The H-theorem and conservation laws are valid for BGK-model, so the second step satisfies conditions (1.8), (1.9), and (1.10).

The main difficulty is to derive the intermediate state f^*. Namely, f^* should represent a physical state (i.e. it should be a non-negative function), and the H-function should monotonically decay along the linear segment which connects f_0 with f^* (condition (1.9) will be obviously satisfied on this segment due to (1.2)). If we have constructed such state f^*, then the two-step approximation (TS) has the form:

$$f_{TS}(a) = \begin{cases} (1-2a)f_0+2af^*, & \text{for } 0\leq a\leq 1/2 \\ \\ 2(1-a)f^*+(2a-1)f_B^0, & \text{for } 1/2\leq a\leq 1 \end{cases} \quad (1.11)$$

Here we have taken $f_{TS}(1/2)=f^*$, without any restriction. Our goal is to derive a physical state f^* on the line

$f_0 + zQ(f_0)$ so that conditions (1.7) and (1.10) should be satisfied for $f_{TS}(a)$ (1.11) as variable a spans the segment $[0, 1/2]$.

In the next section we will derive the state f^* as an equilibrium state of a new satellite kinetic equation, and we will develop an approximate method of calculating this state. In section 3 we will compare the results of TS approximation with the exact Bobylev-Krook-Wu solution of equation (1.1) for Maxwell molecules. Section 4 contains some remarks on a further development of this approximation technique.

2. MARCELIN – DE DONDER EQUILIBRIA

2.1. Marcelin – De Donder Kinetic Equation

In this section we introduce a model kinetic equation which has a rectilinear trajectory running in the direction $Q(f_0)$, and satisfying the conditions (1.7), (1.9), and (1.10). This involves a representation of the function $Q(f_0)$ as a sum of positive and negative parts. Treating $Q(f_0)$ as a function in $\mathbf{v}$, we have:

$$Q(f_0) = Q_\beta - Q_\alpha;$$

$$Q_\beta = \begin{cases} Q(f_0), & \text{if } Q(f_0) > 0 \\ 0, & \text{if } Q(f_0) \leq 0; \end{cases}$$

$$Q_\alpha = \begin{cases} -Q(f_0), & \text{if } Q(f_0) < 0 \\ 0, & \text{if } Q(f_0) \geq 0 \end{cases}$$

(2.1)

In other words, function Q_β is the rate of "probability density" income into the state f_0, while Q_α is the rate of probability density expenditure from the state f_0.

Given the partition (2.1), we consider an equation

$$\frac{\partial f}{\partial t} = k \left[Q_\beta - Q_\alpha \right] \left\{ \exp\left(\int Q_\alpha \ln f \, \mathrm{d}^3 v \right) - \exp\left(\int Q_\beta \ln f \, \mathrm{d}^3 v \right) \right\} \qquad (2.2)$$

Here k is an arbitrary positive constant.

To explain equation (2.2), let us turn to notions of chemical kinetics. Vector $Q(f_0)$ determines a prevailing direction of relaxation in the space of states f during some "short" time after the beginning of relaxation in the initial state f_0. Dynamics within this period can be considered formally as a "chemical reaction", and vector $Q(f_0)$ can be interpreted as a "stoichiometric vector of reaction". Representation (2.1) corresponds to a selection of "stoichiometric coefficients" of the income and of the expenditure of some conventional "substances".

Recall [4] that, for N substances $A_1, \ldots, A_N$, a stoichiometric equation of reaction is:

$$\alpha_1 A_1 + \ldots + \alpha_N A_N \rightarrow \beta_1 A_1 + \ldots + \beta_N A_N \qquad (2.3)$$
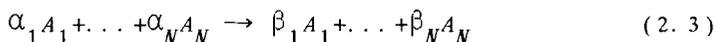
Non-negative numbers α_i and β_i are called stoichiometric coefficient. N-dimensional vector with components $\gamma_i = \beta_i - \alpha_i$ is called the stoichiometric vector of reaction (2.3).

In our case, the "substance number" is the velocity $\mathbf{v}$, and "the amount of substance with the number $\mathbf{v}$" is the value of distribution f in the point $\mathbf{v}$.

Derivation of chemical kinetics equations involves a concept of reactions rates. For stoichiometric equation (2.3), the rate of reaction in the context of Marcelin – De Donder kinetics [4, 5] is:

$$w \propto \exp\left(\sum_{i=1}^{N} \alpha_i \mu_i \right) - \exp\left(\sum_{i=1}^{N} \beta_i \mu_i \right) \qquad (2.4)$$

Here $\mu_i = -k_B^{-1}(\partial s(n_1, \ldots, n_N)/\partial n_i)$ is the divided by $k_B T$ chemical potential of the i-th chemical kind (k_B is the

Boltzmann constant, T is the temperature), i. e. μ_i is proportional to the derivative of the entropy in i-th substance quantity n_i. Expression (2.4) is called the *Marcelin – De Donder kinetic function* [4,5]. Chemical kinetics equation corresponding to stoichiometric equation (2.3) and to reaction rate (2.4) is:

$$\frac{dn_i}{dt}=k\gamma_i w \qquad (2.5)$$

Here $k>0$ is reaction rate constant. The case of a continuous mixture assumes integration in $\mathbf{v}$ instead of summation in numbers of substances. Expression $\ln f(\mathbf{v})=\dfrac{\delta H(f)}{\delta f(\mathbf{v})}$ is the direct analog of chemical potential (for perfect systems). Factor

$$w(f)=\exp\left[\int Q_\alpha \ln f d^3v\right]-\exp\left[\int Q_\beta \ln f d^3v\right] \qquad (2.6)$$

in equation (2.2) is reasonably similar to the Marcelin-De Donder kinetic function (2.4). Model equation (2.2) has a formal analogy with chemical kinetics equation (2.5). For this reason, equation (2.2) will be called *the Marcelin – De Donder equation* (MDD-equation).

A few words should be said about the choice of partition (2.1). There exist infinitely many partitions of function $Q(f_0)$ into positive and negative parts. In the chemical interpretation, any choice reflects a splitting of the given stoichiometric vector γ_i in two sets of the income and of the expenditure stoichiometric coefficient, α_i and β_i. Partition (2.1) makes the sense of splitting the chemical reagents in two groups so that either $\alpha_i \neq 0$ and $\beta_i = 0$, or $\alpha_i = 0$ and $\beta_i \neq 0$. This corresponds to stoichiometric equations (2.3) *without auto-catalysis*. Recall that auto-catalytic step is realized when both α_i and β_i in (2.3) are not equal to zero, at least for a single number i. When

auto-catalytic steps are absent, MDD reaction rate (2.4) for perfect systems transforms into the standard mass action law form (MAL). Hence, partition (2.1) can be called *the MAL-representation* of function $Q(f_0)$. This representation corresponds to partition of velocity space into two domains with non-intersecting interiors, V_β and V_α. The support of function's $Q(f_0)$ positive part coincides with V_β, the support of the negative part of $Q(f_0)$ coincides with V_α. Accordingly, functions Q_α and Q_β are non-negative, and they are concentrated on non-intersecting domains V_α and V_β.

MDD-equation (2.2) possesses a set of properties which are a formal immediate generalization of elementary properties of equations (2.5) onto continuous case [2, 4, 5]:

Property 1. If f_0 is a non-negative function, then solution to equation (2.2) with initial condition f_0 is non-negative for all $t \geq 0$.

Property 2. Solution to equation (2.2) with initial condition f_0 belongs to the straight line $f_0 + zQ(f_0)$.

Property 3. Conservation laws are satisfied in every point of the trajectory of equation (2.2).

Property 4. H-function (1.3) monotonically decreases due to equation (2.2), that is:

$$\frac{\mathrm{d}H(t)}{\mathrm{d}t} = k\int\left[\left(Q_\beta - Q_\alpha\right)\left\{\exp\left(\int Q_\alpha \ln f \mathrm{d}^3 v\right) - \exp\left(\int Q_\beta \ln f \mathrm{d}^3 v\right)\right\}\right]\ln f \mathrm{d}^3 v \leq 0$$

Thus, the trajectory of MDD-equation (2.2) is a segment of a straight line emerging from the initial state f_0 and running in the direction $Q(f_0)$. All states on the MDD-trajectory do make physical sense, conservation laws are satisfied, and the H-function monotonically decays from its value in the initial state f_0 to its value in a final equilibrium state of equation (2.2). This latter state will be called the *MDD-equilibria*, and it will be denoted as f_{MDD}^0. To get

the trajectory of MDD-equation (2.2), we have to derive the state f^0_{MDD}.

2.2. Estimations of MDD-equilibria

Let us consider a functional $A(f)$ which is a direct analog of *affinity* [6]:

$$A(f) = \int Q(f_0) \ln f \, d^3v \qquad (2.7)$$

Condition $A(f)=0$ determines a hyper-surface $D(f)$ where the "chemical potential" $\ln f$ is orthogonal to "stoichiometric vector" $Q(f_0)$. MDD-equilibria f^0_{MDD} is the state where the line $f_0 + zQ(f_0)$ crosses the hyper-surface $D(f)$. Due to Property 2, we have:

$$f^0_{MDD} = f_0 + z_{MDD} Q(f_0) \qquad (2.8)$$

and parameter z_{MDD} is a solution of an equation:

$$A(z) = 0 \qquad (2.9)$$

Here $A(z)$ is the value of affinity $A(f)$ (2.7) on the line $f_0 + zQ(f_0)$:

$$A(z) = \int Q(f_0) \ln(f_0 + zQ(f_0)) d^3v \qquad (2.10)$$

Note that z_{MDD} is correctly defined by equation (2.9), and it is independent of any partition of $Q(f_0)$. For practical aims, MAL-representation (2.1) is most convenient.

Introduce a normalization of MAL-representation (2.1):

$$q_{\alpha, \beta} = q^{-1} Q_{\alpha, \beta} \qquad q(f_0) = q^{-1} Q(f_0), \qquad q = \int Q_\beta d^3v = \int Q_\alpha d^3v \qquad (2.11)$$

After introducing a new variable $b = qz$, we have:

$$f^0_{\text{MDD}} = f_0 + b_{\text{MDD}} q(f_0) \tag{2.12}$$

Parameter $b_{\text{MDD}} = q z_{\text{MDD}}$ is a solution of an equation equivalent to equation (2.9):

$$A_\alpha(b) = A_\beta(b) \tag{2.13}$$

Here

$$A_\alpha(b) = \int q_\alpha \ln(f_0 - bq_\alpha) \mathrm{d}^3 v, \quad A_\beta(b) = \int q_\beta \ln(f_0 + bq_\beta) \mathrm{d}^3 v \tag{2.14}$$

Functions $A_\alpha(b)$ and $A_\beta(b)$ (2.14) have the following properties:

1. The domain of function $A_\alpha(b)$ is an open semi-axis $]-\infty, b_\alpha[$, where $b_\alpha > 0$. The domain of function $A_\beta(b)$ is an open semi-axis $]b_\beta, +\infty[$, where $b_\beta < 0$. Functions $A_\alpha(b)$ and $A_\beta(b)$ have logarithmic singularities in points b_α and b_β respectively.

2. Functions $A_\alpha(b)$ and $A_\beta(b)$ are *monotonic*, that is $\mathrm{d}A_\alpha(b)/\mathrm{d}b < 0$ inside the domain of $A_\alpha(b)$, and $\mathrm{d}A_\beta(b)/\mathrm{d}b > 0$ inside the domain of $A_\beta(b)$.

3. Functions $A_\alpha(b)$ and $A_\beta(b)$ are *concave*, that is $\mathrm{d}^2 A_{\alpha,\beta}(b)/\mathrm{d}b^2 \leqslant 0$ inside corresponding domains.

4. $A_\beta(0) - A_\alpha(0) = q^{-1}\sigma(f_0) < 0$,

where $\sigma(f_0) = \int Q(f_0)\ln f_0 \, \mathrm{d}^3 v$ is the H-function production in initial state f_0 (see (1.4)).

The singular point b_α is the minimal value of the ratio f_0/q_α. More specifically, let us define a parameter $\mathscr{R} = b_\alpha^{-1}$:

$$\mathscr{R} = \sup_{\mathbf{v} \in \mathbb{R}^3} \frac{q_\alpha(\mathbf{v})}{f_0(\mathbf{v})} \tag{2.15}$$

If $\mathscr{R} < \infty$, then for all $\mathbf{v}$ functions $\ln(1 - bq_\alpha(\mathbf{v})/f_0)$ are defined inside the interval $[0, \mathscr{R}^{-1}[$. Further, we shall assume that $\mathscr{R} < \infty$ for the initial state f_0. This means that $f_0(\mathbf{v})$ should decreases sufficiently rapidly

as $|\mathbf{v}|$ tends to infinity (see section 4).

Properties of functions $A_\alpha(b)$ and $A_\beta(b)$ listed guarantee that equation (2.13) has an unique positive solution b_{MDD}.

To get a guaranteed first estimation $b_{MDD}^{(1)}$ located between zero and the unknown solution b_{MDD}, it is sufficient to approximate the function $A_\beta(b)$ from above with a concave function, and to approximate $A_\alpha(b)$ from below with a concave function.

To get an upper estimation for function $A_\beta(b)$, turn to logarithmic coordinates, and consider a function $W_\beta(b)$

$$W_\beta(b)=\exp(A_\beta(b)) \qquad (2.16)$$

It can be shown that function $W_\beta(b)$ is monotonic and concave. Consequently, $W_\beta(b)$ is majorized by a tangent line:

$$W_\beta(b)\leq\exp(A_\beta(0))\left\{\frac{dA_\beta(b)}{db}\bigg|_{b=0} b + 1\right\} \qquad (2.17)$$

Inequality (2.17) yields the upper estimation for function $A_\beta(b)$ inside its domain:

$$A_\beta(b)\leqslant A_\beta(0)+\ln\left(1+\frac{dA_\beta(b)}{db}\bigg|_{b=0} b\right) \qquad (2.18)$$

Lower estimation for function $A_\alpha(b)$ is evident from an inequality being true for $b\in[0,\mathscr{X}^{-1}[$:

$$A_\alpha(b)=A_\alpha(0)+\int q_\alpha\ln(1-b\frac{q_\alpha}{f_0})d^3v\geq A_\alpha(0)+\ln(1-\mathscr{X}b)$$

Hence,

$$A_\alpha(b)\geq A_\alpha(0)+\ln(1-\mathscr{X}b) \qquad (2.19)$$

Equalizing the right hand sides of inequalities

(2.18) and (2.19), we get an explicit linear equation for the approximation $b_{MDD}^{(1)}$ which is located *with a guaranty* between 0 and b_{MDD}. Solving this equation and returning to the variable z, we finally get the first approximation $z_{MDD}^{(1)}$:

$$z_{MDD}^{(1)} = \frac{1 - \exp\left[q^{-1}\sigma(f_0)\right]}{q\mathcal{X} + q\left\{\frac{dA_\beta(b)}{db}\bigg|_{b=0}\right\}\exp\left[q^{-1}\sigma(f_0)\right]} \qquad (2.20)$$

Let us list here the four parameters which should be calculated to obtain the value $z_{MDD}^{(1)}$ (2.20):

$$\sigma(f_0)=\int \varrho(f_0)\ln f_0\, d^3v; \qquad q=\int \varrho_\beta d^3v=\int \varrho_\alpha d^3v;$$

$$\mathcal{X}=\sup_{\mathbf{v}\in\mathbb{R}^3} \frac{q_\alpha(\mathbf{v})}{f_0(\mathbf{v})}; \qquad \frac{dA_\beta(b)}{db}\bigg|_{b=0} = \int \frac{q_\beta^2}{f_0} d^3v \qquad (2.21)$$

Substituting the value $z_{MDD}^{(1)}$ (2.20) instead of z_{MDD} into (2.8), we come to the first approximation for MDD-equilibria which is located with a guaranty between f_0 and f_{MDD}^0. The value (2.20) can be improved by a method of successive approximations. To do this, one should make the estimations (2.18) and (2.19) in the point $b_{MDD}^{(1)}$. This gives a start to a Newton-type process of obtaining the solution b_{MDD}. The sequence of approximations will *monotonically increase* to the point b_{MDD}. We will not discuss the convergency of this sequence in this paper, and we will restrict ourselves to the first approximation (2.20).

Thus, we have constructively determined the state $f^*=f_{MDD}^0$ at which the first step of relaxation ends, and we have completed the two-step approximation (1.11).

3. EXAMPLE: TWO–STEP APPROXIMATION OF BKW–MODE

A model of particles with the binary interaction potential proportional to the inverse forth degree of distance (in the three-dimensional case) is usually called "Maxwell molecules". For them, equation (1.1) is:

$$\frac{\partial f(\mathbf{v}, t)}{\partial t} = \int d^3 v \int d\hat{\mathbf{n}} \alpha(\hat{\mathbf{g}} \cdot \hat{\mathbf{n}}) \left\{ f(\mathbf{v}', t)f(\mathbf{w}', t) - f(\mathbf{v}, t)f(\mathbf{w}, t) \right\} \quad (3.1)$$

Here α depends only on the projection of the unit vector $\hat{\mathbf{g}} = \frac{\mathbf{v} - \mathbf{w}}{|\mathbf{v} - \mathbf{w}|}$ on the scattering direction $\hat{\mathbf{n}} = \frac{\mathbf{v}' - \mathbf{w}'}{|\mathbf{v} - \mathbf{w}|}$. Notations are standard, and follow the paper [7].

An exact automodel solution of equation (3.1) was discovered by Bobylev [8], and Krook and Wu [9] (the BKW-mode). The TAP which represents the BKW-mode is:

$$f_{BKW}(a, c) = \left(\frac{2\pi}{a(1-c)+c} \right)^{-3/2} \exp\left\{ -\frac{(a(1-c)+c)v^2}{2} \right\} \times$$

$$\times \frac{1}{2}\left\{ \left(5 - 3(a(1-c)+c) \right) + (a(1-c)+c)\left[(a(1-c)+c)-1 \right]v^2 \right\} \quad (3.2)$$

Here variable a spans the segment $[0, 1]$, while parameter c labels the initial state of BKW-trajectory (3.2). Parameter c takes the values in a semi-opened interval $[1, \frac{5}{3}[$. Value $c=1$ corresponds to the equilibrium distribution f_B^0 (1.6). For $c>\frac{5}{3}$, function (3.3) becomes negative for some $\mathbf{v}$ at $a=0$. The BKW-trajectory (3.2) begins in the state $f_0(c) \equiv f_{BKW}(0, c)$ at $a=0$, and ends in the equilibrium state $f_B^0 \equiv f_{BKW}(1, c)$ at $a=1$.

Now we will construct the two-step approximation of the BKW-trajectory.

The initial state. Initial states will be chosen on the BKW-trajectory, and they will be labeled with parameter c:

$$f_0(c) = \frac{1}{2}\left[\frac{2\pi}{c}\right]^{-3/2} \exp\left\{-\frac{cv^2}{2}\right\}\left\{(5-3c)+c(c-1)v^2\right\} \qquad (3.3)$$

The final equilibrium state f_B^0 is the same for all initial states $f_0(c)$, and it is given by expression (1.6). Thus, we are going to construct a family of two-step approximations for initial states $f_0(c)$ (3.3), where c takes values between 1 and 5/3.

MAL-representation. Substituting functions (3.3) into the RHS of equation (3.1), we find the functions $Q_0(c) \equiv Q(f_0(c))$ (the values of collision integral in the states (3.3)):

$$Q_0(c) = \frac{\lambda}{2}(c-1)^2\left[\frac{2\pi}{c}\right]^{-3/2} \exp\left\{-\frac{cv^2}{2}\right\}\left\{15-10cv^2+c^2(v^2)^2\right\} \qquad (3.4)$$

Here $\lambda = \frac{1}{8}\int d\hat{\mathbf{n}} \ \alpha(\hat{\mathbf{k}}\cdot\hat{\mathbf{n}})(1-(\hat{\mathbf{k}}\cdot\hat{\mathbf{n}})^2)$.

For a given c, where $1<c<5/3$, function $Q_0(c)$ (3.4) is negative only inside the spheric layer between spheres of radii $v_-(c) = \sqrt{(5-\sqrt{10})/c}$ and $v_+(c) = \sqrt{(5+\sqrt{10})/c}$, centered in the point $\mathbf{v}=0$. MAL-partition of the velocity space is:

$$V_\alpha(c) = \left\{\mathbf{v} \mid \ v_-^2(c) \leqslant v^2 \leqslant v_+^2(c)\right\};$$

$$V_\beta(c) = \left\{\mathbf{v} \mid \ v^2 < v_-^2(c)\right\} \cup \left\{\mathbf{v} \mid \ v^2 > v_+^2(c)\right\} \qquad (3.5)$$

The first approximation of MDD-equilibria. Introducing a dimensionless variable $z'_{MDD}(c)$:

$$z_{MDD}(c) = \frac{1}{\lambda(c-1)^2}z'_{MDD}(c)$$

we can write down the MDD-equilibrium states $f_{MDD}^0(c)$ as:

$$f^0_{MDD}(c) = \frac{1}{2}\left[\frac{2\pi}{c}\right]^{-3/2} \exp\left\{-\frac{cv^2}{2}\right\}\left\{(5-3c+15z'_{MDD}(c)) + \right.$$

$$\left. + ((c-1)-10z'_{MDD}(c))cv^2 + z'_{MDD}(c)c^2(v^2)^2\right\} \qquad (3.6)$$

The first approximation to $z'_{MDD}(c)$ (2.20) gives:

$$z'^{(1)}_{MDD}(c) = \frac{1-\exp(q^{-1}P_3(c))}{P_1(c)+q^{-1}P_2\exp(q^{-1}P_3(c))};$$

$$q = -\int_{\sqrt{5-\sqrt{10}}}^{\sqrt{5+\sqrt{10}}} (15-10t^2+t^4)t^2 e^{-\frac{t^2}{2}}\,dt;$$

$$P_1(c) = -\frac{15-10\tau(c)+\tau^2(c)}{(5-3c)+(c-1)\tau(c)};$$

$$\tau(c) = \frac{\left[(5-3c)^2+5(c-1)(7-3c)\right]^{1/2}-(5-3c)}{(c-1)};$$

$$P_2 = \int_0^{\sqrt{5-\sqrt{10}}} \varphi(t)\,dt + \int_{\sqrt{5+\sqrt{10}}}^{\infty} \varphi(t)\,dt; \quad \varphi(t) = \frac{(15-10t^2+t^4)^2t^2}{(5-3c)+(c-1)t^2}e^{-\frac{t^2}{2}};$$

$$P_3(c) = \int_0^{\infty} (15-10t^2+t^4)t^2 e^{-\frac{t^2}{2}} \ln\left(1+\frac{c-1}{5-3c}t^2\right)dt \qquad (3.7)$$

All integrals in (3.7) can be easily calculated
numerically. The first approximation $z'^{(1)}_{MDD}(c)$ is given

TABLE 1

No	c	$z'^{(1)}_{MDD}$	$z'^{(1)}_{MDD}/z'_{LIM}$
1	1. 06	$8.2484 \cdot 10^{-4}$	0. 1125
2	1. 12	$3.1779 \cdot 10^{-3}$	0. 2221
3	1. 18	$6.8551 \cdot 10^{-3}$	0. 3276
4	1. 24	$1.1660 \cdot 10^{-2}$	0. 4291
5	1. 30	$1.7409 \cdot 10^{-2}$	0. 5268
6	1. 36	$2.3916 \cdot 10^{-2}$	0. 6203
7	1. 42	$3.0969 \cdot 10^{-2}$	0. 7087
8	1. 48	$3.8277 \cdot 10^{-2}$	0. 7895
9	1. 54	$4.5322 \cdot 10^{-2}$	0. 8563
10	1. 59	$5.0791 \cdot 10^{-2}$	0. 8903

First Approximation $z'^{(1)}_{MDD}(c)$ for MDD-equilibria (3.6) (Third Column) and Capacity of its Positiveness (Fourth Column).

in Table 1 (third column) for ten values of parameter c. Substituting $z'^{(1)}_{MDD}(c)$ (3.7) instead of $z'_{MDD}(c)$ into expression $f^0_{MDD}(c)$ (3.6), we finally get the two-step approximation of the BKW-trajectory:

$$f_{TS}(a, c) = \begin{cases} (1-2a)f_0(c) + 2af^0_{MDD}(c) , & \text{for } 0 \le a \le 1/2 \\ \\ 2(1-a)f^0_{MDD}(c) + (2a-1)f^0_B , & \text{for } 1/2 \le a \le 1 \end{cases} \quad (3.8)$$

To make a relevant comparison of TS approximation (3.8) with BKW-trajectory (3.2), we have to eliminate the dependence on a. Consider normalized moments $m_k(f)$:

$$m_k(f) = \int (v^2)^k f \, d^3v \left[\int (v^2)^k f_B^0 \, d^3v \right]^{-1}, \quad k = 0, 1, 2, \ldots \qquad (3.9)$$

We have to obtain the dependencies $m_k(m_1)$ for (3.2) and (3.8) and next to compare these dependencies. Typical dependencies of higher moments $(k \geqslant 3)$ on the lowest nontrivial moment m_2 are presented in Fig. 1 for $c = 1.3$ (a moderate nonequilibrium initial states).

Qualitative behavior. Both the BKW and the TS dependencies $m_k(m_2)$ tend to be more convex with the increase of k. This tendency is more progressive for TS curves at small k. For c not exceeding 1.48, there exists a critical number $k^*(c)$ such that the BKW curve $m_k(m_2)$ does not intersect the BGK-segment of TS for $k \leqslant k^*(c)$. Number $k^*(c)$ falls down with the increase of c ($k^* \approx 110$ for $c = 1.06$, $k^* \approx 6$ for $c = 1.42$). For $k \gg k^*(c)$, the MDD-segment of TS becomes practically horizontal (see Fig. 1d).

Quantitative comparison. Table 2 gives the euclidean distance between the curves $m_k(m_2)$ for BKW and TS (in scaled units where m_k and m_2 have equal total variation), in percents of the total variation of moments. Recall that the distance between two sets, X and Y, is defined as:

$$\text{dist}(X, Y) = \max_{x \in X} \min_{y \in Y} \text{dist}(x, y)$$

In other words, we compare the curves $m_k(m_2)$ for BKW and TS as two sets of points in a plane (m_k, m_2). This is an appropriate way to make a comparison because we consider only geometrical properties of trajectories, while time behavior was not under consideration.

Accounting that TS approximation requires *only the single state* f_{MDD}^0 which is rather "inexpensively"

obtained (i.e. without solving any dynamic equations),
we can see that it is appropriate for *a'priori*
estimations of trajectories. It should be mentioned that
a physically interesting quantitative comparison usually
concerns a dozen of first nontrivial moments while the
higher moments are required to have a qualitative
similarity.

Finishing this section, let us note a remarkable
fact. Example considered shows that the MDD-segment of
the TS approximation *is not small* in comparison with its
BGK-segment. In a physical interpretation, the initial
rate of relaxation $Q(f_0)$ defines the changes of the
initial state f_0 due to a few first collisions of
particles. MDD-equilibria gives the exact upper bound of
changes which the initial state *can* get in the first
collisions, and this bound turns out to be significant.
If this bound were very low, then triangles in Fig. 1
would be very narrow, and TS approximation would give a
qualitatively poor estimation of the real trajectory
(i.e. then the TS approximation would be almost similar
to the BGK-approximation). In other words, the account
of first collisions is substantial to construct an
approximation of the relaxation trajectory in a whole.
To illustrate it once again, let us note that the line
$f_0+zQ(f_0)$ abandons the space of physical states for
$z>z_{LIM}$. It is interesting to compare the limiting size
of the step z_{LIM} along the line $f_0+zQ(f_0)$ with the step
prescribed by MDD-equation. For states (3.6), we can
find exactly such z'_{LIM} so that physically possible
values z'_{MDD} can not exceed z'_{LIM}. The fourth column in
Table 1. shows how far the the first approximation to
$f^0_{MDD}(c)$ is located from the border of physical states
(the exact MDD-equilibria is still closer to the
border). It can be seen that for none of c the step
prescribed by MDD-kinetics is negligible in comparison
with the physically possible step.
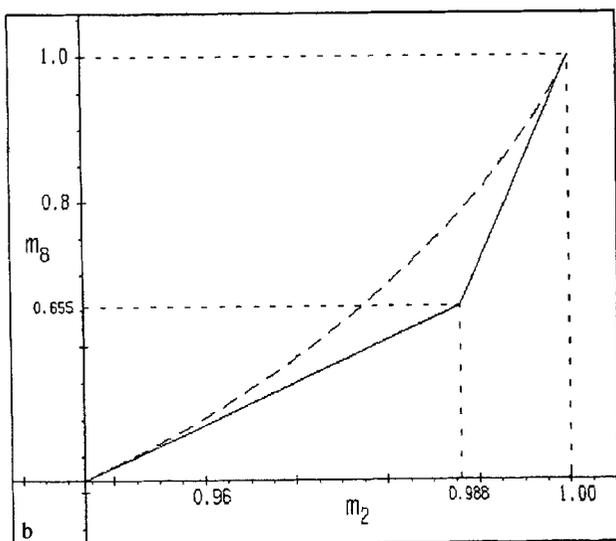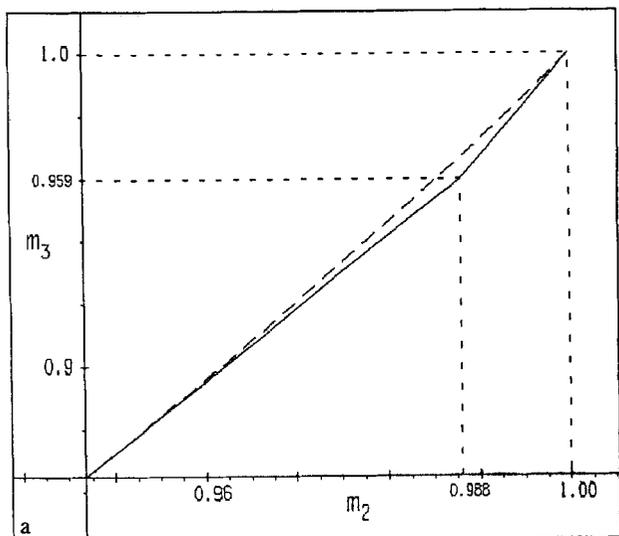
Figure 1.

Dependencies of higher normalized moments m_k ($k \geqslant 3$) on the lowest nontrivial moment m_2 for TS approximation (3.8) (solid lines) and BKW-trajectory (3.2) (dashed lines). Solid lines brake at m_2 corresponding to MDD-equilibria. In all figures $c = 1.3$, $z_{MDD}^{\prime(1)}(c) = 1.7409 \cdot 10^{-2}$, $m_2(f_0) = 0.9467$, $m_2(f_{MDD}^0) = 0.9879$.
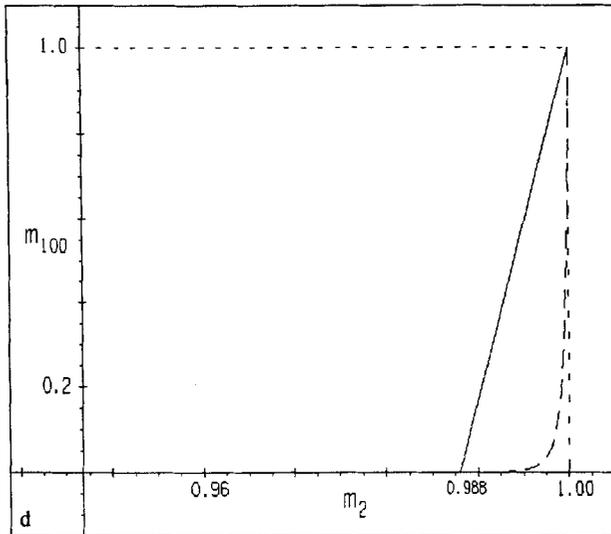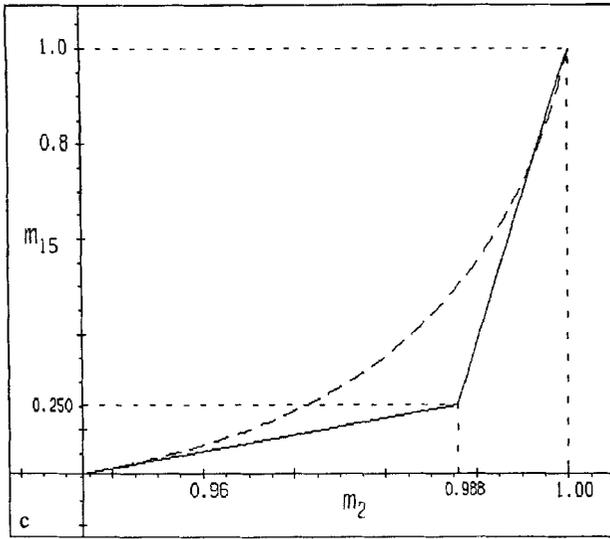
Figure 1. Continued

1a) $k=3$, $m_3(f_0)=0.8648$, $m_3(f_{MDD}^0)=0.9599$.

1b) $k=8$, $m_8(f_0)=0.4168$, $m_8(f_{MDD}^0)=0.6558$.

1c) $k=15$, $m_{15}(f_0)=0.1075$, $m_{15}(f_{MDD}^0)=0.2503$.

1d) $k=100$ $m_{100}(f_0)=0.13\cdot10^{-9}$, $m_{100}(f_{MDD}^0)=1.52\cdot10^{-9}$.

TABLE 2

k	$c=1.12$	$c=1.24$	$c=1.36$	$c=1.48$	$c=1.59$
3	1.4	2.1	2.5	2.6	2.2
4	2.6	3.9	4.6	4.6	3.8
5	3.8	5.6	6.3	6.1	5.0
6	4.9	6.9	7.5	7.2	5.7
7	5.8	8.1	8.6	7.9	6.2
8	6.7	9.0	9.3	8.4	6.2
9	7.6	9.8	9.8	8.5	6.1
10	8.3	10.5	10.2	8.5	5.7
15	11.2	12.1	9.7	6.5	9.6
20	12.8	11.6	7.7	7.5	13.6
40	13.2	5.6	9.2	14.8	21.4
60	9.9	6.3	12.3	17.8	24.1
80	6.5	8.1	13.9	19.2	25.4
100	4.2	9.2	14.9	20.1	26.2
200	5.5	11.6	16.7	21.6	27.5
300	6.5	12.3	17.3	22.0	27.8

Euclidean Distance Between the Curves $m_k(m_2)$ for BKW and TS in Percents to the Total Variation of Moments.

$$\text{dist}(X_k, Y_k) = \max_{x\in X_k} \min_{y\in Y_k} \text{dist}(x,y);$$

$$X_k = (m_2, m_k(m_2))\Big|_{TS}, \quad Y_k = (m_2, m_k(m_2))\Big|_{BKW}.$$

4. FINAL REMARKS AND CONCLUSIONS

It is not much surprising that there are practically no reliable approximate analytic methods for the space-independent Boltzmann equation and similar kinetic systems because there is no a traditional small parameter (we are speaking of methods applicable to equation (1.1) with arbitrary collision integral; the exception are Maxwell molecules and some other similar models, see [7]). In fact, among classical methods of kinetic theory, perhaps only the Grad method [10] is formally applicable which involves a termination of the moment chain equivalent to equation (1.1). However the realization of Grad method for equation (3.1) has shown its poor approximation abilities [11]. Results of section 3 show that, in principle, any approximate method which "begins with the equilibria f_B^0" will face serious difficulties when predicting the trajectory.

The method developed in section 2 is directly applicable to any kinetic equation of the type (1.1) possessing the properties (i) and (ii) of section 1. The method gives explicit approximation of a trajectory satisfying with a guarantee conditions (1.7)-(1.10). It requires the obtainment of parameters (2.21), and so it can be said that the problem is solved "in quadratures". The finiteness of these parameters is the main restriction on the choice of the initial state f_0, and it has a very natural physical meaning: $\sigma(f_0)$ is the H-function production, $\mathcal{X}$ reflects the upper bound of expenditure of positiveness, $(dA_\beta(b)/db)|_{b=0}$ reflects the total income of positiveness. If $\mathcal{X}=\infty$. then $f(\mathbf{v})$ becomes negative for some $\mathbf{v}$ in an infinitely short period after $t=0$. If $(dA_\beta(b)/db)|_{b=0}=\infty$, then the conservation laws will be violated infinitely quickly. To apply the method of section 2, the initial state

should decrease sufficiently rapidly as $|\mathbf{v}|$ tends to infinity. It is sufficient to consider the following initial states:

$$f_0 \propto \exp\ (-cv^2/2)P(\mathbf{v})$$

Here $c \geqslant 1$, and $P(\mathbf{v})$ is a positive function which has a polynomial growth as $|\mathbf{v}|$ tends to infinity.

Finishing this paper, let us list here some further ways in development of TS approximation.

(i)   *Multi-step   approximations.*   When   the (approximate) MDD-equilibria f^0_{MDD} is obtained, we can construct the next MDD-equilibria using f^0_{MDD} instead f_0, and $Q(f^0_{MDD})$ instead of $Q(f_0)$. Continuing this process, we can make n such steps, and we should complete the process with the $n+1$-th BGK-step. The broken line obtained will be a TAP. A better way is to make the first step shorter than it is prescribed by $z^{(1)}_{MDD}$ (2.20). A general recipe might be as follows: make the first step n times shorter than $z^{(1)}_{MDD}$, and next make $n-1$ such steps. It should be stressed that adding new MDD-steps will give a better result *with a guarantee* (in contrast to Grad-type methods where adding higher moments can even result in negative-valued functions).

(ii)   *Smooth   planar   approximations.*   The   three states, f_0, f^0_{MDD}, and f^0_B, form *a triangle* consisting of their convex linear combinations. Each point of this triangle is a physical state, and conservation laws are valid. We can pose a problem of constructing a *smooth* TAP from f_0 to f^0_B inside this triangle, and which is tangent to the MDD-side in f_0. Then we could get a smooth approximation of the trajectory. It is possible, but some efforts should be spend to complete condition (1.10) along this curve. This will be reported in a separate paper.

(iii)   *Time   behavior.*   Though   the   qualitative behavior of the relaxation is sufficient for many

problems (in particular, in chemical kinetics), the time evolution is also interesting. For TAP's, the time behavior should come through a dependence $a(t)$. To get an *ordinary differential equation* for a, we have to project the vectors $Q(f(a))$ onto $\partial f(a)/\partial a$ in every state $f(a)$. There are serious reasons to believe that a general method of thermodynamically correct projecting [12, 13, 14] solves this problem. If so, then the equation for a comes through the entropy balance equation along TAP, and it has the form:

$$da/dt = \sigma(a)(dH(a)/da)^{-1} \qquad (4.1)$$

Here $\sigma(a) = \sigma(f(a))$, $H(a) = H(f(a))$, initial condition is $a(0) = 0$, and we have to distinguish the left and the right derivatives $dH(a)/da$ in the point $a = 1/2$.

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