# 6 Newton Method with Incomplete Linearization

The Newton method with incomplete linearization is developed for solving the invariance equation. It is the basis of an iterative construction of the manifolds of slow motions.

## 6.1 The Method

Let us come back to the invariance equation (3.3),

$$\Delta_y = (1 - P_y)J(F(y)) = 0 \, .$$

One of the most efficient methods to solve this equation is the Newton method with incomplete linearization. Let us linearize the vector field $J$ around $F(y)$:

$$J(F(y) + \delta F(y)) = J(F(y)) + (DJ)_{F(y)}\delta F(y) + o(\delta F(y)) \, . \tag{6.1}$$

Equation of the Newton method with incomplete linearization makes it possible to determine $\delta F(y)$ from a linear system:

$$\begin{cases} P_y \delta F(y) = 0 \, , \\ (1 - P_y)(DJ)_{F(y)}\delta F(y) = (1 - P_y)J(F(y)) \, . \end{cases} \tag{6.2}$$

The crucial point here is that the same projector $P_y$ is used as in the equation (3.3), that is, the variation of the projector $\delta P$ is not computed (hence, the suggested linearization of equation (3.3) is incomplete). We recall that projector $P_y$ depends on the tangent space $T_y = \mathrm{im}(DF)_y$. If the thermodynamic projector (5.25) is used here, then $P_y$ depends also on $\langle|\rangle_{F(y)}$ and on $g = (DS)_{F(y)}$.

Equations of the Newton method with incomplete linearization (6.2) are not differential equations in $y$ anymore, they do not contain derivatives of the unknown $\delta F(y)$ with respect to $y$ (which would be the case if the variation of the projector $\delta P$ has been taken into account). The absence of the derivatives in equation (6.2) significantly simplifies its solving. However, even this is not the main advantage of the incomplete linearization. More essential is the fact that iterations of the Newton method with incomplete linearization are

Alexander N. Gorban and Iliya V. Karlin: *Invariant Manifolds for Physical and Chemical Kinetics*, Lect. Notes Phys. **660**, 139–178 (2005)
www.springerlink.com

expected to converge to slow invariant manifolds, unlike the usual Newton method (with "complete linearization").

In order to clarify this feature of the Newton method with incomplete linearization (6.2), let us consider the case of linear manifolds for linear systems. Let a linear evolution equation be given in the real Hilbert space:

$$\dot{\boldsymbol{x}} = \mathbf{A}\boldsymbol{x} \ ,$$

where $\mathbf{A}$ is negative definite symmetric operator with a simple spectrum. The square of the norm is the Lyapunov function,

$$S(\boldsymbol{x}) = \langle \boldsymbol{x} \mid \boldsymbol{x} \rangle \ .$$

The manifolds we consider are lines, $\boldsymbol{l}(y) = y\boldsymbol{e}$, where $\boldsymbol{e}$ is the unit vector, and $y$ is a scalar. The invariance equation for such manifolds reads:

$$\boldsymbol{e}\langle \boldsymbol{e} \mid \mathbf{A}\boldsymbol{e} \rangle - \mathbf{A}\boldsymbol{e} = 0 \ ,$$

and it is simply the eigenvalue problem for the operator $\mathbf{A}$. Solutions to the latter equation are eigenvectors $\boldsymbol{e}_i$, corresponding to eigenvalues $\lambda_i$.

Assume that we choose an initial approximation, that is the line $\boldsymbol{l}_0 = y\boldsymbol{e}_0$ defined by the unit vector $\boldsymbol{e}_0$. Let the vector $\boldsymbol{e}_0$ be not an eigenvector of $\mathbf{A}$. We seek another line, $\boldsymbol{l}_1 = a\boldsymbol{e}_1$, where $\boldsymbol{e}_1$ is another unit vector, $\boldsymbol{e}_1 = \boldsymbol{x}_1/\|\boldsymbol{x}_1\|$, $\boldsymbol{x}_1 = \boldsymbol{e}_0 + \delta\boldsymbol{x}$. The additional condition in (6.2) reads: $P_y \delta F(y) = 0$, i.e. $\langle \boldsymbol{e}_0 \mid \delta\boldsymbol{x} \rangle = 0$. Then (6.2) becomes

$$[1 - \boldsymbol{e}_0\langle \boldsymbol{e}_0 \mid \cdot \rangle]\mathbf{A}[\boldsymbol{e}_0 + \delta\boldsymbol{x}] = 0 \ .$$

Subject to the additional condition, the unique solution is as follows:

$$\boldsymbol{e}_0 + \delta\boldsymbol{x} = \langle \boldsymbol{e}_0 \mid \mathbf{A}^{-1}\boldsymbol{e}_0 \rangle^{-1}\mathbf{A}^{-1}\boldsymbol{e}_0 \ .$$

Upon rewriting the latter expression in the eigen-basis of $\mathbf{A}$, we have:

$$\boldsymbol{e}_0 + \delta\boldsymbol{y} \propto \sum_i \lambda_i^{-1}\boldsymbol{e}_i\langle \boldsymbol{e}_i \mid \boldsymbol{e}_0 \rangle \ .$$

The leading term in this sum corresponds to the eigenvalue with the *minimal absolute value*. The example indicates that the method (6.2) seeks the direction of the *slowest relaxation*. For this reason, the Newton method with incomplete linearization (6.2) can be recognized as the basis of iterative construction of the manifolds of slow motions.

In an attempt to simplify computations, the question which always can be asked is as follows: To what extend is the choice of the projector essential in the equation (6.2)? This question is a valid one, because if we accept that iterations converge to a relevant slow manifold, and also that the projection on the true invariant manifold is insensible to the choice of the projector, should

one care of the projector on each iteration? In particular, for the moment parameterizations, can one use in equation (6.2) the projector (5.1)? Experience gained from some of the problems studied by this method indicates that this is possible. However, in order to derive physically meaningful equations of motion along the approximate slow manifolds, one has to use the thermodynamic projector (5.25). Otherwise we cannot guarantee the dissipation properties of these equations of motion.

## 6.2 Example: Two-Step Catalytic Reaction

We consider here a two-step four-component reaction with one catalyst $A_2 = Z$ (2.98):

$$A_1 + A_2 \rightleftharpoons A_3 \rightleftharpoons A_2 + A_4 \,. \tag{6.3}$$

We assume the Lyapunov function of the form (2.86), $G = \sum_{i=1}^{4} c_i[\ln(c_i/c_i^{\rm eq}) - 1]$. The kinetic equation for the four-component vector of concentrations, $\boldsymbol{c} = (c_1, c_2, c_3, c_4)$, has the form

$$\dot{\boldsymbol{c}} = \boldsymbol{\gamma}_1 W_1 + \boldsymbol{\gamma}_2 W_2 \,. \tag{6.4}$$

Here $\boldsymbol{\gamma}_{1,2}$ are stoichiometric vectors,

$$\boldsymbol{\gamma}_1 = (-1, -1, 1, 0),\ \boldsymbol{\gamma}_2 = (0, 1, -1, 1) \,, \tag{6.5}$$

while functions $W_{1,2}$ are reaction rates:

$$W_1 = k_1^+ c_1 c_2 - k_1^- c_3,\ W_2 = k_2^+ c_3 - k_2^- c_2 c_4 \,. \tag{6.6}$$

Here $k_{1,2}^{\pm}$ are reaction rate constants. The system under consideration has two conservation laws,

$$c_1 + c_3 + c_4 = B_1,\ c_2 + c_3 = B_2 \,, \tag{6.7}$$

or $(\boldsymbol{b}_{1,2}, \boldsymbol{c}) = B_{1,2}$, where $\boldsymbol{b}_1 = (1, 0, 1, 1)$ and $\boldsymbol{b}_2 = (0, 1, 1, 0)$. The nonlinear system (6.4) is effectively two-dimensional, and we consider one-dimensional manifolds of reduced description.

We have chosen the concentration of the specie $A_1$ as the variable of reduced description: $M = c_1$, and $c_1 = (\boldsymbol{m}, \boldsymbol{c})$, where $\boldsymbol{m} = (1, 0, 0, 0)$. The initial manifold $\boldsymbol{c} = \boldsymbol{c}_0(M)$ (i.e. $\boldsymbol{c} = \boldsymbol{c}_0(c_1, B_1, B_2)$) was taken as the quasi-equilibrium approximation, i.e. the vector function $\boldsymbol{c}_0$ is the solution to the problem:

$$G \to \min \text{ for } (\boldsymbol{m}, \boldsymbol{c}) = c_1,\ (\boldsymbol{b}_1, \boldsymbol{c}) = B_1,\ (\boldsymbol{b}_2, \boldsymbol{c}) = B_2 \,. \tag{6.8}$$

The solution to the problem (6.8) can be computed explicitly:

$$
\begin{aligned}
c_{01} &= c_1 \,, \\
c_{02} &= B_2 - \phi(c_1) \,, \\
c_{03} &= \phi(c_1) \,, \\
c_{04} &= B_1 - c_1 - \phi(c_1) \,, \\
\phi(M) &= A(c_1) - \sqrt{A^2(c_1) - B_2(B_1 - c_1)} \,, \\
A(c_1) &= \frac{B_2(B_1 - c_1^{\mathrm{eq}}) + c_3^{\mathrm{eq}}(c_1^{\mathrm{eq}} + c_3^{\mathrm{eq}} - c_1)}{2c_3^{\mathrm{eq}}} \,.
\end{aligned}
\tag{6.9}
$$

The thermodynamic projector associated with the manifold (6.9) reads:

$$
\boldsymbol{P}_0\boldsymbol{x} = \frac{\partial \boldsymbol{c}_0}{\partial c_1}(\boldsymbol{m}, \boldsymbol{x}) + \frac{\partial \boldsymbol{c}_0}{\partial B_1}(\boldsymbol{b}_1, \boldsymbol{x}) + \frac{\partial \boldsymbol{c}_0}{\partial B_2}(\boldsymbol{b}_2, \boldsymbol{x}) \,. \tag{6.10}
$$

Computing $\boldsymbol{\Delta}_0 = (1 - \boldsymbol{P}_0)\boldsymbol{J}(\boldsymbol{c}_0)$ we find that it is not equal to zero, and thus the quasiequilibrium manifold $\boldsymbol{c}_0$ is not invariant. The first correction, $\boldsymbol{c}_1 = \boldsymbol{c}_0 + \delta\boldsymbol{c}$, is found from the linear algebraic system (6.2)

$$
(1 - \boldsymbol{P}_0)\boldsymbol{L}_0'\delta\boldsymbol{c} = -[1 - \boldsymbol{P}_0]\boldsymbol{J}(\boldsymbol{c}_0) \,, \tag{6.11}
$$

$$
\begin{aligned}
\delta c_1 &= 0 \\
\delta c_1 + \delta c_3 + \delta c_4 &= 0 \\
\delta c_3 + \delta c_2 &= 0 \,,
\end{aligned}
\tag{6.12}
$$

where the symmetric $4 \times 4$ matrix $\boldsymbol{L}_0'$ has the form (we write 0 instead of $\boldsymbol{c}_0$ in the subscript in order to simplify notations):

$$
L'_{0,kl} = -\gamma_{1k}\frac{W_1^+(\boldsymbol{c}_0) + W_1^-(\boldsymbol{c}_0)}{2}\frac{\gamma_{1l}}{c_{0l}} - \gamma_{2k}\frac{W_2^+(\boldsymbol{c}_0) + W_2^-(\boldsymbol{c}_0)}{2}\frac{\gamma_{2l}}{c_{0l}} \tag{6.13}
$$

Here we use the self-adjoint linearization[1].

The explicit solution $\boldsymbol{c}_1(c_1, B_1, B_2)$ to the linear system (6.11) is easily found, and we do not reproduce it here. The process was iterated. On the $k+1$ iteration, the following projector $\boldsymbol{P}_k$ was used:

$$
\boldsymbol{P}_k\boldsymbol{x} = \frac{\partial \boldsymbol{c}_k}{\partial c_1}(\boldsymbol{m}, \boldsymbol{x}) + \frac{\partial \boldsymbol{c}_k}{\partial B_1}(\boldsymbol{b}_1, \boldsymbol{x}) + \frac{\partial \boldsymbol{c}_k}{\partial B_2}(\boldsymbol{b}_2, \boldsymbol{x}) \,. \tag{6.14}
$$

Note that projector $\boldsymbol{P}_k$ (6.14) is thermodynamic only if $k = 0$. In the process of finding the corrections to the manifold, the non-thermodynamic projectors are allowed (we should return to the thermodynamic projector for projection of the vector field onto ansatz manifold). The linear equation at the $k+1$ iteration is thus obtained by replacing $\boldsymbol{c}_0$, $\boldsymbol{P}_0$, and $\boldsymbol{L}_0'$ with $\boldsymbol{c}_k$, $\boldsymbol{P}_k$, and $\boldsymbol{L}_k'$ in all the entries of (6.11) and (6.13).

[1] The self-adjoint linearization was introduced in Chap. 2 (2.33), more detailed discussion follows in Chap. 7 (7.15)

Once the manifold $\boldsymbol{c}_k$ was obtained on the $k$th iteration, we derived the corresponding dynamics by introducing the corresponding thermodynamic projector. The resulting dynamic equation for the variable $c_1$ in the $k$th approximation has the form:

$$(\boldsymbol{\nabla} G\,\big|_{\boldsymbol{c}_k}, \partial \boldsymbol{c}_k/\partial c_1)\dot{c}_1 = (\boldsymbol{\nabla} G\,\big|_{\boldsymbol{c}_k}, \boldsymbol{J}(\boldsymbol{c}_k))\ . \tag{6.15}$$

Here $[\boldsymbol{\nabla} G\,\big|_{\boldsymbol{c}_k}]_i = \ln[c_{ki}/c_i^{\mathrm{eq}}]$.

Analytic results were compared with the results of the numerical integration of the system (6.4). The following set of parameters was used:

$$\begin{gathered} k_1^+ = 1.0,\ k_1^- = 0.5,\ k_2^+ = 0.4,\ k_2^- = 1.0\ ; \\ c_1^{\mathrm{eq}} = 0.5,\ c_2^{\mathrm{eq}} = 0.1,\ c_3^{\mathrm{eq}} = 0.1,\ c_4^{\mathrm{eq}} = 0.4\ , \\ B_1 = 1.0,\quad B_2 = 0.2\ . \end{gathered}$$

Figure 6.1 demonstrates the quasi-equilibrium manifold (6.9) and the first two corrections. It should be stressed that we spent no special effort on the construction of the initial approximation, that is, of the quasi-equilibrium manifold, have not used any information about the Jacobian field (unlike, for example, the ILDM [93] or CSP [90] methods) etc. The initial quasi-equilibrium approximation is in a rather poor agreement with the reduced description. Therefore, it should be appreciated that the further corrections

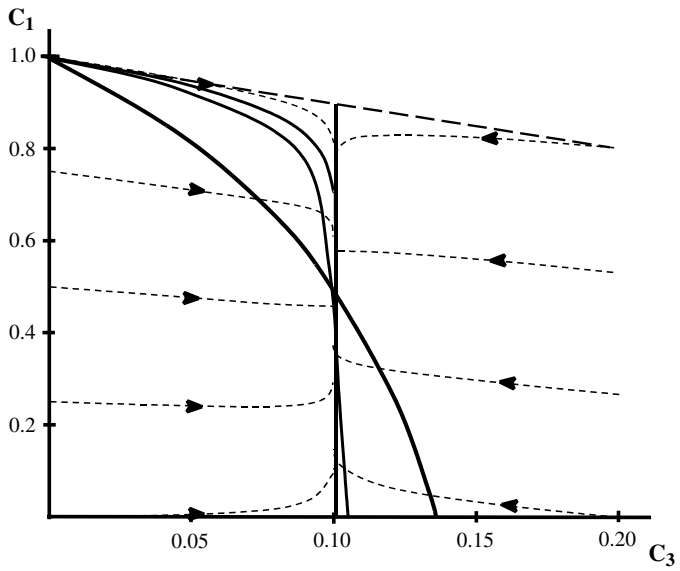


**Fig. 6.1.** Images of the initial quasi-equilibrium manifold (*bold* line) and the first two corrections (*solid* normal lines) in the phase plane $[c_1, c_3]$ for two-step catalytic reaction (6.3). *Dashed* lines are individual trajectories

*rapidly* improve the situation while no small parameter considerations were used. This confirms our expectation of the advantage of using the iteration methods instead of methods based on a small parameter expansions for model reduction problems.

## 6.3 Example: Non-Perturbative Correction of Local Maxvellian Manifold and Derivation of Nonlinear Hydrodynamics from Boltzmann Equation (1D)

We apply here the method of invariant manifold to a particularly important situation when the initial manifold consists of local Maxwellians (5.49) (the LM manifold). This manifold and its corrections play the central role in the problem of derivation of hydrodynamics from the Boltzmann equation. Hence, any method of approximate investigation of the Boltzmann equation should be tested with the LM manifold. Classical methods (the Chapman-Enskog and Hilbert methods) use Taylor-type expansions into powers of a small parameter (the Knudsen number expansion). However, as we have mentioned above, the method of invariant manifold, generally speaking, assumes no small parameters, at least in its formal part where convergency properties are not discussed. We shall develop an appropriate technique to consider the invariance equation of the first iteration. This technique involves ideas of the parametrix expansion of the theory of pseudodifferential and Fourier integral operators [249, 250]. This approach will make it possible to avoid using small parameters.

We seek a correction to the LM manifold in the form (dependence of velocity $\boldsymbol{v}$ will be not displayed whenever possible):

$$f_1(n, \boldsymbol{u}, T) = f_0(n, \boldsymbol{u}, T) + \delta f_1(n, \boldsymbol{u}, T) \, . \tag{6.16}$$

We use the Newton method with incomplete linearization for obtaining the correction $\delta f_1(n, \boldsymbol{u}, T)$, because we are interested in a manifold of slow (hydrodynamic) motions. We introduce the representation:

$$\delta f_1(n, \boldsymbol{u}, T) = f_0(n, \boldsymbol{u}, T)\varphi(n, \boldsymbol{u}, T) \, . \tag{6.17}$$

### 6.3.1 Positivity and Normalization

When seeking corrections, we should be ready to face two problems that are typical for any method of successive approximations in the Boltzmann equation theory. Namely, the first of this problems is that the correction

$$f_{\Omega_{k+1}} = f_{\Omega_k} + \delta f_{\Omega_{k+1}}$$

obtained from the linearized invariance equation of the $k+1$-th iteration may be not a non-negatively defined function and thus it cannot be used directly in order 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 $\mu_f = D_f H(f)$ rather than the process of immediate correcting the distribution functions.

The dual variable $\mu_f$ is:

$$\mu_f\big|_{f=f(\boldsymbol{x},\boldsymbol{v})} = D_f H(f)\big|_{f=f(\boldsymbol{x},\boldsymbol{v})} = D_f H_{\boldsymbol{x}}(f)\big|_{f=f(\boldsymbol{x},\boldsymbol{v})} = \ln f(\boldsymbol{v},\boldsymbol{x}) \; . \quad (6.18)$$

Then, at the $k+1$-th iteration, we obtain a new dual variable $\mu_f\big|_{\Omega_{k+1}}$:

$$\mu_f\big|_{\Omega_{k+1}} = \mu_f\big|_{\Omega_k} + \delta\mu_f\big|_{\Omega_{k+1}} \; . \quad (6.19)$$

Due to the relationship $\mu_f \longleftrightarrow f$, we have:

$$\delta\mu_f\big|_{\Omega_{k+1}} = \varphi_{\Omega_{k+1}} + O(\delta f^2_{\Omega_{k+1}}), \varphi_{\Omega_{k+1}} = f^{-1}_{\Omega_k}\delta f_{\Omega_{k+1}} \; . \quad (6.20)$$

Thus, solving the linear invariance equation of the $k$-th iteration with respect to the unknown function $\delta f_{\Omega_{k+1}}$, we find a correction to the dual variable $\varphi_{\Omega_{k+1}}$(6.20), and we derive the corrected distributions $f_{\Omega_{k+1}}$ as

$$f_{\Omega_{k+1}} = \exp(\mu_f\big|_{\Omega_k} + \varphi_{\Omega_{k+1}}) = f_{\Omega_k}\exp(\varphi_{\Omega_{k+1}}) \; . \quad (6.21)$$

Functions (6.21) are positive, and they satisfy the invariance equation and the additional conditions within the accuracy of $\varphi_{\Omega_{k+1}}$.

However, the second difficulty which might occur is that functions (6.21) might have no finite moments (5.43). In particular, this difficulty can be a result of some approximations used in solving equations. Hence, we have to "regularize" the functions (6.21) in some way. A sketch of an approach to do this regularization is as follows: instead of $f_{\Omega_{k+1}}$(6.21), we consider functions:

$$f^{(\beta)}_{\Omega_{k+1}} = f_{\Omega_k}\exp(\varphi_{\Omega_{k+1}} + \varphi^{\mathrm{reg}}(\beta)) \; . \quad (6.22)$$

Here $\varphi^{\mathrm{reg}}(\beta)$ is a function labeled with $\beta \in B$, and $B$ is a linear space. Then we derive $\beta_*$ from the condition of matching the macroscopic variables.

For example, corrections to the LM distribution in the Chapman-Enskog method [70] and the thirteen-moment Grad approximation [201] are not non-negatively defined functions, while the thirteen-moment quasiequilibrium approximation [224] has no finite integrals (5.42) and (5.43).

### 6.3.2 Galilean Invariance of Invariance Equation

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

$$\frac{\mathrm{d}f}{\mathrm{d}t} = J_u(f), \frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial t} + u_{\boldsymbol{x},s}(f)\frac{\partial f}{\partial x_s} ;$$
$$J_u(f) = -(v_s - u_{\boldsymbol{x},s}(f))\frac{\partial f}{\partial x_s} + Q(f,f) . \tag{6.23}$$

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

$$u_{\boldsymbol{x},s}(f) = n_{\boldsymbol{x}}^{-1}(f)\int v_s f(\boldsymbol{v},\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{v};\ n_{\boldsymbol{x}}(f) = \int f(\boldsymbol{v},\boldsymbol{x})\,\mathrm{d}^3\boldsymbol{v} . \tag{6.24}$$

In particular, this form of the Boltzmann equation vector field is convenient when the initial manifold $\Omega_0$ consists of functions $f_{\Omega_0}$ which depend explicitly on $(\boldsymbol{v}-u_{\boldsymbol{x}}(f))$ (i.e., if functions $f_{\Omega_0} \in \Omega_0$ do not change under velocity shifts: $\boldsymbol{v} \to \boldsymbol{v} + c$, where $c$ is a constant vector). This is also the case of the LM manifold.

Substituting $J_u(f)$ (6.23) instead of $J(f)$ (5.44) into all expressions which depend on the Boltzmann equation vector field, we transfer all procedures developed above into the moving reference system. In particular, we obtain the following invariance equation of the first iteration for a general locally finite dimensional initial approximation $f_0(a(\boldsymbol{x}),\boldsymbol{v})$:

$$(P^{0*}_{a(\boldsymbol{x})}(\cdot) - 1)J^0_{u,\mathrm{lin},a(\boldsymbol{x})}(\delta f_1(a(\boldsymbol{x}),\boldsymbol{v})) + \Delta(f_0(a(\boldsymbol{x}),\boldsymbol{v})) = 0 ; \tag{6.25}$$

where

$$\begin{aligned} J^0_{u,\mathrm{lin},a(\boldsymbol{x})}(g) = &\left\{ n_{\boldsymbol{x}}^{-1}(f_0(a(\boldsymbol{x})))\int v_s g\,\mathrm{d}^3\boldsymbol{v} \right. \\ &\left. + u_{\boldsymbol{x},s}(f_0(a(\boldsymbol{x})))n_{\boldsymbol{x}}^{-1}(f_0(a(\boldsymbol{x})))\int g\,\mathrm{d}^3\boldsymbol{v} \right\}\frac{\partial f_0(a(\boldsymbol{x}),\boldsymbol{v})}{\partial x_s} \\ &- (v_s - u_{\boldsymbol{x},s}(f_0(a(\boldsymbol{x}))))\frac{\partial g}{\partial x_s} + L_{f_0(a(\boldsymbol{x}),\boldsymbol{v})}(g) ; \\ \Delta(f_0(a(\boldsymbol{x}),\boldsymbol{v})) = &(P^*_{a(\boldsymbol{x})}(\cdot) - 1)J_u(f_0(a(\boldsymbol{x}),\boldsymbol{v})) . \end{aligned}$$

Here $a(\boldsymbol{x})$ are coordinates on the manifold at the given space point $\boldsymbol{x}$, $P^*_{a(\boldsymbol{x})}$ is the corresponding thermodynamic projector. Additional conditions do not depend on the vector field, and thus they remain valid for equation (6.25).

### 6.3.3 Equation of the First Iteration

The equation of the first iteration in the form of (6.20) for the correction $\varphi(n,\boldsymbol{u},T)$ is:

$$\begin{aligned} &\{P_{f_0(n,\boldsymbol{u},T)}(\cdot) - 1\}\left\{-(v_s - u_s)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s} + f_0(n,\boldsymbol{u},T)L_{f_0(n,\boldsymbol{u},T)}(\varphi)\right. \\ &-(v_s - u_s)\frac{\partial(f_0(n,\boldsymbol{u},T)\varphi)}{\partial x_s} - n^{-1}(f_0(n,\boldsymbol{u},T))\left(\int v_s f_0(n,\boldsymbol{u},T)\varphi\,\mathrm{d}^3\boldsymbol{v}\right. \\ &\left.\left. + u_s(f_0(n,\boldsymbol{u},T))\int f_0(n,\boldsymbol{u},T)\varphi\,\mathrm{d}^3\boldsymbol{v}\right)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s}\right\} = 0 . \end{aligned} \tag{6.26}$$

Here $P_{f_0(n,\boldsymbol{u},T)}$ is the thermodynamic projector on the LM manifold and $f_0(n,\boldsymbol{u},T)L_{f_0(n,\boldsymbol{u},T)}(\varphi)$ is the linearized Boltzmann collision integral:

$$f_0(n,\boldsymbol{u},T)L_{f_0(n,\boldsymbol{u},T)}(\varphi) = \int w(\boldsymbol{v}',\boldsymbol{v}_1'|\boldsymbol{v},\boldsymbol{v}_1)f_0(n,\boldsymbol{u},T) \times \{\varphi' + \varphi_1' - \varphi_1 - \varphi\}\, \mathrm{d}^3\boldsymbol{v}'\, \mathrm{d}^3\boldsymbol{v}_1'\, \mathrm{d}^3\boldsymbol{v}_1 \,. \tag{6.27}$$

Additional condition for equation (6.26) has the form:

$$P_{f_0(n,\boldsymbol{u},T)}(f_0(n,\boldsymbol{u},T)\varphi) = 0 \,. \tag{6.28}$$

In detail notation:

$$\int 1 \cdot f_0(n,\boldsymbol{u},T)\varphi\, \mathrm{d}^3\boldsymbol{v} = 0,\ \int v_i f_0(n,\boldsymbol{u},T)\varphi\, \mathrm{d}^3\boldsymbol{v} = 0,\ \ i = 1,2,3 \,,$$
$$\int \boldsymbol{v}^2 f_0(n,\boldsymbol{u},T)\varphi\, \mathrm{d}^3\boldsymbol{v} = 0 \,. \tag{6.29}$$

Eliminating in (6.26) the terms containing

$$\int v_s f_0(n,\boldsymbol{u},T)\varphi\, \mathrm{d}^3\boldsymbol{v} \text{ and } \int f_0(n,\boldsymbol{u},T)\varphi\, \mathrm{d}^3\boldsymbol{v}$$

with the use of (6.29), we obtain the following form of equation (6.26):

$$\{P_{f_0(n,\boldsymbol{u},T)}(\cdot) - 1\}\left(-(v_s - u_s)\frac{\partial f_0(n,\boldsymbol{u},T)}{\partial x_s}\right. \tag{6.30}$$
$$\left. + f_0(n,\boldsymbol{u},T)L_{f_0(n,\boldsymbol{u},T)}(\varphi) - (v_s - u_s)\frac{\partial (f_0(n,\boldsymbol{u},T)\varphi)}{\partial x_s}\right) = 0 \,.$$

In order to address the properties of equation (6.30), it proves useful to introduce real Hilbert spaces $G_{f_0(n,\boldsymbol{u},T)}$ with scalar products:

$$(\varphi,\psi)_{f_0(n,\boldsymbol{u},T)} = \int f_0(n,\boldsymbol{u},T)\varphi\psi\, \mathrm{d}^3\boldsymbol{v} \,. \tag{6.31}$$

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

The projector $P_{f_0(n,\boldsymbol{u},T)}$ (5.55) is associated with a projector $\mathit{\Pi}_{f_0(n,\boldsymbol{u},T)}$ which acts in the space $G_{f_0(n,\boldsymbol{u},T)}$:

$$\mathit{\Pi}_{f_0(n,\boldsymbol{u},T)}(\varphi) = f_0^{-1}(n,\boldsymbol{u},T)P_{f_0(n,\boldsymbol{u},T)}(f_0(n,\boldsymbol{u},T)\varphi) \,. \tag{6.32}$$

It is an orthogonal projector, because

$$\mathit{\Pi}_{f_0(n,\boldsymbol{u},T)}(\varphi) = \sum_{s=0}^{4} \psi^{(s)}_{f_0(n,\boldsymbol{u},T)}(\psi^{(s)}_{f_0(n,\boldsymbol{u},T)},\varphi)_{f_0(n,\boldsymbol{u},T)} \,. \tag{6.33}$$

Here $\psi^{(s)}_{f_0(n,\boldsymbol{u},T)}$ are given by the expression (5.57).

We can rewrite the equation of the first iteration (6.30) in the form:

$$L_{f_0(n,\boldsymbol{u},T)}(\varphi) + K_{f_0(n,\boldsymbol{u},T)}(\varphi) = D_{f_0(n,\boldsymbol{u},T)} \; . \tag{6.34}$$

Notations used here are:

$$D_{f_0(n,\boldsymbol{u},T)} = f_0^{-1}(n,\boldsymbol{u},T)\Delta(f_0(n,\boldsymbol{u},T)) \; ; \tag{6.35}$$

$$K_{f_0(n,\boldsymbol{u},T)}(\varphi) = \left\{ \Pi_{f_0(n,\boldsymbol{u},T)}(\cdot) - 1 \right\} f_0^{-1}(n,\boldsymbol{u},T)(v_s - u_s)\frac{\partial(f_0(n,\boldsymbol{u},T)\varphi)}{\partial x_s} \; .$$

The additional condition for equation (6.34) is:

$$(\psi^{(s)}_{f_0(n,\boldsymbol{u},T)}, \varphi)_{f_0(n,\boldsymbol{u},T)} = 0, s = 0, \ldots, 4 \; . \tag{6.36}$$

We list now the properties of the equation (6.34) for usual collision models [70]:

(a) The linear integral operator $L_{f_0(n,\boldsymbol{u},T)}$ is self-adjoint with respect to the scalar product $(\cdot,\cdot)_{f_0(n,\boldsymbol{u},T)}$, and the quadratic form $(\varphi, L_{f_0(n,\boldsymbol{u},T)}(\varphi))$ is negatively definite in $\mathrm{im}L_{f_0(n,\boldsymbol{u},T)}$.
(b) The kernel of $L_{f_0(n,\boldsymbol{u},T)}$ does not depend on $f_0(n,\boldsymbol{u},T)$, and it is the linear hull of the polynomials $\psi_0 = 1, \psi_i = v_i, i = 1,2,3$, and $\psi_4 = v^2$.
(c) The right hand side $D_{f_0(n,\boldsymbol{u},T)}$ is orthogonal to $\ker L_{f_0(n,\boldsymbol{u},T)}$ in the sense of the scalar product $(\cdot,\cdot)_{f_0(n,\boldsymbol{u},T)}$.
(d) The projection operator $\Pi_{f_0(n,\boldsymbol{u},T)}$ is the self-adjoint projector onto $\ker L_{f_0(n,\boldsymbol{u},T)}$:

$$\Pi_{f_0(n,\boldsymbol{u},T)}(\varphi) \in \ \ker L_{f_0(n,\boldsymbol{u},T)} \tag{6.37}$$

Projector $\Pi_{f_0(n,\boldsymbol{u},T)}$ projects orthogonally.
(e) The image of the operator $K_{f_0(n,\boldsymbol{u},T)}$ is orthogonal to $\ker L_{f_0(n,\boldsymbol{u},T)}$.
(f) Additional condition (6.36) requires the solution of equation (6.34) to be orthogonal to $\ker L_{f_0(n,\boldsymbol{u},T)}$.

These properties result in the *necessary condition* for solving the equation (6.34) with the additional constraint (6.36). This means the following: equation (6.34), provided with constraint (6.36), satisfies the condition which is necessary to have the unique solution in $\mathrm{im}L_{f_0(n,\boldsymbol{u},T)}$.

**Remark.** Because of the *differential* part of the operator $K_{f_0(n,\boldsymbol{u},T)}$, we are not able to apply the Fredholm alternative to obtain the *necessary and sufficient* conditions for solvability of equation (6.36). Thus, the condition mentioned here is, rigorously speaking, only the necessary condition. Nevertheless, we shall continue to develop a formal procedure for solving the equation (6.34).

To this end, we paid no attention to the dependence of functions, spaces, operators, etc, on the space variable $\boldsymbol{x}$. It is useful to rewrite once again the equation (6.34) in order to separate the local in $\boldsymbol{x}$ operators from the

differential operators. Furthermore, we shall replace the subscript $f_0(n, \boldsymbol{u}, T)$ with the subscript $\boldsymbol{x}$ in all the expressions. We represent (6.34) as:

$$
\begin{aligned}
&A_{\mathrm{loc}}(\boldsymbol{x},\boldsymbol{v})\varphi - A_{\mathrm{diff}}\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right)\varphi = -D(\boldsymbol{x},\boldsymbol{v})\ ;\\
&A_{\mathrm{loc}}(\boldsymbol{x},\boldsymbol{v})\varphi = -\left\{L_{\boldsymbol{x}}(\boldsymbol{v})\varphi + (\Pi_{\boldsymbol{x}}(\boldsymbol{v})-1)r_{\boldsymbol{x}}\varphi\right\}\ ;\\
&A_{\mathrm{diff}}\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right)\varphi = (\Pi_{\boldsymbol{x}}(\cdot)-1)\left((v_s-u_s)\frac{\partial}{\partial x_s}\varphi\right)\ ;\\
&\Pi_{\boldsymbol{x}}(\boldsymbol{v})g = \sum_{s=0}^{4}\psi^{(s)}_{\boldsymbol{x}}(\psi^{(s)}_{\boldsymbol{x}}, g)\ ;\\
&\psi^{(0)}_{\boldsymbol{x}} = n^{-1/2},\ \psi^{(s)}_{\boldsymbol{x}} = (2/n)^{1/2}c_s(\boldsymbol{x},\boldsymbol{v}),\ s=1,2,3\ ,\\
&\psi^{(4)}_{\boldsymbol{x}} = (2/3n)^{1/2}(c^2(\boldsymbol{x},\boldsymbol{v})-3/2);\ c_i(\boldsymbol{x},\boldsymbol{v}) = (m/2k_BT(\boldsymbol{x}))^{1/2}(v_i-u_i(\boldsymbol{x}))\ ,\\
&r_{\boldsymbol{x}} = (v_s-u_s)\left(\frac{\partial \ln n}{\partial x_s} + \frac{m}{k_BT}(v_i-u_i)\frac{\partial u_i}{\partial x_s} + \left(\frac{m(\boldsymbol{v}-\boldsymbol{u})^2}{2k_BT}-\frac{3}{2}\right)\frac{\partial \ln T}{\partial x_s}\right)\ ;\\
&D(\boldsymbol{x},\boldsymbol{v}) = \left\{\left(\frac{m(\boldsymbol{v}-\boldsymbol{u})^2}{2k_BT}-\frac{5}{2}\right)(v_i-u_i)\frac{\partial \ln T}{\partial x_i}\right.\\
&\left.+\frac{m}{k_BT}\left(((v_i-u_i)(v_s-u_s)-\frac{1}{3}\delta_{is}(\boldsymbol{v}-\boldsymbol{u})^2\right)\frac{\partial u_s}{\partial x_i}\right\}\ .
\end{aligned}
\tag{6.38}
$$

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

The additional condition for this equation is:

$$\Pi_{\boldsymbol{x}}(\varphi) = 0\ . \tag{6.39}$$

Equation (6.38) is linear in $\varphi$. However, the main difficulty in solving this equation is caused by the differential in $\boldsymbol{x}$ operator $A_{\mathrm{diff}}$ which does not commute with the local in $\boldsymbol{x}$ operator $A_{\mathrm{loc}}$.

### 6.3.4 Parametrix Expansion

In this subsection we introduce a method to construct approximate solutions of equation (6.37). This procedure involves an expansion similar to the parametrix expansion in the theory of pseudo-differential (PDO) and Fourier integral operators (FIO).

Considering $\varphi \in \mathrm{im}L_{\boldsymbol{x}}$, we write a formal solution of equation (6.38) as:

$$\varphi(\boldsymbol{x},\boldsymbol{v}) = \left(A_{\mathrm{loc}}(\boldsymbol{x},\boldsymbol{v}) - A_{\mathrm{diff}}\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right)\right)^{-1}(-D(\boldsymbol{x},\boldsymbol{v})) \tag{6.40}$$

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

$$\varphi(\boldsymbol{x},\boldsymbol{v}) = \left(1 - B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right)^{-1} \varphi_{\rm loc}(\boldsymbol{x},\boldsymbol{v}) \; . \tag{6.41}$$

Notations used here are:

$$\begin{aligned} \varphi_{\rm loc}(\boldsymbol{x},\boldsymbol{v}) &= A^{-1}_{\rm loc}(\boldsymbol{x},\boldsymbol{v})(-D(\boldsymbol{x},\boldsymbol{v})) \\ &= [-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]^{-1}(-D(\boldsymbol{x},\boldsymbol{v})) \; ; \\ B_s(\boldsymbol{x},\boldsymbol{v}) &= A^{-1}_{\rm loc}(\boldsymbol{x},\boldsymbol{v})(\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(v_s - u_s) \\ &= [-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]^{-1}(\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(v_s - u_s) \; . \end{aligned} \tag{6.42}$$

We shall now discuss in more details the properties of the terms in (6.42).

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

$$-L_{\boldsymbol{x}}(\boldsymbol{v})\varphi_{\rm loc} - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(r_{\boldsymbol{x}}\varphi_{\rm loc}) = (-D(\boldsymbol{x},\boldsymbol{v})) \tag{6.43}$$

This latter linear integral equation has the unique solution in $\mathrm{im}L_{\boldsymbol{x}}(\boldsymbol{v})$. Indeed,

$$\begin{aligned} \ker A^{+}_{\rm loc}(\boldsymbol{x},\boldsymbol{v}) &= \ker(L_{\boldsymbol{x}}(\boldsymbol{v}) + (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}})^{+} \\ &= \ker(L_{\boldsymbol{x}}(\boldsymbol{v}))^{+} \bigcap \ker((\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}})^{+} \\ &= \ker(L_{\boldsymbol{x}}(\boldsymbol{v}))^{+} \bigcap \ker(r_{\boldsymbol{x}}(\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)) \; , \\ &\quad \text{and } G_{\boldsymbol{x}} \bigcap \Pi_{\boldsymbol{x}}(\boldsymbol{v})G_{\boldsymbol{x}} = \{0\} \; . \end{aligned} \tag{6.44}$$

Thus, the existence of the unique solution of equation (6.43) follows from the Fredholm alternative.

Let us consider the operator $R(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v})$:

$$R\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right) = \left(1 - B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right)^{-1} \; . \tag{6.45}$$

One can represent it as a formal series:

$$R\left(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v}\right) = \sum_{m=0}^{\infty} \left[B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right]^m \; . \tag{6.46}$$

Here

$$\left[B_s(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_s}\right]^m = B_{s_1}(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_{s_1}} \ldots B_{s_m}(\boldsymbol{x},\boldsymbol{v})\frac{\partial}{\partial x_{s_m}} \; . \tag{6.47}$$

Every term of the type (6.47) can be represented as a finite sum of operators which are superpositions of the following two operations: of the integral in $\boldsymbol{v}$ operations with kernels depending on $\boldsymbol{x}$, and of differential in $\boldsymbol{x}$ operations.

Our goal is to obtain explicit representation of the operator $R(\boldsymbol{x}, \frac{\partial}{\partial \boldsymbol{x}}, \boldsymbol{v})$ (6.45) as an integral operator. If the operator $B_s(\boldsymbol{x}, \boldsymbol{v})$ would not depend on $\boldsymbol{x}$ i.e., if no dependence on spatial variables would occur in kernels of integral operators, in $B_s(\boldsymbol{x}, \boldsymbol{v})$), then we could reach our goal via the usual Fourier transform. However, operators $B_s(\boldsymbol{x}, \boldsymbol{v})$ and $\frac{\partial}{\partial x_k}$ do not commute, and thus this elementary approach does not work. We shall develop a method to obtain the required explicit representation using the ideas of PDO and IOF technique.

We start with the representation (6.46). Our strategy is to transform every summand (6.47) in order to place integral in $\boldsymbol{v}$ operators $B_s(\boldsymbol{x}, \boldsymbol{v})$ on the left of the differential operators $\frac{\partial}{\partial x_k}$. The commutation of every pair $\frac{\partial}{\partial x_k} B_s(\boldsymbol{x}, \boldsymbol{v})$ yields an elementary transform:

$$\frac{\partial}{\partial x_k} B_s(\boldsymbol{x}, \boldsymbol{v}) \to B_s(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_k} - \left[ B_s(\boldsymbol{x}, \boldsymbol{v}), \frac{\partial}{\partial x_k} \right] . \tag{6.48}$$

Here $[M, N] = MN - NM$ denotes the commutator of operators $M$ and $N$. We can represent (6.47) as:

$$\begin{aligned} \left[ B_s(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_s} \right]^m &= B_{s_1}(\boldsymbol{x}, \boldsymbol{v}) \dots B_{s_m}(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_{s_1}} \dots \frac{\partial}{\partial x_{s_m}} \\ &+ O\left( \left[ B_{s_i}(\boldsymbol{x}, \boldsymbol{v}), \frac{\partial}{\partial x_{s_k}} \right] \right) . \end{aligned} \tag{6.49}$$

Here $O([B_{s_i}(\boldsymbol{x}, \boldsymbol{v}), \frac{\partial}{\partial x_{s_k}}])$ denotes the terms which contain one or more pairs of brackets $[\cdot, \cdot]$. The first term in (6.49) contains no 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 (6.47).

In this section we consider explicitly the zeroth-order term of this commutator expansion. Neglecting all the terms with brackets in (6.49), we write:

$$\left[ B_s(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_s} \right]_0^m = B_{s_1}(\boldsymbol{x}, \boldsymbol{v}) \dots B_{s_m}(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_{s_1}} \dots \frac{\partial}{\partial x_{s_m}} . \tag{6.50}$$

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

We should now substitute expressions $[B_s(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_s}]_0^m$ (6.50) instead of expressions $[B_s(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_s}]^m$ (6.47) into the series (6.46):

$$R_0\left( \boldsymbol{x}, \frac{\partial}{\partial x}, \boldsymbol{v} \right) = \sum_{m=0}^{\infty} \left[ B_s(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_s} \right]_0^m . \tag{6.51}$$

The action of every summand (6.50) might be defined via the Fourier transform with respect to spatial variables.

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

$$Fg(\boldsymbol{x}, \boldsymbol{v}) \equiv \hat{g}(\boldsymbol{k}, \boldsymbol{v}) = \int g(\boldsymbol{x}, \boldsymbol{v}) \exp(-ik_s x_s)\, \mathrm{d}^p \boldsymbol{x} \,. \tag{6.52}$$

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

$$g(x, \boldsymbol{v}) \equiv F^{-1}\hat{g}(\boldsymbol{k}, \boldsymbol{v}) = (2\pi)^{-p} \int \hat{g}(\boldsymbol{k}, \boldsymbol{v}) \exp(ik_s x_s)\, \mathrm{d}^p \boldsymbol{k} \,. \tag{6.53}$$

The action of the operator (6.50) on a function $g(\boldsymbol{x}, \boldsymbol{v})$ is defined as:

$$\begin{aligned}
&\left[B_s(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_s}\right]_0^m g(\boldsymbol{x}, \boldsymbol{v}) \\
&= \left(B_{s_1}(\boldsymbol{x}, \boldsymbol{v}) \ldots B_{s_m}(\boldsymbol{x}, \boldsymbol{v}) \frac{\partial}{\partial x_{s_1}} \ldots \frac{\partial}{\partial x_{s_m}}\right) (2\pi)^{-p} \int \hat{g}(\boldsymbol{k}, \boldsymbol{v}) e^{ik_s x_s}\, \mathrm{d}^p \boldsymbol{k} \\
&= (2\pi)^{-p} \int \exp(ik_s x_s)[ik_l B_l(\boldsymbol{x}, \boldsymbol{v})]^m \hat{g}(\boldsymbol{k}, \boldsymbol{v})\, \mathrm{d}^p \boldsymbol{k} \,.
\end{aligned} \tag{6.54}$$

Taking into account (6.54) in (6.51) yields the following definition of the operator $R_0$:

$$R_0 g(\boldsymbol{x}, \boldsymbol{v}) = (2\pi)^{-p} \int e^{ik_s x_s} (1 - ik_l B_l(\boldsymbol{x}, \boldsymbol{v}))^{-1} \hat{g}(\boldsymbol{k}, \boldsymbol{v})\, \mathrm{d}^p \boldsymbol{k} \,. \tag{6.55}$$

This is the *Fourier integral operator* (note that the kernel of this integral operator depends on $\boldsymbol{k}$ and on $\boldsymbol{x}$). The commutator expansion introduced above is a version of the *parametrix expansion* [249, 250], while expression (6.55) is the leading term of this expansion. The kernel $(1 - ik_l B_l(\boldsymbol{x}, \boldsymbol{v}))^{-1}$ is called the *main symbol of the parametrix*.

The account of (6.55) in the formula (6.41) yields the zeroth-order term of parametrix expansion $\varphi_0(\boldsymbol{x}, \boldsymbol{v})$:

$$\varphi_0(\boldsymbol{x}, \boldsymbol{v}) = F^{-1}(1 - ik_l B_l(\boldsymbol{x}, \boldsymbol{v}))^{-1} F\varphi_{\mathrm{loc}} \,. \tag{6.56}$$

In detail notation:

$$\begin{aligned}
&\varphi_0(\boldsymbol{x}, \boldsymbol{v}) = (2\pi)^{-p} \int \int \exp(ik_s(x_s - y_s)) \\
&\times (1 - ik_s[-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]^{-1} (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)(v_s - u_s(\boldsymbol{x})))^{-1} \\
&\times [-L_{\boldsymbol{y}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{y}}(\boldsymbol{v}) - 1)r_{\boldsymbol{y}}]^{-1} (-D(\boldsymbol{y}, \boldsymbol{v}))\, \mathrm{d}^p \boldsymbol{y}\, \mathrm{d}^p \boldsymbol{k} \,.
\end{aligned} \tag{6.57}$$

We shall now list the steps to calculate the function $\varphi_0(\boldsymbol{x}, \boldsymbol{v})$ (6.57).

**Step 1**. Solve the linear integral equation

$$[-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v}) - 1)r_{\boldsymbol{x}}]\varphi_{\mathrm{loc}}(\boldsymbol{x}, \boldsymbol{v}) = -D(\boldsymbol{x}, \boldsymbol{v}) \,. \tag{6.58}$$

and obtain the function $\varphi_{\mathrm{loc}}(\boldsymbol{x}, \boldsymbol{v})$.

**Step 2.** Calculate the Fourier transform $\hat{\varphi}_{\rm loc}(\boldsymbol{k},\boldsymbol{v})$:

$$\hat{\varphi}_{\rm loc}(\boldsymbol{k},\boldsymbol{v}) = \int \varphi_{\rm loc}(\boldsymbol{y},\boldsymbol{v})\exp(-ik_s y_s)\,\mathrm{d}^p\boldsymbol{y}\ . \tag{6.59}$$

**Step 3**. Solve the linear integral equation

$$\begin{aligned}&[-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v})-1)(r_{\boldsymbol{x}} + ik_s(v_s - u_s(\boldsymbol{x}))]\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v}) = -\hat{D}(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})\ ;\\ &-\hat{D}(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v}) = [-L_{\boldsymbol{x}}(\boldsymbol{v}) - (\Pi_{\boldsymbol{x}}(\boldsymbol{v})-1)r_{\boldsymbol{x}}]\hat{\varphi}_{\rm loc}(\boldsymbol{k},\boldsymbol{v})\ .\end{aligned} \tag{6.60}$$

and obtain the function $\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$.
**Step 4.** Calculate the inverse Fourier transform $\varphi_0(\boldsymbol{x},\boldsymbol{v})$:

$$\varphi_0(\boldsymbol{x},\boldsymbol{v}) = (2\pi)^{-p}\int \hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})\exp(ik_s x_s)\,\mathrm{d}^p\boldsymbol{k}\ . \tag{6.61}$$

Completing these four steps, we obtain an explicit expression for the zeroth-order term of parametrix expansion $\varphi_0(\boldsymbol{x},\boldsymbol{v})$(6.56).

As we have already mentioned it above, equation (6.58) of Step 1 has the unique solution in $\mathrm{im}L_{\boldsymbol{x}}(\boldsymbol{v})$. Equation (6.60) of Step 3 has the same property. Indeed, for every $\boldsymbol{k}$, the right hand side $-\hat{D}(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$ is orthogonal to $\mathrm{im}\Pi_{\boldsymbol{x}}(\boldsymbol{v})$, and thus the existence and the uniqueness of the formal solution $\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$ follows again from the Fredholm alternative.

Thus, in Step 3, we obtain the unique solution $\hat{\varphi}_0(\boldsymbol{x},\boldsymbol{k},\boldsymbol{v})$. For every $\boldsymbol{k}$, this is a function which belongs to $\mathrm{im}L_{\boldsymbol{x}}(\boldsymbol{v})$. Because the LM distribution $f_0(\boldsymbol{x},\boldsymbol{v}) = f_0(n(\boldsymbol{x}),\boldsymbol{u}(\boldsymbol{x}),T(\boldsymbol{x}),\boldsymbol{v})$ has no explicit dependency on $\boldsymbol{x}$, we see that the inverse Fourier transform of Step 4 gives $\varphi_0(\boldsymbol{x},\boldsymbol{v}) \in \mathrm{im}L_{\boldsymbol{x}}(\boldsymbol{v})$.

Equations (6.58)–(6.61) provide us with the scheme of constructing the zeroth-order term of parametrix expansion. Closing this section, we 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:

$$R = \sum_{m=0}^{\infty}(AB)^m\ . \tag{6.62}$$

In every term of this series, we want to place operators $A$ on the left to operators $B$. In order to do this, we have to commute $B$ with $A$ from left to right. The commutation of every pair $BA$ yields the elementary transform, $BA \to AB - [A,B]$, 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:

$$R = R_0 + R_1 + (\text{terms with more than two brackets})\ . \tag{6.63}$$

Here

$$R_0 = \sum_{m=0}^{\infty} A^m B^m \; ; \tag{6.64}$$

$$R_1 = -\sum_{m=2}^{\infty} \sum_{i=2}^{\infty} i A^{m-i} [A, B] A^{i-1} B^{i-1} B^{m-i} \; . \tag{6.65}$$

Operator $R_0$ (6.64) is the zeroth-order term of parametrix expansion derived above. Operator $R_1$ (the *first-order term of parametrix expansion*) can be represented as follows:

$$R_1 = -\sum_{m=1}^{\infty} m A^m [A, B] \left( \sum_{i=0}^{\infty} A^i B^i \right) B^m = -\sum_{m=1}^{\infty} m A^m C B^m \; ,$$
$$C = [A, B] R_0 \; . \tag{6.66}$$

This expression can be considered as an *ansatz* for the formal series (6.62), 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.

In the next subsection we shall consider in more detail the zero-order term of parametrix expansion.

### 6.3.5 Finite-Dimensional Approximations to Integral Equations

Dealing further only with the zeroth-order term of parametrix expansion (6.57), we have to solve two linear integral equations, (6.58) and (6.60). These equations satisfy the Fredholm alternative, and thus they have unique solutions. After the problem is reduced to solving linear integral equations, we are at the same level of complexity as in the Chapman-Enskog method. The usual approach is to replace integral operators with some appropriate finite-dimensional operators.

First we remind some standard objectives of finite-dimensional approximations, considering equation (6.58). Let $p_i(\boldsymbol{x}, \boldsymbol{v})$, where $i = 1, 2, \ldots$, be a basis in $\mathrm{im} L_{\boldsymbol{x}}(\boldsymbol{v})$. Every function $\varphi(\boldsymbol{x}, \boldsymbol{v}) \in \mathrm{im} L_{\boldsymbol{x}}(\boldsymbol{v})$ can be represented in this basis as:

$$\varphi(\boldsymbol{x}, \boldsymbol{v}) = \sum_{i=1}^{\infty} a_i(\boldsymbol{x}) p_i(\boldsymbol{x}, \boldsymbol{v}); a_i(\boldsymbol{x}) = (\varphi(\boldsymbol{x}, \boldsymbol{v}), p_i(\boldsymbol{x}, \boldsymbol{v}))_{\boldsymbol{x}} \; . \tag{6.67}$$

Equation (6.58) is equivalent to an infinite set of linear algebraic equations with respect to unknowns $a_i(\boldsymbol{x})$:

$$\sum_{i=1}^{\infty} m_{ki}(\boldsymbol{x}) a_i(\boldsymbol{x}) = d_k(\boldsymbol{x}), \quad k = 1, 2, \ldots \; . \tag{6.68}$$

Here

$$m_{ki}(\boldsymbol{x}) = (p_k(\boldsymbol{x},\boldsymbol{v}), A_{\rm loc}(\boldsymbol{x},\boldsymbol{v})p_i(\boldsymbol{x},\boldsymbol{v}))_{\boldsymbol{x}} \; ;$$
$$d_k(\boldsymbol{x}) = -(p_k(\boldsymbol{x},\boldsymbol{v}), D(\boldsymbol{x},\boldsymbol{v}))_{\boldsymbol{x}} \; . \tag{6.69}$$

For a finite-dimensional approximation of equation (6.68) we use a projection onto a finite number of basis functions $p_i(\boldsymbol{x},\boldsymbol{v}), i = i_1,\ldots,i_n$. Then, instead of (6.67), we search for the function $\varphi_{\rm fin}$:

$$\varphi_{\rm fin}(\boldsymbol{x},\boldsymbol{v}) = \sum_{s=1}^{n} a_{i_s}(\boldsymbol{x}) p_{i_s}(\boldsymbol{x},\boldsymbol{v}) \; . \tag{6.70}$$

Infinite set of equations (6.68) is replaced with a finite set of linear algebraic equations with respect to $a_{i_s}(\boldsymbol{x})$, where $s = 1,\ldots,n$:

$$\sum_{l=1}^{n} m_{i_s i_l}(\boldsymbol{x}) a_{i_l}(\boldsymbol{x}) = d_{i_s}(\boldsymbol{x}), \quad s = 1,\ldots,n \; . \tag{6.71}$$

There are no a priori restrictions upon the choice of the basis, as well as upon the choice of its finite-dimensional approximations. Here we use the standard basis of irreducible Hermite tensors (see, for example, [112,201]). The simplest finite-dimensional approximation occurs if the finite set of Hermite tensors is chosen as:

$$p_k(\boldsymbol{x},\boldsymbol{v}) = c_k(\boldsymbol{x},\boldsymbol{v})(c^2(\boldsymbol{x},\boldsymbol{v}) - (5/2)), k = 1,2,3 \; ;$$
$$p_{ij}(\boldsymbol{x},\boldsymbol{v}) = c_i(\boldsymbol{x},\boldsymbol{v})c_j(\boldsymbol{x},\boldsymbol{v}) - \frac{1}{3}\delta_{ij}c^2(\boldsymbol{x},\boldsymbol{v}), \quad i,j = 1,2,3 \; ;$$
$$c_i(\boldsymbol{x},\boldsymbol{v}) = \boldsymbol{v}_T^{-1}(\boldsymbol{x})(v_i - u_i(\boldsymbol{x})), \quad v_T(\boldsymbol{x}) = (2k_B T(\boldsymbol{x})/m)^{1/2} \; . \tag{6.72}$$

It is important to stress here that "good" properties of orthogonality of Hermite tensors, as well as of other similar polynomial systems in the Boltzmann equation theory, have the local in $\boldsymbol{x}$ character, i.e. when these functions are treated as polynomials in $c(\boldsymbol{x},\boldsymbol{v})$ rather than polynomials in $\boldsymbol{v}$. For example, functions $p_k(\boldsymbol{x},\boldsymbol{v})$ and $p_{ij}(\boldsymbol{x},\boldsymbol{v})$(6.72) are orthogonal in the sense of the scalar product $(\cdot,\cdot)_{\boldsymbol{x}}$:

$$(p_k(\boldsymbol{x},\boldsymbol{v}), p_{ij}(\boldsymbol{x},\boldsymbol{v}))_{\boldsymbol{x}} \propto \int e^{-c^2(\boldsymbol{x},\boldsymbol{v})} p_k(\boldsymbol{x},\boldsymbol{v}) p_{ij}(\boldsymbol{x},\boldsymbol{v})\, {\rm d}^3 c(\boldsymbol{x},\boldsymbol{v}) = 0 \; . \tag{6.73}$$

On the contrary, functions $p_k(\boldsymbol{y},\boldsymbol{v})$ and $p_{ij}(\boldsymbol{x},\boldsymbol{v})$ are not orthogonal neither in the sense of the scalar product $(\cdot,\cdot)_{\boldsymbol{y}}$, nor in the sense of the scalar product $(\cdot,\cdot)_{\boldsymbol{x}}$, if $\boldsymbol{y} \neq \boldsymbol{x}$. This distinction is important for constructing the parametrix expansion. Further, we omit the dependencies on $\boldsymbol{x}$ and $\boldsymbol{v}$ in the dimensionless velocity $c_i(\boldsymbol{x},\boldsymbol{v})$(6.72) if no confusion might occur.

In this section we consider the case of one-dimensional in $\boldsymbol{x}$ equations. We assume that:

$$u_1(\boldsymbol{x}) = u(x_1)\,, \quad u_2 = u_3 = 0\,, \quad T(\boldsymbol{x}) = T(x_1), \quad n(\boldsymbol{x}) = n(x_1)\,. \quad (6.74)$$

We write $x$ instead of $x_1$ below. Finite-dimensional approximation (6.72) requires only two functions:

$$p_3(x,\boldsymbol{v}) = c_1^2(x,\boldsymbol{v}) - \frac{1}{3}c^2(x,\boldsymbol{v})\,, \quad p_4(x,\boldsymbol{v}) = c_1(x,\boldsymbol{v})(c^2(x,\boldsymbol{v}) - (5/2))\,,$$
$$c_1(x,\boldsymbol{v}) = v_T^{-1}(x)(v_1 - u(x))\,, \quad c_{2,3}(x,\boldsymbol{v}) = v_T^{-1}(x)v_{2,3}\,. \quad (6.75)$$

We shall now perform a step-by-step calculation of the zeroth-order term of the parametrix expansion, in the one-dimensional case, for the finite-dimensional approximation (6.75).

**Step 1.** *Calculation of* $\varphi_{\mathrm{loc}}(x,\boldsymbol{v})$ *from equation* (6.58).

We seek the function $\varphi_{\mathrm{loc}}(x,\boldsymbol{v})$ in the approximation (6.75) as:

$$\varphi_{\mathrm{loc}}(x,\boldsymbol{v}) = a_{\mathrm{loc}}(x)(c_1^2 - (1/3)c^2) + b_{\mathrm{loc}}(x)c_1(c^2 - (5/2))\,. \quad (6.76)$$

Finite-dimensional approximation (6.71) of integral equation (6.58) in the basis (6.75) yields:

$$m_{33}(x)a_{\mathrm{loc}}(x) + m_{34}(x)b_{\mathrm{loc}}(x) = \alpha_{\mathrm{loc}}(x)\,;$$
$$m_{43}(x)a_{\mathrm{loc}}(x) + m_{44}(x)b_{\mathrm{loc}}(x) = \beta_{\mathrm{loc}}(x)\,. \quad (6.77)$$

Notations used are:

$$m_{33}(x) = n(x)\lambda_3(x) + \frac{11}{9}\frac{\partial u}{\partial x}\,; \qquad m_{44}(x) = n(x)\lambda_4(x) + \frac{27}{4}\frac{\partial u}{\partial x}\,;$$
$$m_{34}(x) = m_{43}(x) = \frac{v_T(x)}{3}\left(\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right)\,;$$
$$\lambda_{3,4}(x) = -\frac{1}{\pi^{3/2}}\int e^{-c^2(\boldsymbol{x},\boldsymbol{v})}p_{3,4}(x,\boldsymbol{v})L_{\boldsymbol{x}}(\boldsymbol{v})p_{3,4}(\boldsymbol{x},\boldsymbol{v})\,\mathrm{d}^3c(\boldsymbol{x},\boldsymbol{v}) > 0\,;$$
$$\alpha_{\mathrm{loc}}(x) = -\frac{2}{3}\frac{\partial u}{\partial x}\,; \qquad \beta_{\mathrm{loc}}(x) = -\frac{5}{4}v_T(x)\frac{\partial \ln T}{\partial x}\,. \quad (6.78)$$

Parameters $\lambda_3(x)$ and $\lambda_4(x)$ are easily expressed via the so-called Enskog integral brackets, and they are calculated in [70] for a wide class of molecular models.

Solving equation (6.77), we obtain coefficients $a_{\mathrm{loc}}(x)$ and $b_{\mathrm{loc}}(x)$ in the expression (6.76):

$$a_{\mathrm{loc}} = \frac{A_{\mathrm{loc}}(x)}{Z(x,0)}\,; \quad b_{\mathrm{loc}} = \frac{B_{\mathrm{loc}}(x)}{Z(x,0)}\,; \quad Z(x,0) = m_{33}(x)m_{44}(x) - m_{34}^2(x)\,;$$
$$A_{\mathrm{loc}}(x) = \alpha_{\mathrm{loc}}(x)m_{44}(x) - \beta_{\mathrm{loc}}(x)m_{34}(x)\,;$$
$$B_{\mathrm{loc}}(x) = \beta_{\mathrm{loc}}(x)m_{33}(x) - \alpha_{\mathrm{loc}}(x)m_{34}(x)\,;$$
$$a_{\mathrm{loc}} = \frac{-\frac{2}{3}\frac{\partial u}{\partial x}\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) + \frac{5}{12}v_T^2\frac{\partial \ln T}{\partial x}\left(\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right)}{\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right)\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) - \frac{v_T^2}{9}\left(\frac{\partial \ln n}{\partial x} + \frac{11}{2}\frac{\partial \ln T}{\partial x}\right)^2}\,;$$

$$b_{\rm loc}=\frac{-\frac{5}{4}v_T\frac{\partial\ln T}{\partial x}\left(n\lambda_3+\frac{11}{9}\frac{\partial u}{\partial x}\right)+\frac{2}{9}v_T\frac{\partial u}{\partial x}\left(\frac{\partial\ln n}{\partial x}+\frac{11}{2}\frac{\partial\ln T}{\partial x}\right)}{\left(n\lambda_3+\frac{11}{9}\frac{\partial u}{x}\right)\left(n\lambda_4+\frac{27}{4}\frac{\partial u}{\partial x}\right)-\frac{v_T^2}{9}\left(\frac{\partial\ln n}{x}+\frac{11}{2}\frac{\partial\ln T}{x}\right)^2}\,. \tag{6.79}$$

These expressions complete Step 1.

**Step 2.** *Calculation of Fourier transform of $\varphi_{loc}(x,\boldsymbol{v})$ and its expression in the local basis.*

In this step we make two operations:

(i) The Fourier transformation of the function $\varphi_{\rm loc}(x,\boldsymbol{v})$:

$$\hat\varphi_{\rm loc}(k,\boldsymbol{v})=\int_{-\infty}^{+\infty}\exp(-iky)\varphi_{\rm loc}(y,\boldsymbol{v})\,{\rm d}y\,. \tag{6.80}$$

(ii) The representation of $\hat\varphi_{\rm loc}(k,\boldsymbol{v})$ in the local basis $\{p_0(x,\boldsymbol{v}),\dots,p_4(x,\boldsymbol{v})\}$:

$$p_0(x,\boldsymbol{v})=1, p_1(x,\boldsymbol{v})=c_1(x,\boldsymbol{v}), p_2(x,\boldsymbol{v})=c^2(x,\boldsymbol{v})-(3/2)\,, \tag{6.81}$$
$$p_3(x,\boldsymbol{v})=c_1^2(x,\boldsymbol{v})-(1/3)c^2(x,\boldsymbol{v}), p_4(x,\boldsymbol{v})=c_1(x,\boldsymbol{v})(c^2(x,\boldsymbol{v})-(5/2))\,.$$

Operation (ii) is necessary for completing Step 3 because there we deal with $x$-dependent operators. Obviously, the function $\hat\varphi_{\rm loc}(k,\boldsymbol{v})$ (6.80) is a finite-order polynomial in $\boldsymbol{v}$, and thus representation (ii) is exact.

We obtain in (ii):

$$\hat\varphi_{\rm loc}(x,k,\boldsymbol{v})\equiv\hat\varphi_{\rm loc}(x,k,c(x,\boldsymbol{v}))=\sum_{i=0}^{4}\hat h_i(x,k)p_i(x,\boldsymbol{v})\,. \tag{6.82}$$

Here

$$\hat h_i(x,k)=(p_i(x,\boldsymbol{v}),p_i(x,\boldsymbol{v}))_x^{-2}(\hat\varphi_{\rm loc}(k,\boldsymbol{v}),p_i(x,\boldsymbol{v}))_x\,. \tag{6.83}$$

Let us introduce notations:

$$\vartheta\equiv\vartheta(x,y)=(T(x)/T(y))^{1/2}\,,\quad \gamma\equiv\gamma(x,y)=\frac{u(x)-u(y)}{v_T(y)}\,. \tag{6.84}$$

Coefficients $\hat h_i(x,k)$(6.83) have the following explicit form:

$$\begin{aligned}
\hat h_i(x,k)&=\int_{-\infty}^{+\infty}\exp(-iky)h_i(x,y)\,{\rm d}y;\, h_i(x,y)=Z^{-1}(y,0)g_i(x,y)\\
g_0(x,y)&=B_{\rm loc}(y)(\gamma^3+\frac{5}{2}\gamma(\vartheta^2-1))+\frac{2}{3}A_{\rm loc}(y)\gamma^2\,;\\
g_1(x,y)&=B_{\rm loc}(y)(3\vartheta\gamma^2+\frac{5}{2}\vartheta(\vartheta^2-1))+\frac{4}{3}A_{\rm loc}(y)\vartheta\gamma\,;\\
g_2(x,y)&=\frac{5}{3}B_{\rm loc}(y)\vartheta^2\gamma\,;\\
g_3(x,y)&=B_{\rm loc}(y)2\vartheta\gamma+A_{\rm loc}(y)\vartheta^2\,;\\
g_4(x,y)&=B_{\rm loc}(y)\vartheta^3\,.
\end{aligned} \tag{6.85}$$

Here $Z(y,0), B_{\rm loc}(y)$ and $A_{\rm loc}(y)$ are the functions defined in (6.79)

**Step 3.** *Calculation of the function $\hat{\varphi}_0(x,k,\boldsymbol{v})$ from equation (6.60).*

Linear integral equation (6.60) is similar to equation (6.58). We search for the function $\hat{\varphi}_0(x,k,\boldsymbol{v})$ in the basis (6.75) as:

$$\hat{\varphi}_0(x,k,\boldsymbol{v}) = \hat{a}_0(x,k)p_3(x,\boldsymbol{v}) + \hat{b}_0(x,k)p_4(x,\boldsymbol{v}) \; . \tag{6.86}$$

Finite-dimensional approximation of the integral equation (6.60) in the basis (6.75) yields the following equations for unknowns $\hat{a}_0(x,k)$ and $\hat{b}_0(x,k)$:

$$\begin{aligned} m_{33}(x)\hat{a}_0(x,k) + \left[m_{34}(x) + \frac{1}{3}ikv_T(x)\right]\hat{b}_0(x,k) &= \hat{\alpha}_0(x,k) \; ; \\ \left[m_{43}(x) + \frac{1}{3}ikv_T(x)\right]\hat{a}_0(x,k) + m_{44}(x)\hat{b}_0(x,k) &= \hat{\beta}_0(x,k) \; . \end{aligned} \tag{6.87}$$

Notations used here are:

$$\hat{\alpha}_0(x,k) = m_{33}(x)\hat{h}_3(x,k) + m_{34}(x)\hat{h}_4(x,k) + \hat{s}_\alpha(x,k) \; ; \tag{6.88}$$

$$\begin{aligned} \hat{\beta}_0(x,k) &= m_{43}(x)\hat{h}_3(x,k) + m_{44}(x)\hat{h}_4(x,k) + \hat{s}_\beta(x,k) \; ; \\ \hat{s}_{\alpha,\beta}(x,k) &= \int_{-\infty}^{+\infty} \exp(-iky)s_{\alpha,\beta}(x,y)\,{\rm d}y \; ; \\ s_\alpha(x,y) &= \frac{1}{3}v_T(x)\left(\frac{\partial \ln n}{\partial x} + 2\frac{\partial \ln T}{\partial x}\right)h_1(x,y) \\ &\quad + \frac{2}{3}\frac{\partial u}{\partial x}(h_0(x,y) + 2h_2(x,y)) \; ; \\ s_\beta(x,y) &= \frac{5}{4}v_T(x)\left(\frac{\partial \ln n}{\partial x}h_2(x,y) + \frac{\partial \ln T}{\partial x}(3h_2(x,y) + h_0(x,y))\right) \\ &\quad + \frac{2\partial u}{3\partial x}h_1(x,y) \; . \end{aligned} \tag{6.89}$$

Solving equations (6.87), we obtain functions $\hat{a}_0(x,k)$ and $\hat{b}_0(x,k)$ in (6.86):

$$\begin{aligned} \hat{a}_0(x,k) &= \frac{\hat{\alpha}_0(x,k)m_{44}(x) - \hat{\beta}_0(x,k)(m_{34}(x) + \frac{1}{3}ikv_T(x))}{Z(x,\frac{1}{3}ikv_T(x))} \; ; \\ \hat{b}_0(x,k) &= \frac{\hat{\beta}_0(x,k)m_{33}(x) - \hat{\alpha}_0(x,k)(m_{34}(x) + \frac{1}{3}ikv_T(x))}{Z(x,\frac{1}{3}ikv_T(x))} \; . \end{aligned} \tag{6.90}$$

Here

$$\begin{aligned} Z(x,\frac{1}{3}ikv_T(x)) &= Z(x,0) + \frac{k^2v_T^2(x)}{9} + \frac{2}{3}ikv_T(x)m_{34}(x) \\ &= \left(n\lambda_3 + \frac{11\partial u}{9\partial x}\right)\left(n\lambda_4 + \frac{27\partial u}{4\partial x}\right) \end{aligned}$$

$$-\frac{v_T^2(x)}{9}\left(\frac{\partial \ln n}{\partial x}+\frac{11\partial \ln T}{2\partial x}\right)^2$$
$$+\frac{k^2v_T^2(x)}{9}+\frac{2}{9}ikv_T^2(x)\left(\frac{\partial \ln n}{\partial x}+\frac{11\partial \ln T}{2\partial x}\right) . \quad (6.91)$$

**Step 4**. *Calculation of the inverse Fourier transform of the function* $\hat{\varphi}_0(x,k,\boldsymbol{v})$.

The inverse Fourier transform of the function $\hat{\varphi}_0(x,k,\boldsymbol{v})$ (6.86) yields:

$$\varphi_0(x,\boldsymbol{v}) = a_0(x)p_3(x,\boldsymbol{v}) + b_0(x)p_4(x,\boldsymbol{v}) . \quad (6.92)$$

Here

$$a_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp(ikx)\hat{a}_0(x,k)\,\mathrm{d}k ,$$
$$b_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\exp(ikx)\hat{b}_0(x,k)\,\mathrm{d}k . \quad (6.93)$$

Taking into account expressions (6.79), (6.90)–(6.91), and (6.85), we obtain finally the explicit expression for the *finite-dimensional approximation of the zeroth-order term of parametrix expansion* (6.92):

$$a_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\mathrm{d}y\int_{-\infty}^{+\infty}\mathrm{d}k\exp(ik(x-y))Z^{-1}(x,\frac{1}{3}ikv_T(x))$$
$$\times\{Z(x,0)h_3(x,y)+[s_\alpha(x,y)m_{44}(x)-s_\beta(x,y)m_{34}(x)]$$
$$-\frac{1}{3}ikv_T(x)[m_{34}(x)h_3(x,y)+m_{44}(x)h_4(x,y)+s_\beta(x,y)]\Big\} ;$$
$$b_0(x) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}dy\int_{-\infty}^{+\infty}\mathrm{d}k\exp(ik(x-y))Z^{-1}(x,\frac{1}{3}ikv_T(x))$$
$$\times\{Z(x,0)h_4(x,y)+[s_\beta(x,y)m_{33}(x)-s_\alpha(x,y)m_{34}(x)]$$
$$-\frac{1}{3}ikv_T(x)[m_{34}(x)h_4(x,y)+m_{33}(x)h_3(x,y)+s_\alpha(x,y)]\Big\} . \quad (6.94)$$

### 6.3.6 Hydrodynamic Equations

Now we discuss the utility of obtained results for hydrodynamics.

The correction to the LM manifold $f_0(n,\boldsymbol{u},T)$(5.49) has the form:

$$f_1(n,\boldsymbol{u},T) = f_0(n,\boldsymbol{u},T)(1+\varphi_0(n,\boldsymbol{u},T)) \quad (6.95)$$

Here the function $\varphi_0(n,\boldsymbol{u},T)$ is given explicitly by expressions (6.92)–(6.94).

The usual form of closed hydrodynamic equations for $n,\boldsymbol{u}$, and $T$, where the traceless stress tensor $\sigma_{ik}$ and the heat flux vector $q_i$ are expressed via hydrodynamic variables, will be obtained if we substitute the function (6.95)

into balance equations of the density, of the momentum, and of the energy. For the LM approximation, these balance equations result in the Euler equation of the nonviscid liquid (i.e. $\sigma_{ik}(f_0) \equiv 0$, and $q_i(f_0) \equiv 0$). For the correction $f_1$ (6.95), 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 one-dimensional situation under consideration):

$$\sigma = \frac{1}{3} n a_0 \ , \quad q = \frac{5}{4} n b_0 \ . \tag{6.96}$$

Here $a_0$ and $b_0$ are given by expression (6.94).

From the geometrical viewpoint, hydrodynamic equations with the stress tensor and the heat flux vector (6.96) have the following interpretation: we take the corrected manifold $\Omega_1$ which consists of functions $f_1$ (6.95), and we project the Boltzmann equation vectors $J_{\boldsymbol{u}}(f_1)$ onto the tangent spaces $T_{f_1}$ using the quasiequilibrium projector $P_{f_0}$ (5.55).

### 6.3.7 Nonlocality

Expressions (6.94) include nonlocal spatial dependence, and, hence, the corresponding hydrodynamic equations are nonlocal. This nonlocality enters in two different ways. The first source of nonlocality might be called a *frequency-response nonlocality*, and it enters through explicit non-polynomial $k$-dependence of integrands in (6.94). This latter dependence has the form:

$$\int_{-\infty}^{+\infty} \frac{A(x,y) + ikB(x,y)}{C(x,y) + ikD(x,y) + k^2 E(x,y)} \exp(ik(x-y))\, \mathrm{d}k \ . \tag{6.97}$$

Integration over $k$ in (6.97) can be completed via auxiliary functions.

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

### 6.3.8 Acoustic Spectra

The frequency-response nonlocality in hydrodynamic equations is relevant to small perturbations of the uniform equilibrium. The stress tensor $\sigma$ and the heat flux $q$(6.96) are:

$$\begin{aligned} \sigma &= -(2/3) n_0 T_0 R \left( 2\varepsilon \frac{\partial u}{\partial \xi}' - 3\varepsilon^2 \frac{\partial^2 T}{\partial \xi^2} \right) \ ; \\ q &= -(5/4) T_0^{3/2} n_0 R \left( 3\varepsilon \frac{\partial T}{\partial \xi}' - (8/5)\varepsilon^2 \frac{\partial^2 u}{\partial \xi^2} \right) \ . \end{aligned} \tag{6.98}$$

Here

$$R = \left(1 - (2/5)\varepsilon^2 \frac{\partial^2}{\partial \xi^2}\right) - 1 \,. \tag{6.99}$$

In (6.98), we have expressed parameters $\lambda_3$ and $\lambda_4$ via the viscosity coefficient $\mu$ of the Chapman-Enskog method [70] (it is easy to see from (6.78) 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 $\delta u, \delta T, \delta n$ 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 used the system of units with $k_B = m = 1$.

In the linear case, the parametrix expansion degenerates, and its zeroth-order term (6.61) gives the exact solution to equation (6.38).

The dispersion relationship for the approximation (6.98) is:

$$\begin{aligned} &\omega^3 + (23k^2/6D)\omega^2 + \left\{k^2 + (2k^4/D^2) + (8k^6/5D^2)\right\}\omega + (5k^4/2D) = 0 \,; \\ &D = 1 + (4/5)k^2 \,. \end{aligned} \tag{6.100}$$

Here $k$ is the wave vector.

The acoustic spectrum given by the dispersion relationship (6.100) contains no nonphysical short-wave instability, unlike the Burnett approximation (Fig. 6.2). The regularization of the Burnett approximation [43, 44] gives a similar result. Both of these approximations predict a limit of the decrement $\mathrm{Re}\omega$ for short waves. These issues will be addressed in more detail in Chap. 8.

### 6.3.9 Nonlinearity

Nonlinear dependence 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 $\varphi_{\mathrm{loc}}$(6.79). In order to outline some features of this nonlinearity, we represent the zeroth-order term of the expansion of $a_{\mathrm{loc}}$(6.79) into powers of $\frac{\partial \ln T}{\partial x}$ and $\frac{\partial \ln n}{\partial x}$:

$$a_{\mathrm{loc}} = -\frac{2}{3}\frac{\partial u}{\partial x}\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right)^{-1} + O\left(\frac{\partial \ln T}{\partial x}, \frac{\partial \ln n}{\partial x}\right) \,. \tag{6.101}$$

This expression describes the asymptotic of the "purely nonlinear" contribution to the stress tensor $\sigma$(6.96) for a strong divergency of a flow. The account of nonlocality yields instead of (6.98):

$$\begin{aligned} a_0(x) = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} dy \int_{-\infty}^{+\infty} \mathrm{d}k \exp(ik(x-y)) \frac{2}{3}\frac{\partial u}{\partial y}\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial y}\right)^{-1} \\ \times \left[\left(n\lambda_3 + \frac{11}{9}\frac{\partial u}{\partial x}\right)\left(n\lambda_4 + \frac{27}{4}\frac{\partial u}{\partial x}\right) + \frac{k^2 v_T^2}{9}\right]^{-1} \end{aligned}$$

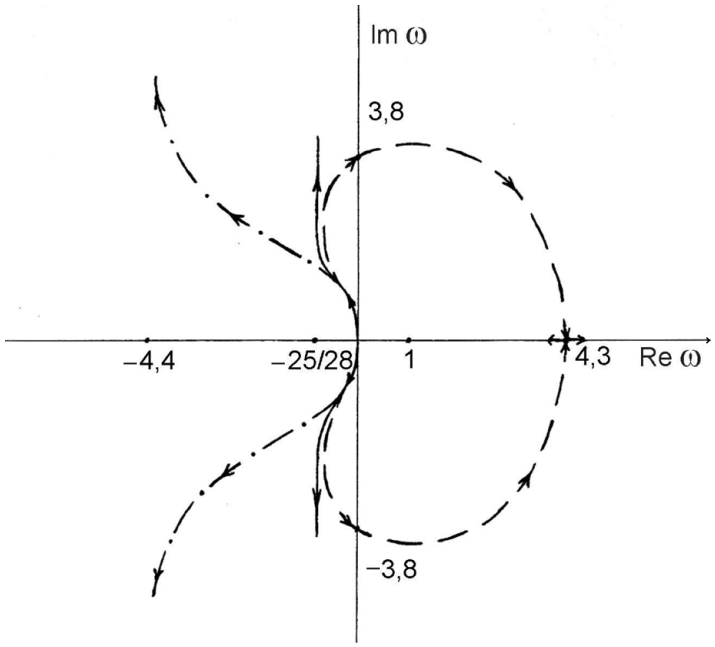


**Fig. 6.2.** Acoustic dispersion curves for approximation (6.98) (*solid* line), for second (the Burnett) approximation of the Chapman-Enskog expansion [72] (*dashed* line) and for the regularization of the Burnett approximation via partial summing of the Chapman-Enskog expansion [43,44] (punctuated *dashed* line). Arrows indicate the direction of increase of $k^2$

$$\times\left[\left(n\lambda_3+\frac{11}{9}\frac{\partial u}{\partial x}\right)\left(n\lambda_4+\frac{27}{4}\frac{\partial u}{\partial x}\right)\right.$$
$$\left.+\frac{4}{9}\left(n\lambda_4+\frac{27}{4}\frac{\partial u}{\partial dy}\right)\frac{\partial u}{\partial x}v_T^{-2}(u(x)-u(y))^2-\frac{2}{3}ik\frac{\partial u}{\partial x}(u(x)-u(y))\right]$$
$$+O\left(\frac{\partial \ln T}{\partial x},\frac{\partial \ln n}{\partial x}\right)\ . \tag{6.102}$$

Both expressions, (6.101) and (6.102) become singular when

$$\frac{\partial u}{\partial y}\to\left(\frac{\partial u}{\partial y}\right)^*=-\frac{9n\lambda_3}{11}\ . \tag{6.103}$$

Hence, the stress tensor (6.97) becomes infinite if $\frac{\partial u}{\partial y}$ tends to $\frac{\partial u}{\partial y}^*$ in any point $y$. In other words, the flow becomes "infinitely viscous" 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 damping" at $\frac{\partial u}{\partial y}^*$. This peculiarity was detected in

[43, 44] as a result of partial summation of the Chapman-Enskog expansion. In particular, partial summing for the simplest nonlinear situation [45, 233] yields the following expression for the stress tensor $\sigma$:

$$\sigma = \sigma_{\mathrm{I}R} + \sigma_{\mathrm{II}R}\,; \quad \sigma_{\mathrm{I}R} = -\frac{4}{3}\left(1 - \frac{5}{3}\varepsilon^2\frac{\partial^2}{\partial\xi^2}\right)^{-1}\left(\varepsilon\frac{\partial u'}{\partial\xi} + \varepsilon^2\frac{\partial^2\theta'}{\partial\xi^2}\right)\,;$$
$$\theta' = T' + n'\,; \quad \sigma_{\mathrm{II}R} = \frac{28}{9}\left(1 + \frac{7}{3}\varepsilon\frac{\partial u'}{\partial\xi}\right)^{-1}\frac{\partial^2 u'}{\partial\xi^2}\,. \tag{6.104}$$

Notations here follow (6.98) and (6.99). Expression (6.104) might be considered as a scetch of the "full" stress tensor defined by $a_0$(6.94). It takes into account both the frequency-response and the nonlinear contributions ($\sigma_{\mathrm{I}R}$ and $\sigma_{\mathrm{II}R}$, respectively) in a simple form of a sum. However, the superposition of these contributions in (6.94) is more complicated. Moreover, the explicit correlative nonlocality of expression (6.94) was detected neither in [45], nor in numerous examples of partial summation [233].

Nevertheless, approximation (6.104) contains the peculiarity of viscosity similar to that in (6.101) and (6.102). In dimensionless variables and $\varepsilon = 1$, expression (6.104) predicts the infinite threshold at velocity divergency equal to $-(3/7)$, rather than $-(9/11)$ in (6.101) and (6.102). Viscosity tends to zero as the divergency tends to positive infinity in both approximations. A physical interpretation of these phenomena was given in [45]: large *positive* values of $\frac{\partial u}{\partial x}$ means that the 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 (6.104) and $-(9/11)$) for (6.101) and (6.102)) describe a strong compression of the flow. Strong deceleration results in a "solid fluid" limit with an infinite viscosity (Fig. 6.3).

Thus, hydrodynamic equations for approximation (6.95) are both nonlinear and nonlocal. This result is not surprising, accounting for the integro-differential nature of equation (6.38).

It is important that no small parameters were used neither when we were deriving equation (6.38) nor when we were obtaining the correction (6.95).

## 6.4 Example: Non-Perturbative Derivation of Linear Hydrodynamics from the Boltzmann Equation (3D)

In this example we shall discuss a bit more about the linear hydrodynamics obtained by the Newtom method with incomplete linearization. Using the Newton method instead of power series, a model of linear hydrodynamics is derived from the Boltzmann equation for regimes where the Knudsen number is of order unity. The model demonstrates no violation of stability of acoustic spectra in contrast to the Burnett hydrodynamics.

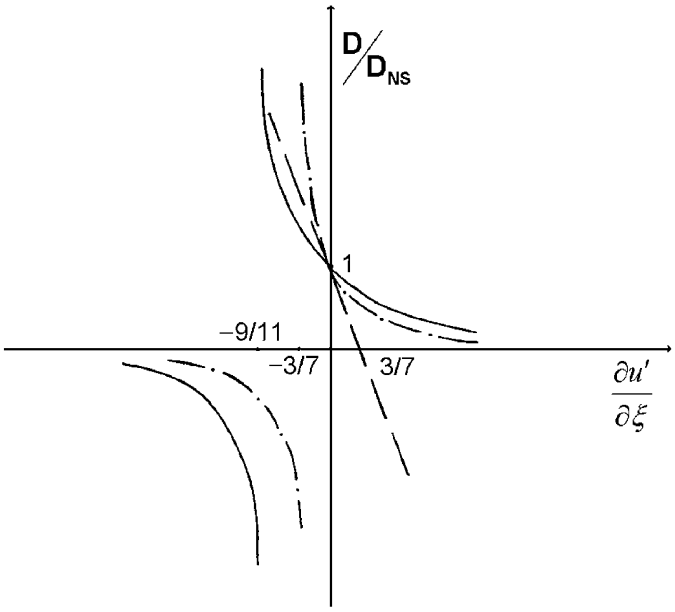


**Fig. 6.3.** Dependency of viscosity on compression for approximation (6.101) (*solid* line), for partial summing (6.104) (punctuated *dashed* line), and for the Burnett approximation [45,233] (*dashed* line). The latter changes the sign at a regular point and, hence, nothing prevents the flow to transfer into the nonphysical region

The Knudsen number $\varepsilon$ (a ratio between the mean free path, $l_c$, and a scale of hydrodynamic flows, $l_h$) is a smalness parameter when hydrodynamics is derived from the Boltzmann equation [239]. The Chapman–Enskog method [70] derives the Navier-Stokes hydrodynamic equations as the first-order correction to the Euler hydrodynamics at $\varepsilon \to 0$, and it also derives formal corrections of order $\varepsilon^2$, $\varepsilon^3$, ... (known as the Burnett and super-Burnett corrections). These corrections are important outside the strictly hydrodynamic domain $\varepsilon \ll 1$, and has to be considered for an exension of hydrodynamic description into a highly nonequilidrium domain $\varepsilon \leq 1$. Not much is known about high-order in $\varepsilon$ hydrodynamics, especially in nonlinear case. Nonetheless, in linear case, some definite information can be obtained. On the one hand, experiments on sound propagation in noble gases are considerably better explained with the Burnett and super-Burnett hydrodynamics rather than with the Navier-Stokes approximation alone [241]. On the other hand, direct calculation shows non-physical behavior of the Burnett hydrodynamics for ultra-short waves: acoustic waves increase instead of decay [72]. The latter failure of the Burnett approximation cannot be ignored. For the Navier-Stokes approximation no such violation is observed.

These two results indicate that, at least in a linear regime, it makes sense to consider hydrodynamics at $\varepsilon \sim 1$, but the Chapman-Enskog method of

deriving such hydrodynamics is problematic. The problem of constructing solutions to the Boltzmann equation valid when $\varepsilon$ is of order one is one of the main open problems of classical kinetic theory [239].

The main idea of the present example is to formulate the problem of a finding a correction to the Euler hydrodynamics in such a fashion that expansions in $\varepsilon$ do not appear as a necessary element of analysis. This will be possible by using the Newton method instead of Taylor expansions to get such correction. Resulting hydrodynamic equations do not exhibit the mentioned violation.

The starting point is the set of local Maxwell distribution functions (LM) $f_0(n, \boldsymbol{u}, T; \boldsymbol{v})$, where $\boldsymbol{v}$ is the particle's velocity, and $n$, $\boldsymbol{u}$, and $T$ are local number density, average velocity, and temperature. We write the Boltzmann equation as before in the co-moving reference frame (6.23):

$$\frac{\mathrm{d}f}{\mathrm{d}t} = J(f), \quad J(f) = -(v-u)_i \cdot \partial_i f + Q(f,f)\,, \tag{6.105}$$

where $\mathrm{d}/\mathrm{d}t = \partial/\partial t + u_i \cdot \partial_i$ is the material derivative, $\partial_i = \partial/\partial x_i$, while $Q$ is the Boltzmann collision integral.

On the one hand, calculating right hand site of (6.105) in the LM-states, we obtain $J(f_0)$, a time derivative of the LM-states due to the Boltzmann equation. On the other hand, calculating a time derivative of the LM-states due to the Euler dynamics, we obtain $P_0 J(f_0)$, where $P_0$ is the thermodynamic projector operator onto the LM manifold (see [11] and (5.55)):

$$P_0 J = \frac{f_0}{n}\left\{\int J\,\mathrm{d}\boldsymbol{c} + 2c_i \cdot \int c_i J\,\mathrm{d}\boldsymbol{c} + \frac{2}{3}\left(c^2 - \frac{3}{2}\right)\int \left(c^2 - \frac{3}{2}\right) J\,\mathrm{d}\boldsymbol{c}\right\}\,, \tag{6.106}$$

Since the LM functions are not solutions to the Boltzmann equation (6.105) (except for constant $n$, $\boldsymbol{u}$, and $T$), a difference $\Delta(f_0)$ between $J(f_0)$ and $P_0 J(f_0)$ is not equal to zero (5.59):

$$\begin{aligned}\Delta(f_0) &= J(f_0) - P_0 J(f_0) \\ &= -f_0\left\{2(\partial_i u_k)\left(c_i c_k - \frac{1}{3}\delta_{ik}c^2\right) + v_T \frac{\partial_i T}{T} c_i \left(c^2 - \frac{5}{2}\right)\right\}\,.\end{aligned} \tag{6.107}$$

here $\boldsymbol{c} = v_T^{-1}(\boldsymbol{v} - \boldsymbol{u})$, and $v_T = \sqrt{2k_B T/m}$ is the thermal velocity. Note that the latter expression gives the complete invariance defect of the linearized local Maxwell approximation, and it is neither big nor small by itself. An unknown hydrodynamic solution of (6.105), $f_\infty(n, \boldsymbol{u}, T; \boldsymbol{v})$, satisfies the following invariance equation:

$$\Delta(f_\infty) = J(f_\infty) - P_\infty J(f_\infty) = 0\,, \tag{6.108}$$

where $P_\infty$ is an unknown projecting operator. Both $P_\infty$ and $f_\infty$ are unknown in (6.108), but, nontheless, one is able to consider a sequence of corrections

$\{f_1, f_2, \ldots\}$, $\{P_1, P_2, \ldots\}$ to the initial approximation $f_0$ and $P_0$. Above it was shown, how to ensure the $H$-theorem on every step of approximations by choosing appropriate projecting operators $P_n$. In the present illustrative example we do not consider projectors other than $P_0$.

Let us apply the Newton method with incomplete linearization to (6.108) with $f_0$ as initial approximation for $f_\infty$ and with $P_0$ as an initial approximation for $P_\infty$. Writing $f_1 = f_0 + \delta f$, we get the first iteration:

$$L(\delta f/f_0) + (P_0 - 1)(v - u)_i \partial_i \delta f + \Delta(f_0) = 0 \,, \tag{6.109}$$

where $L$ is a linearized collision integral.

$$\begin{aligned} &L(g) \\ &= f_0(\boldsymbol{v}) \int w(\boldsymbol{v}_1', \boldsymbol{v}'; \boldsymbol{v}_1, \boldsymbol{v}) f_0(\boldsymbol{v}_1) \{g(\boldsymbol{v}_1') + g(\boldsymbol{v}') - g(\boldsymbol{v}_1) - g(\boldsymbol{v})\} \, \mathrm{d}\boldsymbol{v}_1' \, \mathrm{d}\boldsymbol{v}' \, \mathrm{d}\boldsymbol{v}_1 \,. \end{aligned} \tag{6.110}$$

Here $w$ is a probability density of velocities change, $(\boldsymbol{v}, \boldsymbol{v}_1) \leftrightarrow (\boldsymbol{v}', \boldsymbol{v}_1')$, of a pair of molecules after their encounter. When deriving (6.109), we have accounted $P_0 L = 0$, and an additional condition which fixes the same values of $n$, $\boldsymbol{u}$, and $T$ in states $f_1$ as in LM states $f_0$:

$$P_0 \delta f = 0 \,. \tag{6.111}$$

Equation (6.109) is basic in what follows. Note that it contains no Knudsen number explicitly. Our strategy will be to treat equation (6.109) in such a way that the Knudsen number will appear explicitly only at the latest stage of computations.

The two further approximations will be adopted. The first concerns a linearization of (6.109) about the global equilibria $F_0$. The second concerns a finite-dimensional approximation of integral operator in (6.109) in velocity space. It is worthwhile noting here that none of these approximations concerns an assumption about the smallness of the Knudsen number.

Following the first of the approximations mentioned, denote as $\delta n$, $\delta \boldsymbol{u}$, and $\delta T$ deviations of hydrodynamic variables from their equilibrium values $n_0$, $\boldsymbol{u}_0 = 0$, and $T_0$. Introduce also dimensionless variables $\Delta n = \delta n/n_0$, $\Delta \boldsymbol{u} = \delta \boldsymbol{u}/v_T^0$, and $\Delta T = \delta T/T_0$, where $v_T^0$ is a heat velocity in equilibria, and a dimensionless relative velocity $\xi = \boldsymbol{v}/v_T^0$. Correction $f_1$ in the approximation, linear in deviations from $F_0$, reads:

$$f_1 = F_0(1 + \varphi_0 + \varphi_1) \,,$$

where

$$\varphi_0 = \Delta n + 2\Delta u_i \xi_i + \Delta T(\xi^2 - 3/2)$$

is a linearized deviation of LM from $F_0$, and $\varphi_1$ is an unknown function. The latter is to be obtained from a linearized version of (6.109).

Following the second approximation, we seek $\varphi_1$ in a form:

$$\varphi_1 = A_i(\boldsymbol{x})\xi_i\left(\xi^2 - \frac{5}{2}\right) + B_{ik}(\boldsymbol{x})\left(\xi_i\xi_k - \frac{1}{3}\delta_{ik}\xi^2\right) + \ldots \tag{6.112}$$

where dots denote terms of an expansion of $\varphi_1$ in velocity polynomials, orthogonal to $\xi_i(\xi^2 - 5/2)$ and $\xi_i\xi_k - 1/3\delta_{ik}\xi^2$, as well as to 1, to $\boldsymbol{\xi}$, and to $\xi^2$. These terms do not contribute to shear stress tensor and heat flux vector in hydrodynamic equations. Independency of functions $A$ and $B$ from $\xi^2$ amounts to the first Sonine polynomial approximation of viscosity and heat transfer coefficients. Thus, we consider a projection onto a finite-dimensional subspace spanned by $\xi_i(\xi^2 - 5/2)$ and $\xi_i\xi_k - 1/3\delta_{ik}\xi^2$. Our goal is to derive functions $A$ and $B$ from a linearized version of (6.109). Knowing $A$ and $B$, we get the following expressions for shear stress tensor $\boldsymbol{\sigma}$ and heat flux vector $\boldsymbol{q}$:

$$\sigma = p_0 B, \;\; \boldsymbol{q} = \frac{5}{4}p_0 v_T^0 A \;, \tag{6.113}$$

where $p_0$ is equilibrium pressure of ideal gas.

Linearizing (6.109) near $F_0$, using an ansatz for $\varphi_1$ cited above, and turning to Fourier transform in space, we derive:

$$\begin{aligned} &\frac{5p_0}{3\eta_0}a_i(\boldsymbol{k}) + iv_T^0 b_{ij}(\boldsymbol{k})k_j = -\frac{5}{2}iv_T^0 k_i\tau(\boldsymbol{k}) \;; \\ &\frac{p_0}{\eta_0}b_{ij}(\boldsymbol{k}) + iv_T^0\overline{k_i a_j(\boldsymbol{k})} = -2iv_T^0\overline{k_i\gamma_j(\boldsymbol{k})} \;, \end{aligned} \tag{6.114}$$

where $i = \sqrt{-1}$, $\boldsymbol{k}$ is the wave vector, $\eta_0$ is the first Sonine polynomial approximation of shear viscosity coefficient, $\boldsymbol{a}(\boldsymbol{k})$, $\boldsymbol{b}(\boldsymbol{k})$, $\tau(\boldsymbol{k})$ and $\boldsymbol{\gamma}(\boldsymbol{k})$ are Fourier transforms of $\boldsymbol{A}(\boldsymbol{x})$, $\boldsymbol{B}(\boldsymbol{x})$, $\Delta T(\boldsymbol{x})$, and $\Delta\boldsymbol{u}(\boldsymbol{x})$, respectively, and the over-bar denotes a symmetric traceless dyad:

$$\overline{a_i b_j} = 2a_i b_j - \frac{2}{3}\delta_{ij}a_s b_s \;.$$

Introducing a dimensionless wave vector $\boldsymbol{f} = [(v_T^0\eta_0)/(p_0)]\boldsymbol{k}$, solution to (6.114) may be written:

$$\begin{aligned} &b_{lj}(\boldsymbol{k}) = -\frac{10}{3}i\overline{\gamma_l(\boldsymbol{k})f_j}[(5/3) + (1/2)f^2]^{-1} \\ &+\frac{5}{3}i(\gamma_s(\boldsymbol{k})f_s)\overline{f_l f_j}[(5/3)+(1/2)f^2]^{-1}[5+2f^2]^{-1} - \frac{15}{2}\tau(\boldsymbol{k})\overline{f_l f_j}[5+2f^2]^{-1} \;; \\ &a_l(\boldsymbol{k}) = -\frac{15}{2}if_l\tau(\boldsymbol{k})[5+2f^2]^{-1} \\ &-[5+2f^2]^{-1}[(5/3)+(1/2)f^2]^{-1}[(5/3)f_l(\gamma_s(\boldsymbol{k})f_s) + \gamma_l(\boldsymbol{k})f^2(5+2f^2)] \;. \end{aligned} \tag{6.115}$$

Considering $z$-axis as a direction of propagation and denoting $k_z$ as $k$, $\gamma$ as $\gamma_z$, we obtain from (6.114) the $k$-dependence of $a = a_z$ and $b = b_{zz}$:

$$a(k) = -\frac{\frac{3}{2}p_0^{-1}\eta_0 v_T^0 ik\tau(k) + \frac{4}{5}p_0^{-2}\eta_0^2(v_T^0)^2k^2\gamma(k)}{1+\frac{2}{5}p_0^{-2}\eta_0^2(v_T^0)^2k^2}\,, \tag{6.116}$$
$$b(k) = -\frac{\frac{4}{3}p_0^{-1}\eta_0 v_T^0 ik\gamma(k) + p_0^{-2}\eta_0^2(v_T^0)^2k^2\tau(k)}{1+\frac{2}{5}p_0^{-2}\eta_0^2(v_T^0)^2k^2}\,.$$

Using expressions for $\sigma$ and $\boldsymbol{q}$ cited above, and also using (6.116), it is an easy matter to close the linearized balance equations (given in Fourier terms):

$$\frac{1}{v_T^0}\partial_t\nu(k) + ik\gamma_k = 0\,, \tag{6.117}$$
$$\frac{2}{v_T^0}\partial_t\gamma(k) + ik(\tau(k)+\nu(k)) + ikb(k) = 0\,,$$
$$\frac{3}{2v_T^0}\partial\tau + ik\gamma(k) + \frac{5}{4}ika(k) = 0\,.$$

The equations (6.117), together with expressions (6.116), complete our derivation of hydrodynamic equations.

To this end, the Knudsen number was not penetrating our derivations. Now it is worthwhile to introduce it. The Knudsen number will appear most naturally if we turn to dimensionless form of (6.116). Taking $l_c = v_T^0\eta_0/p_0$ ($l_c$ is of order of a mean free path), and introducing a hydrodynamic scale $l_h$, so that $k = \kappa/l_h$, where $\kappa$ is a not-dimensional wave vector, we obtain in (6.116):

$$a(\kappa) = -\frac{\frac{3}{2}i\varepsilon\kappa\tau(\kappa) + \frac{4}{5}\varepsilon^2\kappa^2\gamma_\kappa}{1+\frac{2}{5}\varepsilon^2\kappa^2}\,, \tag{6.118}$$
$$b(\kappa) = -\frac{\frac{4}{3}i\varepsilon\kappa\gamma(\kappa) + \varepsilon^2\kappa^2\tau(\kappa)}{1+\frac{2}{5}\varepsilon^2\kappa^2}\,,$$

where $\varepsilon = l_c/l_h$. Considering the limit $\varepsilon \to 0$ in (6.118), we come back to the familiar Navier-Stokes expressions: $\sigma_{zz}^{NS} = -\frac{4}{3}\eta_0\partial_z\delta u_z$, $q_z^{NS} = -\lambda_0\partial_z\delta T$, where $\lambda_0 = 15k_B\eta_0/4m$ is the first Sonine polynomial approximation of heat conductivity coefficient.

Since we were not assuming smallness of the Knudsen number $\varepsilon$ while deriving (6.118), we can write $\varepsilon = 1$. With all the approximations mentioned above, (6.117) and (6.116) (or, equivalently, (6.117) and (6.118)) may be considered as a model of a linear hydrodynamics at $\varepsilon$ of order one. The most interesting feature of this model is a non-polynomial dependence on $\kappa$. This amounts to that share stress tensor and heat flux vector depend on spatial derivatives of $\delta\boldsymbol{u}$ and of $\delta T$ to arbitrary high order.

To find out a result of the non-polynomial behavior (6.118), it is most informative to calculate a dispersion relation for plane waves. Let us introduce a dimensionless frequency $\lambda = \omega l_h/v_T^0$, where $\omega$ is a complex frequency of a

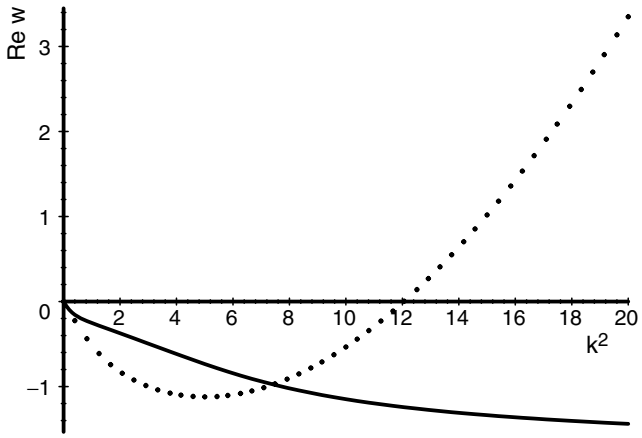


**Fig. 6.4.** Attenuation rate of sound waves. *Dotts*: the Burnett approximation. Bobylev's instability occurs when the curve intersects the horizontal axis. *Solid*: First iteration of the Newton method on the invariance equation

wave $\sim\exp(\omega t+ikz)$ (Re$\omega$ is a damping rate, and Im$\omega$ is a circular frequency). Making use of (6.117) and (6.118), writing $\varepsilon = 1$, we obtain the following dispersion relation $\lambda(\kappa)$:

$$12(1+\frac{2}{5}\kappa^2)^2\lambda^3+23\kappa^2(1+\frac{2}{5}\kappa^2)\lambda^2+2\kappa^2(5+5\kappa^2+\frac{6}{5}\kappa^4)\lambda+\frac{15}{2}\kappa^4(1+\frac{2}{5}\kappa^2)=0\ . \tag{6.119}$$

Figure 6.4 presents a dependence Re$\lambda(\kappa^2)$ for acoustic waves obtained from (6.119) and for the Burnett approximation [72]. The violation in the latter occurs when the curve crosses the horizontal axis. In contrast to the Burnett approximation [72], the acoustic spectrum (6.119) is stable for all $\kappa$. Moreover, Re$\lambda(\kappa^2)$ demonstrates a finite limit, as $\kappa^2 \to \infty$.

A discussion of results concerns the following two items:

1. The approach used avoids expansion into powers of the Knudsen number, and thus we obtain a hydrodynamics valid (at least formally) for moderate Knudsen numbers as an immediate correction to the Euler hydrodynamics. This is in a contrast to the usual treatment of high-order hydrodynamics as "(the well established) Navier-Stokes approximation + high-order terms". The Navier-Stokes hydrodynamics is recovered a posteriori, as a limiting case, but not as a necessary intermediate step of computations.
2. Linear hydrodynamics derived is stable for all $k$, same as the Navier-Stokes hydrodynamics alone. The $(1+\alpha k^2)^{-1}$ "cut-off", as in (6.116) and (6.118), was earlier found in a "partial summing" of Enskog series [42, 43].

Thus, we come to the following two conclusions:

1. A positive answer is given to the question of whether is it possible to construct solutions of the Boltzmann equation valid for the Knudsen number of order one.
2. Linear hydrodynamics derived can be used as a model for $\varepsilon = 1$ without a violation of acoustic spectra at large $k$.

## 6.5 Example: Dynamic Correction to Moment Approximations

### 6.5.1 Dynamic Correction or Extension of the List of Variables?

Considering the Grad moment ansatz as a suitable first approximation to a closed finite-moment dynamics, the correction is derived from the Boltzmann equation. The correction consists of two parts, local and nonlocal. Locally corrected thirteen-moment equations are demonstrated to contain exact transport coefficients. Equations resulting from the nonlocal correction give a microscopic justification to some phenomenological theories of extended hydrodynamics.

A considerable part of the modern development of nonequilibrium thermodynamics is based on the idea of extension of the list of relevant variables. Various phenomenological and semi-phenomenological theories in this domain are known under the common title of the extended irreversible thermodynamics (EIT) [235]. With this, the question of a microscopic justification of the EIT becomes important. Recall that a justification for some of the versions of the EIT was found witin the well known Grad moment method [201].

Originally, the Grad moment approximation was introduced for the purpose of solving the Boltzmann-like equations of the classical kinetic theory. The Grad method is used in various kinetic problems, e.g., in plasma and in phonon transport. We mention also that Grad equations assist in understanding asymptotic features of gradient expansions, both in linear and nonlinear domains [40, 42, 205, 219, 233].

The essence of the Grad method is to introduce an approximation to the one-particle distribution function $f$ which would depend only on a finite number $N$ of moments, and, subsequently, to use this approximation to derive a closed system of $N$ moment equations from the kinetic equation. The number $N$ (the level at which the moment transport hierarchy is truncated) is not specified in the Grad method. One particular way to choose $N$ is to obtain an estimation of the transport coefficients (viscosity and heat conductivity) sufficiently close to their exact values provided by the Chapman–Enskog method (CE) [70]. In particular, for the thirteen-moment Grad approximation it is well known that transport coefficients are equal to the first Sonine polynomial approximation to the exact CE values. Accounting for higher moments with

$N > 13$ can improve this approximation (good for neutral gases but poor for plasmas [231]). However, what should be done, starting with the thirteen-moment approximation, to come to the exact CE transport coefficients is an open question. It is also well known [204] that the Grad method provides a poorly converging approximation when applied to strongly nonequilibrium problems (such as shock and kinetic layers).

Another question comes from the approximate character of the Grad equations, and is discussed in frames of the EIT: while the Grad equations are strictly hyperbolic at any level $N$ (i.e., predicting a finite speed of propagation), whether this feature will be preserved in the further corrections.

These two questions are special cases of a more general one, namely, how to derive a closed description with a given number of moments? Such a description is sometimes called mesoscopic [251] since it occupies an intermediate level between the hydrodynamic (macroscopic) and the kinetic (microscopic) levels of description.

Here we aim at deriving the mesoscopic dynamics of thirteen moments [21] in the simplest case when the kinetic description satisfies the linearized Boltzmann equation. Our approach will be based on the two assumptions:

(i) The mesoscopic dynamics of thirteen moments exists, and is invariant with respect to the microscopic dynamics,
(ii) The thirteen-moment Grad approximation is a suitable first approximation to this mesoscopic dynamics.

The assumption (i) is realized as the invariance equation for the (unknown) mesoscopic distribution function. Following the assumption (ii), we solve the invariance equation iteratively, taking the Grad approximation for the input approximation, and consider the first iteration (further we refer to this as to the dynamic correction, to distinguish from constructing another ansatz). We demonstrate that the correction results in the exact CE transport coefficients. We also demonstrate how the dynamic correction modifies the hyperbolicity of the Grad equations. A similar viewpoint on derivation of hydrodynamics was earlier developed in [11] (see previous examples). We shall return to a comparison below.

### 6.5.2 Invariance Equation for Thirteen-Moment Parameterization

We denote as $n_0$, $\boldsymbol{u}_0 = 0$, and $p_0$ the equilibrium values of the hydrodynamic parameters ($n$ is the number density, $\boldsymbol{u}$ is the average velocity, and $p = nk_BT$ is the pressure). The global Maxwell distribution function $F$ is

$$F = n_0(v_T)^{-3}\pi^{-3/2}\exp(-c^2)\ ,$$

where $v_T = \sqrt{2k_{\mathrm{B}}T_0m^{-1}}$ is the equilibrium thermal velocity, and $\boldsymbol{c} = \boldsymbol{v}/v_T$ is the peculiar velocity of a particle. The near-equilibrium dynamics of the

distribution function, $f = F(1+\varphi)$, is due to the linearized Boltzmann equation:

$$\partial_t \varphi = \hat{J}\varphi \equiv -v_T c_i \partial_i \varphi + \hat{L}\varphi \ ,$$
$$\hat{L}\varphi = \int w F(\boldsymbol{v}_1)[\varphi(\boldsymbol{v}_1') + \varphi(\boldsymbol{v}') - \varphi(\boldsymbol{v}_1) - \varphi(\boldsymbol{v})]\, \mathrm{d}\boldsymbol{v}_1' \, \mathrm{d}\boldsymbol{v}' \, \mathrm{d}\boldsymbol{v}_1 \ ,$$

where $\hat{L}$ is the linearized collision operator, and $w$ is the probability density of pair encounters. Furthermore, $\partial_i = \partial/\partial x_i$, and summation convention in two repeated indices is assumed.

Let $n = \delta n/n_0$, $\boldsymbol{u} = \delta \boldsymbol{u}/v_T$, $p = \delta p/p_0$ ($p = n + T$, $T = \delta T/T_0$), be dimensionless deviations of the hydrodynamic variables, while $\boldsymbol{\sigma} = \delta\boldsymbol{\sigma}/p_0$ and $\boldsymbol{q} = \delta \boldsymbol{q}/(p_0 v_T)$ are dimensionless deviations of the stress tensor $\boldsymbol{\sigma}$, and of the heat flux $\boldsymbol{q}$. The linearized thirteen-moment Grad distribution function is $f_0 = F(\boldsymbol{c})\,[1+\varphi_0]$, where

$$\begin{aligned} \varphi_0 &= \varphi_1 + \varphi_2 \ , \\ \varphi_1 &= n + 2u_i c_i + T\left[c^2 - (3/2)\right] \ , \\ \varphi_2 &= \sigma_{ik}\overline{c_i c_k} + (4/5) q_i c_i \left[c^2 - (5/2)\right] \ . \end{aligned} \tag{6.120}$$

The overline denotes a symmetric traceless dyad. We use the following convention:

$$\overline{a_i b_k} = a_i b_k + a_k b_i - \frac{2}{3}\delta_{ik} a_l b_l \ ,$$
$$\overline{\partial_i f_k} = \partial_i f_k + \partial_k f_i - \frac{2}{3}\delta_{ik}\partial_l f_l \ .$$

The thirteen-moment Grad's equations are derived in two steps: first, the Grad's distribution function (6.120) is inserted into the linearized Boltzmann equation to give a formal expression, $\partial_t \varphi_0 = \hat{J}\varphi_0$, second, projector $P_0$ is applied to this expression, where $P_0 = P_1 + P_2$, and operators $P_1$ and $P_2$ act as follows:

$$P_1 J = \frac{F}{n_0}\left\{ X_0 \int X_0 J \, \mathrm{d}\boldsymbol{v} + X_i \int X_i J \, \mathrm{d}\boldsymbol{v} + X_4 \int X_4 J \, \mathrm{d}\boldsymbol{v} \right\} \ , \tag{6.121}$$
$$P_2 J = \frac{F}{n_0}\left\{ Y_{ik} \int Y_{ik} J d\boldsymbol{v} + Z_i \int Z_i J d\boldsymbol{v} \right\} \ .$$

Here $X_0 = 1$, $X_i = \sqrt{2} c_i$, where $i = 1,2,3$, $X_4 = \sqrt{2/3}\left(c^2 - \frac{3}{2}\right)$, $Y_{ik} = \sqrt{2}\overline{c_i c_k}$, and $Z_i = \frac{2}{\sqrt{5}} c_i \left(c^2 - \frac{5}{2}\right)$. The resulting equation,

$$P_0[F\partial_t \varphi_0] = P_0[F\hat{J}\varphi_0] \ ,$$

is a compressed representation for the thirteen-moment Grad equations for the macroscopic variables $M_{13} = \{n, \boldsymbol{u}, T, \boldsymbol{\sigma}, \boldsymbol{q}\}$.

Now we turn our attention to the main purpose of this example, and derive the dynamic invariance correction to the thirteen-moment distribution function (6.120). The assumption (i) [existence of closed dynamics of thirteen moments] implies the invariance equation for the true mesoscopic distribution function, $\tilde{f}(M_{13}, \boldsymbol{c}) = F[1 + \tilde{\varphi}(M_{13}, \boldsymbol{c})]$, where we have stressed that this function depends parametrically on the same thirteen macroscopic parameters, as the original Grad approximation. The invariance condition for $\tilde{f}(M_{13}, \boldsymbol{c})$ reads [11]:

$$(1 - \tilde{P})[F\hat{J}\tilde{\varphi}] = 0 \,, \tag{6.122}$$

where $\tilde{P}$ is the projector associated with $\tilde{f}$. Generally speaking, the projector $\tilde{P}$ depends on the distribution function $\tilde{f}$ [11,231]. In the following, we use the projector $P_0$ (6.121) which will be consistent with our approximate treatment of (6.122).

Following the assumption (ii) [Grad's distribution function (6.120) is a good initial approximation], the Grad's function $f_0$, and the projector $P_0$, are chosen as the input data for solving the equation (6.122) iteratively. The dynamic correction amounts to the first iterate. Let us consider these steps in a more detail.

Substituting $\varphi_0$ (6.120) and $P_0$ (6.121) instead of $\varphi$ and $P$ in the equation (6.122), we get: $(1 - P_0)[F\hat{J}\varphi_0] \equiv \Delta_0 \neq 0$, which demonstrates that (6.120) is not a solution to the equation (6.122). Moreover, $\Delta_0$ splits in two natural pieces: $\Delta_0 = \Delta_0^{\mathrm{loc}} + \Delta_0^{\mathrm{nloc}}$, where

$$\begin{aligned} \Delta_0^{\mathrm{loc}} &= (1 - P_2)[F\hat{L}\varphi_2] \,, \\ \Delta_0^{\mathrm{nloc}} &= (1 - P_0)[-v_T F c_i \partial_i \varphi_0] \,. \end{aligned} \tag{6.123}$$

Here we have accounted for $P_1[F\hat{L}\varphi] = 0$, and $\hat{L}\varphi_1 = 0$. The first piece of (6.123), $\Delta_0^{\mathrm{loc}}$, can be termed *local* because it does not account for spatial gradients. Its origin is twofold. In the first place, recall that we are performing our analysis in a non-local-equilibrium state (the thirteen-moment Grad's approximation is not a zero point of the Boltzmann collision integral, hence $\hat{L}\varphi_0 \neq 0$). In the second place, specializing to the linearized case under consideration, functions $\overline{\boldsymbol{cc}}$ and $\boldsymbol{c}[c^2 - (5/2)]$, in general, are not the eigenfunctions of the linearized collision integral, and hence $P_2[F\hat{L}\varphi_0] \neq F\hat{L}\varphi_0$, resulting in $\Delta_0^{\mathrm{loc}} \neq 0$[2].

The nonlocal part may be written as:

$$\Delta_0^{\mathrm{nloc}} = -v_T F(\Pi_{1|krs}\partial_k \sigma_{rs} + \Pi_{2|ik}\overline{\partial_k q_i} + \Pi_3 \partial_k q_k) \,, \tag{6.124}$$

where $\Pi$ are velocity polynomials:

[2] Except for Maxwell molecules (interaction potential $U \sim r^{-4}$) for which $\hat{L}\varphi_0 \neq 0$ but $P_2[F\hat{L}\varphi_{\mathrm{G}}] = F\hat{L}\varphi_0$. Same goes for the relaxation time approximation of the collision integral ($\hat{L} = -\tau^{-1}$).

$$\begin{aligned}\Pi_{1|krs} &= c_k\left[c_r c_s - (1/3)\delta_{rs}c^2\right] - (2/5)\delta_{ks}c_r c^2 \ ,\\ \Pi_{2|ik} &= (4/5)\left[c^2 - (7/2)\right]\left[c_i c_k - (1/3)\delta_{ik}c^2\right] \ ,\\ \Pi_3 &= (4/5)\left[c^2 - (5/2)\right]\left[c^2 - (3/2)\right] - c^2 \ .\end{aligned}$$

We seek the dynamic correction of the form:

$$f = F[1 + \varphi_0 + \phi] \ .$$

Substituting $\varphi = \varphi_0 + \phi$, and $P = P_0$, into (6.122), we derive an equation for the correction $\phi$:

$$(1 - P_2)[F\hat{L}(\varphi_2 + \phi)] = (1 - P_0)[v_T F c_i \partial_i(\varphi_0 + \phi)] \ . \tag{6.125}$$

The equation (6.125) should be supplied with the additional condition, $P_0[F\phi] = 0$.

### 6.5.3 Solution of the Invariance Equation

Let us apply the usual ordering to solve (6.125), introducing a small parameter $\epsilon$, multiplying the collision integral $\hat{L}$ with $\epsilon^{-1}$, and expanding $\phi = \sum_n \epsilon^n \phi^{(n)}$. Subject to the additional condition, the resulting sequence of linear integral equations is uniquely soluble. Let us consider the first two orders in $\epsilon$.

Because $\Delta_0^{\rm loc} \neq 0$, the leading correction is of the order $\epsilon^0$, i.e. of the same order as the initial approximation $\varphi_0$. The function $\phi^{(0)}$ is due the following equation:

$$(1 - P_2)[F\hat{L}(\varphi_2 + \phi^{(0)})] = 0 \ , \tag{6.126}$$

subject to the condition, $P_0[F\phi^{(0)}] = 0$. The equation (6.126) has the unique solution: $\varphi_2 + \phi^{(0)} = \sigma_{ik}Y_{ik}^{(0)} + q_i Z_i^{(0)}$, where functions, $Y_{ik}^{(0)}$ and $Z_i^{(0)}$, are solutions to the integral equations:

$$\hat{L}Y_{ik}^{(0)} = bY_{ik} \ , \quad \hat{L}Z_i^{(0)} = aZ_i \ , \tag{6.127}$$

subject to the conditions, $P_1[F\mathsf{Y}^{(0)}] = 0$ and $P_1[F\mathbf{Z}^{(0)}] = 0$. Factors $a$ and $b$ are:

$$\begin{aligned}a &= \pi^{-3/2}\int e^{-c^2} Z_i^{(0)}\hat{L}Z_i^{(0)}\,{\rm d}\boldsymbol{c} \ ,\\ b &= \pi^{-3/2}\int e^{-c^2} Y_{ik}^{(0)}\hat{L}Y_{ik}^{(0)}\,{\rm d}\boldsymbol{c} \ .\end{aligned}$$

Now we are able to notice that the equation (6.127) coincides with the CE equations [70] for the *exact transport coefficients* (viscosity and temperature conductivity). Emergency of these well known equations in the present context is important and rather unexpected: *when the moment transport equations are closed with the locally corrected function* $f^{\rm loc} = F(1+\varphi_0+\phi^{(0)})$, *we*

*come to a closed set of thirteen equations containing the exact CE transport coefficients.*

Let us analyze the next order ($\epsilon^1$), where $\Delta_0^{\rm nloc}$ comes into play. To simplify matters, we neglect the difference between the exact and the approximate CE transport coefficients. The correction $\phi^{(1)}$ is due to the equation,

$$(1-P_2)[F\hat{L}\phi^{(1)}] + \Delta_0^{\rm nloc} = 0 \,, \tag{6.128}$$

the additional condition is: $P_0[F\phi^{(1)}] = 0$. The problem (6.128) reduces to three integral equations of a familiar form:

$$\hat{L}\Psi_{1|krs} = \Pi_{1|krs} \,, \quad \hat{L}\Psi_{2|ik} = \Pi_{2|ik} \,, \quad \hat{L}\Psi_3 = \Pi_3 \,, \tag{6.129}$$

subject to conditions: $P_1[F\Psi_{1|krs}] = 0$, $P_1[F\Psi_{2|ik}] = 0$, and $P_1[F\Psi_3] = 0$. Integral equations (6.129) are of the same structure as are the integral equations appearing in the CE method, and the methods to handle them are well developed [70]. In particular, a reasonable and simple approximation is to take $\Psi_{\alpha|\ldots} = -A_\alpha \Pi_{\alpha|\ldots}$. Then

$$\phi^{(1)} = -v_T(A_1\Pi_{1|krs}\partial_k\sigma_{rs} + A_2\Pi_{2|ik}\overline{\partial_k q_i} + A_3\Pi_3\partial_k q_k) \,, \tag{6.130}$$

where $A_\alpha$ are the approximate values of the kinetic coefficients, and which are expressed via matrix elements of the linearized collision integral:

$$A_\alpha^{-1} \propto -\int \exp(-c^2)\Pi_{\alpha|\ldots}\hat{L}\Pi_{\alpha|\ldots}\,{\rm d}\boldsymbol{c} > 0 \,. \tag{6.131}$$

The evaluation can be extended to a computational scheme for any given molecular model (e.g., for the Lennard-Jones potential), in the manner of the transport coefficients computations in the classical Chapman–Enskog method.

### 6.5.4 Corrected Thirteen-Moment Equations

To summarize the results of the dynamic correction, we quote first the unclosed equations for the variables $M_{13} = M_{13} = \{n, \boldsymbol{u}, T, \boldsymbol{\sigma}, \boldsymbol{q}\}$:

$$(1/v_T^0)\partial_t n + \partial_i u_i = 0 \,, \tag{6.132}$$

$$(2/v_T^0)\partial_t u_i + \partial_i(T+n) + \partial_k\sigma_{ik} = 0 \,, \tag{6.133}$$

$$(1/v_T^0)\partial_t T + (2/3)\partial_i u_i + (2/3)\partial_i q_i = 0 \,, \tag{6.134}$$

$$(1/v_T^0)\partial_t\sigma_{ik} + 2\overline{\partial_i u_k} - (2/3)\overline{\partial_i q_k} + \partial_l h_{ikl} = R_{ik} \,, \tag{6.135}$$

$$(2/v_T)\partial_t q_i - (5/2)\partial_i p - (5/2)\partial_k\sigma_{ik} + \partial_k g_{ik} = R_i \,. \tag{6.136}$$

Terms spoiling the closure are: the higher moments of the distribution function,

$$h_{ikl} = 2\pi^{-3/2} \int e^{-c^2} \varphi c_i c_k c_l d\boldsymbol{c} \,,$$
$$g_{ik} = 2\pi^{-3/2} \int e^{-c^2} \varphi c_i c_k c^2 \, \mathrm{d}\boldsymbol{c} \,,$$

and the scattering rates,

$$R_{ik} = \frac{2}{v_T} \pi^{-3/2} \int e^{-c^2} c_i c_k \hat{L} \varphi \, \mathrm{d}\boldsymbol{c} \,,$$
$$R_i = \frac{2}{v_T} \pi^{-3/2} \int e^{-c^2} c_i c^2 \hat{L} \varphi \, \mathrm{d}\boldsymbol{c} \,.$$

Grad's distribution function (6.120) provides the zeroth-order closure approximation to both the higher-order moments and the scattering rates:

$$R_{ik}^{(0)} = -\mu_0^{-1} \sigma_{ik}, \; R_i^{(0)} = -\lambda_0^{-1} q_i \,, \tag{6.137}$$
$$\partial_l h_{ikl}^{(0)} = (2/3)\delta_{ik} \partial_l q_l + (4/5)\overline{\partial_i q_k} \,,$$
$$\partial_l g_{lk}^{(0)} = (5/2)\partial_k (p + T) + (7/2)\partial_l \sigma_{lk} \,,$$

where $\mu_0$ and $\lambda_0$ are the first Sonine polynomial approximations to the viscosity and the temperature conductivity coefficients [70], respectively.

The local correction improves the closure of the scattering rates:

$$R_{ik} = -\mu_{\mathrm{CE}}^{-1} \sigma_{ik}, \quad R_i = -\lambda_{\mathrm{CE}}^{-1} q_i \,, \tag{6.138}$$

where the subscript CE corresponds to the *exact* Chapman–Enskog values of the transport coefficients.

The nonlocal correction adds the following terms to the higher-order moments:

$$\partial_l g_{lk} = \partial_l g_{lk}^{(0)} - A_3 \partial_k \partial_l q_l - A_2 \partial_l \overline{\partial_l q_k} \,, \tag{6.139}$$
$$\partial_l h_{ikl} = \partial_l h_{ikl}^{(0)} - A_1 \partial_l \partial_l \sigma_{ik} \,,$$

where $A_i$ are the kinetic coefficients derived above.

In order to illustrate what changes in Grad equations with the nonlocal correction, let us consider a model with two scalar variables, $T(x,t)$ and $q(x,t)$ (a simplified case of the one-dimensional corrected thirteen-moment system where one retains only the variables responsible for heat conduction):

$$\partial_t T + \partial_x q = 0, \quad \partial_t q + \partial_x T - a\partial_x^2 q + q = 0 \,. \tag{6.140}$$

Parameter $a \geq 0$ controls "turning on" the nonlocal correction. Using $\{q(k,\omega), T(k,\omega)\} \exp(\omega t + ikx)$, we come to a dispersion relation for the two roots $\omega_{1,2}(k)$. Without the correction ($a = 0$), there are two domains of $k$: for $0 \leq k < k_-$, dispersion is diffusion-like ($\mathrm{Re}\omega_{1,2}(k) \leq 0$, $\mathrm{Im}\omega_{1,2}(k) = 0$), while as $k \geq k_-$, dispersion is wave-like ($\omega_1(k) = \omega_2^*(k)$, $\mathrm{Im}\omega_1(k) \neq 0$). For

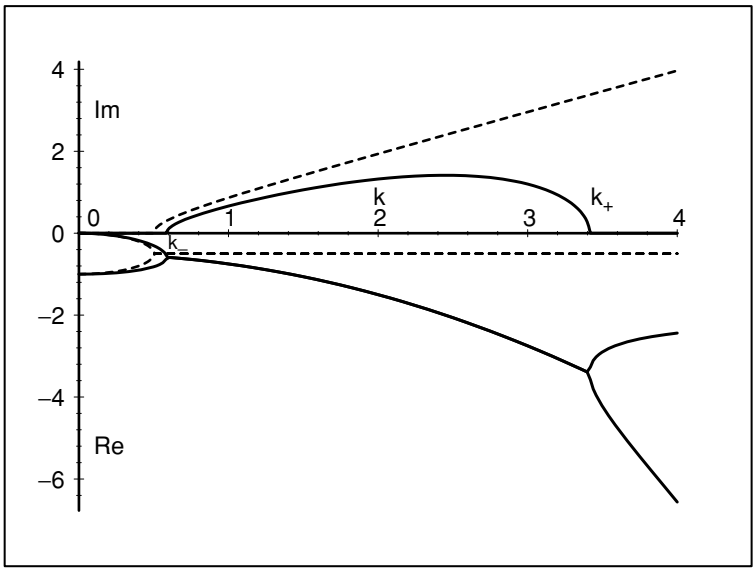


**Fig. 6.5.** Attenuation $\mathrm{Re}\omega_{1,2}(k)$ (*lower* pair of curves), frequency $\mathrm{Im}\omega_{1,2}(k)$ (*upper* pair of curves). *Dashed* lines – Grad case ($a = 0$), drawn lines – dynamic correction ($a = 0.5$)

$a$ between 0 and 1, the dispersion modifies in the following way: The wave-like domain becomes bounded, and exists for $k \in ]k_-(a), k_+(a)[$, while the diffusion-like domain consists of two pieces, $k < k_-(a)$ and $k > k_+(a)$.

The dispersion relation for $a = 1/2$ is shown in Fig. 6.5. As $a$ increases to 1, the boundaries of the wave-like domain, $k_-(a)$ and $k_+(a)$, move towards each other, and collapse at $a = 1$. For $a > 1$, the dispersion relation becomes purely diffusive ($\mathrm{Im}\omega_{1,2} = 0$) for all $k$.

### 6.5.5 Discussion: Transport Coefficients, Destroying the Hyperbolicity, etc.

1. Considering the thirteen-moment Grad's ansatz as a suitable approximation to the closed dynamics of thirteen moments, we have found that the first correction leads to the exact Chapman–Enskog transport coefficients. Further, the nonlocal part of this correction extends the Grad equations with terms containing spatial gradients of the heat flux and of the stress tensor, destroying the hyperbolic nature of Grad's moment system. Corresponding kinetic coefficients are explicitly derived for the Boltzmann equation.
2. Extension of Grad equations with terms like in (6.139) was mentioned in the EIT [252]. These derivations were based on phenomenological and semi-phenomenological argument. In particular, the extension of the heat

flux with appealing to nonlocality effects in *dense* fluids. Here we have derived the similar contribution from the *simplest* (i.e. dilute gas) kinetics, in fact, from the assumption about existence of the mesoscopic dynamics. The advantage of using the simplest kinetics is that corresponding kinetic coefficients (6.131) become a matter of a *computation* for any molecular model.

3. When the invariance principle is applied to derive hydrodynamics (closed equations for the variables $n$, $\boldsymbol{u}$ and $T$) then [11] the local Maxwellian $f_{lm}$ is chosen as the input distribution function for the invariance equation. In the linear domain, $f_{lm} = F[1 + \varphi_1]$, and the projector is $P_{lm} = P_1$, see (6.120) and (6.121). When the latter expressions are substituted into the invariance equation (6.122), we obtain $\Delta_{lm} = \Delta_{lm}^{\mathrm{nloc}} = -v_T F\{2\partial_i u_k \overline{c_i c_k} + \partial_i T c_i[c^2 - (5/2)]\}$, while $\Delta_{lm}^{\mathrm{loc}} \equiv 0$ because the local Maxwellians are zero points of the Boltzmann collision integral. Consequently, the dynamic correction begins with the order $\epsilon$, and the analog of the equation (6.128) reads:
$$\hat{L}\phi_{lm}^{(1)} = v_T\{2\partial_i u_k \overline{c_i c_k} + \partial_i T c_i[c^2 - (5/2)]\} \ ,$$
subject to a condition, $P_1[F\phi_{lm}^{(1)}] = 0$. The latter is the familiar Chapman-Enskog equation, resulting in the Navier-Stokes correction to the Euler equations [70]. Thus, *the nonlocal dynamic correction is related to the thirteen-moment Grad equations entirely in the same way as the Navier-Stokes are related to the Euler equations.*
4. Let us discuss briefly the further corrections. The first local correction (the functions $\mathsf{Y}_1$ and $\mathbf{Z}_1$ in (6.127)) is not the limiting point of our iterational procedure. When the latter is continued, the subsequent local corrections are found from integral equations, $\hat{L}\mathsf{Y}_{n+1} = b_{n+1}\mathsf{Y}_n$, and $\hat{L}\mathbf{Z}_{n+1} = a_{n+1}\mathbf{Z}_n$. Thus, we are led to the following two eigenvalue problems: $\hat{L}\mathsf{Y}_\infty = b_\infty \mathsf{Y}_\infty$, and $\hat{L}\mathbf{Z}_\infty = a_\infty \mathbf{Z}_\infty$, where $a_\infty$ and $b_\infty$ are the closest to zero eigenvalues among all the eigenvalue problems with the given tensorial structure [248].
5. Approach of this example [21] can be extended to derive dynamic corrections to other (non-moment) approximations of interest in the kinetic theory. The above analysis has demonstrated, in particular, the importance of the local correction, generically relevant to an approximation which is not a zero point of the collision integral. Very recently, this approach was successfully applied to improve the nonlinear Grad's thirteen-moment equations [253].