9 Relaxation Methods

The "large stepping" relaxation method for solution of the invariance equation is developed.

9.1 "Large Stepping" for the Equation of the Film Motion

Relaxation method is an alternative to the Newton iteration method described in Chap. 6: The initial approximation to the invariant manifold F_0 is moved with the film extension (4.5),

$$\frac{\mathrm{d}F_t(y)}{\mathrm{d}t} = (1 - P_{t,y})J(F_t(y)) = \Delta_{F(y)} \ ,$$

until a fixed point is reached. The advantage of this method is a relative freedom in its implementation: equation (4.5) needs not to be solved exactly, one is interested only in finding fixed points. Therefore, a "large stepping" in the direction of the defect, $\Delta_{F(y)}$ is possible, while the termination point is defined by the condition that the vector field becomes orthogonal to $\Delta_{F(y)}$. For simplicity, let us consider the procedure of termination in the linear approximation. Let $F_0(y)$ be the initial approximation to the invariant manifold, and we seek the first correction,

$$F_1(y) = F_0(y) + \tau_1(y)\Delta_{F_0(y)} \ ,$$

where function $\tau_1(y)$ has the dimension of time, and is found from the condition that the linearized vector field attached to the points of the new manifold is orthogonal to the initial defect,

$$\langle \Delta_{F_0(y)} | (1 - P_y)[J(F_0(y)) + \tau_1(y)(D_x J)_{F_0(y)}\Delta_{F_0(y)}] \rangle_{F_0(y)} = 0 \ . \tag{9.1}$$

Explicitly,

$$\tau_1(y) = -\frac{\langle \Delta_{F_0(y)} | \Delta_{F_0(y)} \rangle_{F_0(y)}}{\langle \Delta_{F_0(y)} | (D_x J)_{F_0(y)} | \Delta_{F_0(y)} \rangle_{F_0(y)}} \ . \tag{9.2}$$

Further steps $\tau_k(y)$ are found in the same way. It is clear from the above that the step of the relaxation method for the film extension is equivalent to

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the Galerkin approximation for solving the iteration of the Newton method with incomplete linearization. Actually, the relaxation method was first introduced in these terms in [24]. It was implemented in the method of invariant grids [105] for the grid-based numerical representations of manifolds (see Chap. 10). An idea of using the explicit Euler method to approximate the finite-dimensional inertial manifold was proposed earlier in [25]. In our approach the special choice of the projector field is important. For recent development of the numerical Euler-type methods for the solution of the invariance equation see [28].

The advantage of the equation (9.2) is the explicit form of the size of the steps $\tau_k(y)$. This method was successfully applied to the closure problem in the context of the Fokker-Planck equation [24].

9.2 Example: Relaxation Method for the Fokker-Planck Equation

We address here the problem of closure for the Fokker-Planck equation (FPE) (2.60) in a general setting. First, we review the maximum entropy principle as a source of suitable quasiequilibrium initial approximations for closures. We also discuss a version of the maximum entropy principle, valid for a near-equilibrium dynamics, and which results in explicit formulas for arbitrary potential U and diffusion matrix D.

In this Example we consider the FPE of the form (2.60):

$$\partial_t W(\boldsymbol{x}, t) = \partial_x \cdot \{D \cdot [W \partial_x U + \partial_x W]\} \ . \tag{9.3}$$

Here $W(\boldsymbol{x}, t)$ is the probability density over the configuration space $\boldsymbol{x}$, at the time t, while $U(\boldsymbol{x})$ and $D(\boldsymbol{x})$ are the potential and the positively semi-definite $(y \cdot D \cdot y \geq 0)$ diffusion matrix.

9.2.1 Quasi-Equilibrium Approximations for the Fokker-Planck Equation

The quasiequilibrium closures are almost never invariants of the true moment dynamics. For corrections to the quasiequilibrium closures, we apply the method of invariant manifold, which is carried out (subject to certain approximations explained below) to explicit recurrence formulas for one-moment near-equilibrium closures for arbitrary U and D. As a by-product, these formulas provide also a method for computing the lowest eigenvalue of the problem, which dominates the near-equilibrium FPE dynamics. Results are tested with model potentials, including the FENE-like potentials [151–153]. A generalization of the present approach to many-moment closures is also straightforward.

Let us denote as M the set of linearly independent moments,

$$\{M_0, M_1, \ldots, M_k\}, \text{ where } M_i[W] = \int m_i(x) W(x)\, \mathrm{d}x, \; m_0 = 1 \; .$$

We assume that there exists a function $W^*(M, x)$ which extremizes the entropy S (2.61) under the constraints of fixed M. This quasiequilibrium distribution function may be written as

$$W^* = W_{\mathrm{eq}} \exp \left[\sum_{i=0}^{k} \Lambda_i m_i(x) - 1 \right] \; , \tag{9.4}$$

where $\Lambda = \{\Lambda_0, \Lambda_1, \ldots, \Lambda_k\}$ are Lagrange multipliers. Closed-form equations for moments M are derived in two steps. First, the quasiequilibrium distribution (9.4) is substituted into the FPE (9.3) or (2.62) to give a formal expression:

$$\partial_t W^* = \hat{M}_{W^*} (\delta S / \delta W) \big|_{W=W^*}$$

, where $\hat{M}_{W^*}$ is given by (2.62). Second, introducing the quasiequilibrium projector Π^*,

$$\Pi^* \bullet = \sum_{i=0}^{k} (\partial W^* / \partial M_i) \int m(x) \bullet \, \mathrm{d}x \; ,$$

and applying Π^* on both sides of the formal expression, we derive closed for M in the quasiequilibrium approximation. Further processing requires explicit solution to the constraints, $\int W^*(\Lambda, x) m_i(x)\, \mathrm{d}x = M_i$, to get the dependence of Lagrange multipliers Λ on the moments M. Though typically the functions $\Lambda(M)$ are not known explicitly, one general remark about the moment equations is readily available. Specifically, the moment equations in the quasiequilibrium approximation have the form:

$$\dot{M}_i = \sum_{j=0}^{k} M^*_{ij}(M) (\partial S^*(M) / \partial M_j) \; , \tag{9.5}$$

where $S^*(M) = S[W^*(M)]$ is the quasiequilibrium entropy, and where M^*_{ij} is an M-dependent $(k+1) \times (k+1)$ matrix:

$$M^*_{ij} = \int W^*(M, x) [\partial_x m_i(x)] \cdot D(x) \cdot [\partial_x m_i(x)] \, \mathrm{d}x \; .$$

The matrix M^*_{ij} is symmetric, positive semi-definite, and its kernel is the vector δ_{0i}. Thus, *the quasiequilibrium closure reproduces the gradient structure on the macroscopic level* (2.62), the vector field of quasiequilibrium equations (9.5) is a transform of the gradient of the quasiequilibrium entropy given by the symnmetric positive operator.

The following version of the quasiequilibrium closures makes it possible to derive more explicit results in the general case [233, 246–248]: In many cases,

one can split the set of moments M in two parts, $M_I = \{M_0, M_1, \ldots, M_l\}$ and $M_{II} = \{M_{l+1}, \ldots, M_k\}$, in such a way that the quasiequilibrium distribution can be constructed explicitly for M_I as $W_I^*(M_I, x)$. The full quasiequilibrium problem for $M = \{M_I, M_{II}\}$ in the "shifted" formulation reads (see the "triangle entropy method" in Chap. 5): extremize the functional $S[W_I^* + \Delta W]$ with respect to ΔW, under the constraints $M_I[W_I^* + \Delta W] = M_I$ and $M_{II}[W_I^* + \Delta W] = M_{II}$. Let us denote as $\Delta M_{II} = M_{II} - M_{II}(M_I)$ deviations of the moments M_{II} from their values in the quasiequilibrium state W_I^*. For small deviations, the entropy is well approximated with its quadratic part

$$\Delta S = -\int \Delta W \left[1 + \ln \frac{W_I^*}{W_{\rm eq}}\right] \mathrm{d}x - \frac{1}{2}\int \frac{\Delta W^2}{W_I^*}\,\mathrm{d}x\ .$$

Taking into account the fact that $M_I[W_I^*] = M_I$, we come to the following maximizaton problem:

$$\Delta S[\Delta W] \to max,\ \ M_I[\Delta W] = 0,\ \ M_{II}[\Delta W] = \Delta M_{II}\ . \tag{9.6}$$

The solution to the problem (9.6) is always explicitly found from a $(k+1)\times(k+1)$ system of linear algebraic equations for Lagrange multipliers. This triangle entropy method for Boltzmann equations was discussed in details in Sect. 5.6.

In the remainder of this section we deal solely with one-moment near-equilibrium closures: $M_I = M_0$, (i. e. $W_I^* = W_{\rm eq}$), and the set M_{II} contains a single moment $M = \int mW\,\mathrm{d}x$, $m(x) \neq 1$. We shall specify notations for the near-equilibrium FPE, writing the distribution function as $W = W_{\rm eq}(1+\Psi)$, where the function Ψ satisfies an equation:

$$\partial_t \Psi = W_{\rm eq}^{-1}\hat{J}\Psi\ , \tag{9.7}$$

where $\hat{J} = \partial_x\cdot[W_{\rm eq}D\cdot\partial_x]$. The triangle one-moment quasiequilibrium function reads:

$$W^{(0)} = W_{\rm eq}\left[1 + \Delta M m^{(0)}\right] \tag{9.8}$$

where

$$m^{(0)} = [\langle mm\rangle - \langle m\rangle^2]^{-1}[m - \langle m\rangle]\ . \tag{9.9}$$

Here brackets $\langle\ldots\rangle = \int W_{\rm eq}\ldots\,\mathrm{d}x$ denote equilibrium averaging. The superscript (0) indicates that the triangle quasiequilibrium function (9.8) will be considered as the initial approximation to the procedure which we address below. Projector for the approximation (9.8) has the form

$$\Pi^{(0)}\bullet = W_{\rm eq}\frac{m^{(0)}}{\langle m^{(0)}m^{(0)}\rangle}\int m^{(0)}(x)\,\bullet\,\mathrm{d}x\ . \tag{9.10}$$

Substituting the function (9.8) into the FPE (9.7), and applying the projector (9.10) on both the sides of the resulting formal expression, we derive the equation for M:

$$\dot{M} = -\lambda_0 \Delta M \ , \tag{9.11}$$

where $1/\lambda_0$ is an effective relaxation time of the moment M to its equilibrium value, in the quasiequilibrium approximation (9.8):

$$\lambda_0 = \langle m^{(0)} m^{(0)} \rangle^{-1} \langle \partial_x m^{(0)} \cdot D \cdot \partial_x m^{(0)} \rangle \ . \tag{9.12}$$

9.2.2 The Invariance Equation for the Fokker-Planck Equation

Both the quasiequilibrium and the triangle quasiequilibrium closures are almost never invariants of the FPE dynamics. That is, the moments M of solutions of the FPE (9.3) and the solutions of the closed moment equations like (9.5), are different functions of time, even if the initial values coincide. These variations are generally significant even for the near-equilibrium dynamics. Therefore, we ask for corrections to the quasiequilibrium closures to end up with the invariant closures. This problem falls precisely into the framework of the method of invariant manifold [11] (Chap. 6), and we shall apply this method to the one-moment triangle quasiequilibrium closure approximations, as a simple example.

First, the invariant one-moment closure is given by an unknown distribution function $W^{(\infty)} = W_{\text{eq}}[1 + \Delta M m^{(\infty)}(x)]$ which satisfies the invariance equation

$$[1 - \Pi^{(\infty)}] \hat{J} m^{(\infty)} = 0 \ . \tag{9.13}$$

Here $\Pi^{(\infty)}$ is the projector, associated with function $m^{(\infty)}$, and which is also yet unknown. Equation (9.13) is a formal expression of the invariance principle for a one-moment near-equilibrium closure: considering $W^{(\infty)}$ as a manifold in the space of distribution functions, parameterized with the values of the moment M, we require that the microscopic vector field $\hat{J} m^{(\infty)}$ be equal to its projection, $\Pi^{(\infty)} \hat{J} m^{(\infty)}$, onto the tangent space of the manifold $W^{(\infty)}$.

Now we turn our attention to solving the invariance equation (9.13) iteratively, beginning with the triangle one-moment quasiequilibrium approximation $W^{(0)}$ (9.8). We apply the following iteration process to (9.13):

$$[1 - \Pi^{(k)}] \hat{J} m^{(k+1)} = 0 \ , \tag{9.14}$$

where $k = 0, 1, \ldots$, and where $m^{(k+1)} = m^{(k)} + \mu^{(k+1)}$, and the correction satisfies the condition $\langle \mu^{(k+1)} m^{(k)} \rangle = 0$. The projector is updated after each iteration, and it has the form

$$\Pi^{(k+1)} \bullet = W_{\text{eq}} \frac{m^{(k+1)}}{\langle m^{(k+1)} m^{(k+1)} \rangle} \int m^{(k+1)}(x) \bullet \, \mathrm{d}x \ . \tag{9.15}$$

Applying $\Pi^{(k+1)}$ to the formal expression,

$$W_{\text{eq}} m^{(k+1)} \dot{M} = \Delta M [1 - \Pi^{(k+1)}] m^{(k+1)} \ ,$$

we derive the $(k+1)$th update of the effective time (9.12):

$$\lambda_{k+1} = \frac{\langle \partial_x m^{(k+1)} \cdot D \cdot \partial_x m^{(k+1)} \rangle}{\langle m^{(k+1)} m^{(k+1)} \rangle} \ . \tag{9.16}$$

Specializing to the one-moment near-equilibrium closures, and following the general argument of Chap. 6, solutions to the invariance equation (9.13) are eigenfunctions of the operator $\hat{J}$, while the limit of the iteration process (9.14) is the eigenfunction which corresponds to the eigenvalue with the minimal nonzero absolute value.

9.2.3 Diagonal Approximation

In order to obtain more explicit results, we shall now proceed with to an approximate solution to the problem (9.14) *at each iteration*. The correction $\mu^{(k+1)}$ satisfyes the condition $\langle m^{(k)} \mu^{(k+1)} \rangle = 0$, and can be decomposed as follows: $\mu^{(k+1)} = \alpha_k e^{(k)} + e_\perp^{(k)}$. Here $e^{(k)}$ is the defect of the kth approximation: $e^{(k)} = W_{\rm eq}^{-1}[1 - \Pi^{(k)}]\hat{J} m^{(k)} = \lambda_k m^{(k)} + R^{(k)}$, where

$$R^{(k)} = W_{\rm eq}^{-1} \hat{J} m^{(k)} \ . \tag{9.17}$$

The function $e_\perp^{(k)}$ is orthogonal to both $e^{(k)}$ and $m^{(k)}$ ($\langle e^{(k)} e_\perp^{(k)} \rangle = 0$, and $\langle m^{(k)} e_\perp^{(k)} \rangle = 0$).

Our *diagonal approximation* (DA) consists in neglecting the part $e_\perp^{(k)}$. In other words, we seek an improvement of the non-invariance of the kth approximation *along its defect*, $\Delta = e^{(k)}$. Specifically, we consider the following ansatz at the kth iteration:

$$m^{(k+1)} = m^{(k)} + \alpha_k e^{(k)} \ . \tag{9.18}$$

Substituting the ansatz (9.18) into (9.14), we integrate the latter expression with the functon $e^{(k)}$ to evaluate the coefficient α_k:

$$\alpha_k = \frac{A_k - \lambda_k^2}{\lambda_k^3 - 2\lambda_k A_k + B_k} \ , \tag{9.19}$$

where functions A_k and B_k are represented by the following equilibrium averages:

$$\begin{aligned} A_k &= \langle m^{(k)} m^{(k)} \rangle^{-1} \langle R^{(k)} R^{(k)} \rangle \\ B_k &= \langle m^{(k)} m^{(k)} \rangle^{-1} \langle \partial_x R^{(k)} \cdot D \cdot \partial_x R^{(k)} \rangle \ . \end{aligned} \tag{9.20}$$

Finally, putting together (9.16), (9.17), (9.18), (9.19), and (9.20), we arrive at the following DA recurrence solution:

$$m^{(k+1)} = m^{(k)} + \alpha_k[\lambda_k m^{(k)} + R^{(k)}] \,, \tag{9.21}$$

$$\lambda_{k+1} = \frac{\lambda_k - (A_k - \lambda_k^2)\alpha_k}{1 + (A_k - \lambda_k^2)\alpha_k^2} \,. \tag{9.22}$$

Notice that the stationary points of the DA process (9.22) are the true solutions to the invariance equation (9.13). What *may be* lost within the DA is the convergence to the true limit of the procedure (9.14), i.e. to the *minimal* eigenvalue. In a general situation this is highly improbable, though.

In order to test the convergence of the DA process (9.22) we considered two potentials U in the FPE (9.3) with a constant diffusion matrix D. The first test was with the square potential $U = x^2/2$, in the three-dimensional configuration space, since for this potential the spectrum is well-known. We have considered two examples of the initial one-moment quasiequilibrium closures with $m^{(0)} = x_1 + 100(x^2 - 3)$ (example 1), and $m^{(0)} = x_1 + 100x^6x_2$ (example 2), in (9.9). The result of performance of the DA for λ_k is presented in Table 9.1, together with the error δ_k which was estimated as the norm of the variance at each iteration: $\delta_k = \langle e^{(k)} e^{(k)} \rangle / \langle m^{(k)} m^{(k)} \rangle$. In both examples, we see a good monotonic convergency to the minimal eigenvalue $\lambda_\infty = 1$, corresponding to the eigenfunction x_1. This convergence is even striking in the example 1, where the initial choice was very close to a different eigenfunction $x^2 - 3$, and which can be seen in the non-monotonic behavior of the variance. Thus, we have an example to trust the DA approximation as converging to the proper object.

Table 9.1. Iterations λ_k and the error δ_k for $U = x^2/2$

		0	1	4	8	12	16	20
Ex. 1	λ	1.99998	1.99993	1.99575	1.47795	1.00356	1.00001	1.00000
	δ	$0.16 \cdot 10^{-4}$	$0.66 \cdot 10^{-4}$	$0.42 \cdot 10^{-2}$	0.24	$0.35 \cdot 10^{-2}$	$0.13 \cdot 10^{-4}$	$0.54 \cdot 10^{-7}$
		0	1	2	3	4	5	6
Ex. 2	λ	3.399	2.437	1.586	1.088	1.010	1.001	1.0002
	δ	1.99	1.42	0.83	0.16	$0.29 \cdot 10^{-1}$	$0.27 \cdot 10^{-2}$	$0.57 \cdot 10^{-3}$

For the second test, we have taken a one-dimensional potential $U = -50\ln(1 - x^2)$, the configuration space is the segment $|x| \leq 1$. Potentials of this type (a so-called FENE potential) are used in applications of the FPE to models of polymer solutions [151–153]. Results are given in Table 9.2 for the two initial functions, $m^{(0)} = x^2 + 10x^4 - \langle x^2 + 10x^4 \rangle$ (example 3), and $m^{(0)} = x^2 + 10x^8 - \langle x^2 + 10x^8 \rangle$ (example 4). Both examples demonstrate a stabilization of the λ_k at the same value after some ten iterations.

In conclusion, we have developed the principle of invariance to obtain moment closures for the Fokker-Planck equation (9.3), and have derived explicit results for the one-moment near-equilibrium closures, particularly important to get information about the spectrum of the FP operator.

Table 9.2. Iterations λ_k for $U = -50\ln(1-x^2)$

		0	1	2	3	4	5	6	7	8
Ex. 3	λ	213.17	212.186	211.914	211.861	211.849	211.845	211.843	211.842	211.841
Ex. 4	λ	216.586	213.135	212.212	211.998	211.929	211.899	211.884	211.876	211.871

9.3 Example: Relaxational Trajectories: Global Approximations

Here we describe semi-analytical approximate methods for nonlinear space-independent dissipative systems equipped with the entropy functional. The key point of the analysis is an upper limiting state in the beginning of the relaxation. Extremal properties of this state are described, and explicit estimations are derived. This limiting state is used to construct explicit approximations of the trajectories. Special effort is paid to accomplish positivity, smoothness and the entropy growth along the approximate trajectories. The method is tested for the space-independent Boltzmann equation with various collision mechanisms.

9.3.1 Initial Layer and Large Stepping

For relaxing systems, it is a common place to distinguish three subsequent regimes on a way from an initial non-equilibrium state $f_0(\Gamma)$ to the final equilibrium state $f^0(\Gamma)$, where Γ is the phase variable: the early-time relaxation immediately after the system leaves the initial state f_0, the intermediate regime, and the final regression to the equilibrium state f^0. This model picture is only approximate. For gases, the early-time relaxation occurs in a few first collisions of the molecules, and can be singled out from the whole relaxational process and investigated separately.

Considering the beginning of the relaxation, we may expect that it is dominated by a rate of processes in the initial state. In the case of a dilute gas, in particular, this rate is given by the Boltzmann collision integral, $Q(f)$, evaluated in the state f_0, and equal to $Q_0 = Q(f_0)$. The latter expression is the known function of the phase variable, $Q_0(\Gamma)$. Put differently, our expectation is that states which the system passes through in the beginning are close to those on a ray, $f(\Gamma, a)$:

$$f(\Gamma, a) = f_0(\Gamma) + aQ_0(\Gamma)\,, \tag{9.23}$$

where $a \geq 0$ is a scalar variable (we use dimensionless variables). It is clear that such an approximation can be valid if only a "is not too large". On the other hand, nothing tells us ultimatively that a must be "strictly infinitesimal" if we want to obtain at least a moderate by accuracy approximation. In general, this consideration can be relevant if the parameter a in (9.23) does not exceed some certain upper value a^*.

In this Example we give an answer to the following question: what is the upper limiting state, f^*, the system *cannot* overcome when driven with the initial rate Q_0? As long as we can consider Q_0 as the dominant direction in the early-time relaxation, the answer amounts to an upper estimate of the parameter a in (9.23), and thus the limiting state f^* is:

$$f^*(\Gamma) = f(\Gamma, a^*) = f_0(\Gamma) + a^* Q_0(\Gamma) \,, \tag{9.24}$$

where the value a^* is the subject of the analysis to be performed.

Our approach will be based on the following consideration. Denote as $S(f)$ the entropy of the state $f(\Gamma)$, and as $S(a)$ its value in the state $f(\Gamma, a)$ (9.23). A state $f(\Gamma, a')$ can be regarded *accessible* from the initial state $f(\Gamma, 0) = f_0(\Gamma)$ in the course of the Q_0-dominated dynamics, if and only if the function $S(a)$ increases with an increase of the variable a from 0 to a'. The upper limiting value, a^*, is thus characterized by the following two properties:

1. $S(a)$ increases, as a increases from 0 to a^*.
2. $S(a)$ decreases, as a exceeds a^*.

Assuming the usual convexity properties of the entropy, we conclude that the state $f(\Gamma, a^*)$ with these properties is unique.

In the next subsection, "Extremal properties of the limiting state," we derive an equation for the limiting state $f(\Gamma, a^*)$ in two ways: firstly, as a direct consequence of the two properties just mentioned, and, secondly, as an equilibrium state of an appropriately chosen kinetic model of the Q_0-dominated relaxation. Next we introduce a method to obtain the explicit estimate of the function $f(\Gamma, a^*)$ (details are given in special Subsect. 9.3.5 "Estimations"). With this, we get the answer to the question posed above.

The derivation of the state $f(\Gamma, a^*)$ plays the key role in the section "Approximate phase trajectories". There we aim at constructing explicit approximations to trajectories of a given space-independent kinetic equation. Namely, we construct an explicit function $f(\Gamma, a)$, where parameter a spans a segment $[0, 1]$, and which satisfies the following conditions:

1. $f(\Gamma, 0) = f_0(\Gamma)$.
2. $f(\Gamma, 1) = f^0(\Gamma)$.
3. $f(\Gamma, a)$ is a non-negative function of Γ for each a.
4. $C(a) \equiv C(f(a)) = \text{const}$, where $C(f)$ are linear conserved quantities.
5. $S(a) \equiv S(f(a))$ is a monotonically increasing function of a.
6. $\partial f(\Gamma, a)/\partial a|_{a=0} = kQ_0(\Gamma)$, where $k > 0$.

Function $f(\Gamma, a)$ is a path from the initial state f_0 to the equilibrium state f^0 (conditions 1 and 2). All states of the path make physical sense (condition 3), conserved quantities remain fixed, and the entropy monotonically increases along the path (conditions 4 and 5). Finally, condition 6 requires that the path is tangent to the exact trajectory in their common initial state f_0. A function $f(\Gamma, a)$ with the properties 1-6 is, of course, not unique but a construction of

a *definite* example is a rather non-trivial task. Indeed, the major difficulty is to take into account the tangency condition 6 together with the rest of the requirements.

The simplest function with the properties 1-6, and which depends *smoothly* on a, is constructed explicitly in the Subsect. 9.3.3 "Approximate trajectories" (details of the procedure are given in Subsect. 9.3.5). We also discuss the question of the time dependence $f(\Gamma, a(t))$. In the section "Relaxation of the Boltzmann gas", the method is applied to the space-independent nonlinear Boltzmann equation for several collisional mechanisms. In particular, we compare our approximations with the celebrated BKW-mode [255, 256, 262] for the Maxwell molecules, and with solutions to the two-dimensional very hard particles model (VHP) [257, 258].

Before to proceeding any further, it is worthwhile to give here a brief comment on the status of the approximate trajectories considered below. It is well known that the space-independent problem for dissipative kinetic equations is one of the most developed branches of kinetic theory with respect to existence and uniqueness theorems [259–261]. The exact treatment of specific models is also avaiable [263, 286]. On the other hand, there exists a gap of *approximate semi-analytical* methods in this problem. This is not surprising because most of the techniques of the kinetic theory [239] are based on a small parameter expansions, and this is simply not the case of the initial layer problem. The present study fills out this gap. Indeed, as the examples demonstrate, the smooth approximations $f(a, \Gamma)$ constructed below provide a reasonable (and simple) approximation to the exact trajectories.

Moreover, these functions serve for the initial approximation in an iterative method of constructing the exact trajectories for the dissipative systems [26]. This method, in turn, is based on a more general consideration of the paper [11] (Chap. 6). We give additional comments on this iterative method below, as well as we provide an illustration of the correction.

9.3.2 Extremal Properties of the Limiting State

Let us first come to the equation for the limiting state $f(\Gamma, a^*)$ (9.24) in an informal way. The two features of the function $f(\Gamma, a^*)$ indicated above tell us that this is the state of the entropy maximum on the ray $f(\Gamma, a)$ (9.23)[1]. The extremum condition in this state reads:

$$D_f S|_{f=f(\Gamma,a^*)} \left(\frac{\partial f(\Gamma, a)}{\partial a} \right) = \int \frac{\partial f(\Gamma, a)}{\partial a} \frac{\delta S(f)}{\delta f} \bigg|_{f=f(\Gamma,a^*)} \mathrm{d}\Gamma = 0 \,, \quad (9.25)$$

where $\delta S/\delta f$ denotes the (functional) derivative of the entropy evaluated at the state $f(\Gamma, a^*)$. For a particularly interesting case of

[1] The entropy $S(a)$ increases when a runs from zero to a^*, and $S(a)$ starts to decrease when a exceeds a^*.

$$S_B(f) = -\int f(\Gamma)\ln f(\Gamma)\,\mathrm{d}\Gamma$$

(the Boltzmann entropy), and $\int Q(f)\,\mathrm{d}\Gamma = 0$ (conservation of the number of particles), (9.25) gives:

$$\int Q_0(\Gamma)\ln\{f_0(\Gamma) + a^* Q_0(\Gamma)\}\;\mathrm{d}\Gamma = 0\,. \tag{9.26}$$

In order to avoid a duplication of formulas, and in a view of the examples considered below, we shall restrict our consideration to the Boltzmann entropy case. The (unique) positive solution to (9.26) is the value a^* which gives the desired upper estimate.

In order to derive (9.26) more formally, an explicit presentation is required for a model dynamics dominated by Q_0. Let us introduce a partition of the phase space into two domains, Γ_+ and Γ_-, in such a way that the function $Q_0(\Gamma)$ is positive on Γ_+, and is negative on Γ_-, and thus $Q_0(\Gamma) = Q_0^+(\Gamma) - Q_0^-(\Gamma)$, where both the functions $Q_0^+(\Gamma)$ and $Q_0^-(\Gamma)$ are positive and concentrated on Γ_+ and Γ_-, respectively[2]. Let us consider the following kinetic equation:

$$\partial_t f = k_1(Q_0^+(\Gamma) - Q_0^-(\Gamma))(w^-(f) - w^+(f))\,, \tag{9.27}$$

where

$$w^-(f) = \exp\left(\int_{\Gamma_-} Q_0^-(\Gamma)\ln f(\Gamma,t)\,\mathrm{d}\Gamma\right)\,, \tag{9.28}$$

$$w^+(f) = \exp\left(\int_{\Gamma_+} Q_0^+(\Gamma)\ln f(\Gamma,t)\,\mathrm{d}\Gamma\right)\,,$$

and $k_1 > 0$ is an arbitrary positive constant. When supplied with the initial condition $f(\Gamma,0) = f_0(\Gamma)$, equation (9.27) has a formal solution of the form:

$$f(\Gamma,t) = f_0(\Gamma) + a(t)Q_0(\Gamma), \tag{9.29}$$

provided that $a(t)$ is the solution of the ordinary differential equation

$$\frac{\mathrm{d}a}{\mathrm{d}t} = k_1(w^-(a) - w^+(a))\,,$$

with the initial condition $a(0) = 0$. Here $w^\pm(a) = w^\pm(f(a))$.

The solution (9.29) describes a relaxation from the initial state f_0 to the equilibrium state f^*, as t tends to infinity[3] . The entropy S_B monotonically

[2] For the Boltzmann collision integral, this partition should not be confused with the natural representation in the "gain−loss form" as $\int w(\mathbf{v_1'v'}|\mathbf{v_1v})(f'f_1' - ff_1)\,\mathrm{d}\mathbf{v}_1'\,\mathrm{d}\mathbf{v}'\,\mathrm{d}\mathbf{v}_1$.

[3] The equilibrium state f^* of the model kinetic equation (9.27) is not the global equilibrium f^0, exept for the BGK model of the collision integral.

increases along this solution up to the value $S_B^* = S_B(f^*)$ in the state f^*. Substituting $f^* = f_0 + a^* Q_0$ into the right-hand side of (9.27), we derive the equation for the equilibrium state f^* in the form of the detailed balance:

$$w^-(a^*) = w^+(a^*) \; . \tag{9.30}$$

The latter equation is precisely (9.26). Note that the parameter k_1 in (9.27) does not appears in the final result (9.26) since it is responsible only for the rate of the approach to the equilibrium state f^* due to the dynamics (9.27) but not for the location of this state on the ray (9.23).

Let us discuss the idea behind the model dynamics presented by (9.27). As long as we disregard any change of Q in the beginning of the relaxation, the function $Q_0(\Gamma)$ represents a distinguished direction of relaxation in the space of states. The partition of the phase space $\Gamma_+ \cup \Gamma_-$ corresponds then to specification of the *gain* (Γ_+) and of the *loss* (Γ_-) of the phase density, while the factors w^+ and w^- (9.28),

$$w^\pm(f) \sim \exp\left\{ - \int_{\Gamma_\pm} Q_0^\pm(\Gamma) \frac{\delta S(f)}{\delta f(\Gamma)} \, \mathrm{d}\Gamma \right\} \; , \tag{9.31}$$

are the rates of the gain and and of the loss in the current state f, respectively. Equation (9.27) implements these processes in the familiar "gain minus loss" form, while the state f^* corresponds to the balance of the gain and of the loss (9.30). One can also observe a formal analogy of the structure of (9.27) with that of the so-called Marcelin-De Donder equations of chemical kinetics [81, 245] (see Chap. 2).

Thus, the limiting state $f^* = f_0 + a^* Q_0$ is described as the equilibrium state of the kinetic equation (9.27), and solves (9.26). Note that the parameter a^* is correctly defined by (9.26), independently of the partition introduced in the (9.27). The existence of the model relaxational equation (9.27) guarantees that f^* is a physical state (f^* is a non-negative function).

In order to complete the analysis, we have to learn to solve the one-dimensional nonlinear equation (9.26). In general, a method of successive approximation is required to find the solution a^* as a limit of a sequence $a_1^*, a_2^*, \ldots$. Some care should be taken in order to get all the approximations a_i^* not greater than the unknown exact value a^*, since only the states $f(a, \Gamma)$ with $a \le a^*$ are relevant. Moreover, what one actually needs in computations is *some* definite approximation $a_1^* \le a^*$. In Subsect. 9.3.5, a corresponding method is developed, which is based on the partition of Q_0 introduced above. In particular, the first approximation a_1^* reads:

$$a_1^* = \frac{1 - \exp\{-\sigma_0/q\}}{\alpha + \beta \exp\{-\sigma_0/q\}} \; , \tag{9.32}$$

where q, σ_0, α, and β are numerical coefficients:

$$\sigma_0 = -\int Q_0(\Gamma)\ln f_0(\Gamma)\,\mathrm{d}\Gamma\,, \tag{9.33}$$

$$q = \int_{\Gamma_+} Q_0^+(\Gamma)\,\mathrm{d}\Gamma = \int_{\Gamma_-} Q_0^-(\Gamma)\,\mathrm{d}\Gamma\,,$$

$$\alpha = \sup_{\Gamma\in\Gamma_-}\frac{Q_0^-(\Gamma)}{f_0(\Gamma)}\,,$$

$$\beta = \int_{\Gamma_+}\frac{(Q_0^+(\Gamma))^2}{qf_0(\Gamma)}\,\mathrm{d}\Gamma\,.$$

In the latter expressions, σ_0 is the entropy production in the initial state, q is the normalization factor, α and β reflect the maximal loss and the total gain of the phase density in the initial state, respectively. Finiteness of the parameters collected in (9.33) gives a restriction on the initial state f_0 for wich the estimate (9.32) is valid.

9.3.3 Approximate Trajectories

In this subsection we shall demonstrate how to use the states f^* (9.24) in the problem of constructing the approximate trajectories of the space-independent relaxational equations

$$\partial_t f = Q(f)\,. \tag{9.34}$$

Here $Q(f)$ is a kinetic operator (the collision integral in the case of the Boltzmann equation). We assume that (9.34) describes a relaxation to the global equilibrium state $f^0(\Gamma)$, and the entropy $S_B(f)$ increases monotonically along the solutions. Let $c_1(\Gamma),\dots c_k(\Gamma)$ be the conserved densities, i.e.

$$\int c_i Q(f)\,\mathrm{d}\Gamma = 0\,.$$

Then the quantities $C_i(f) = \int c_i f\,\mathrm{d}\Gamma$ are conserved along the solution. Assume that the set of conserved densities $c_1(\Gamma),\dots c_k(\Gamma)$ is full. In this case

$$\ln f^0(\Gamma) = \sum_1^k a_i c_i(\Gamma)\,,$$

where a_i are some numbers. A standard example of (9.34) is the space-independent Boltzmann equation which we consider below.

Let $f(\Gamma,t)$ be the solution to (9.34) with the initial condition $f(\Gamma,0) = f_0(\Gamma)$. The trajectory of this solution can be represented as a function $f(\Gamma,a)$, where a varies from 0 to 1. For each a, the function $f(\Gamma,a)$ is a non-negative function of Γ, and

$$f(\Gamma,0)=f_0(\Gamma)\;,\quad f(\Gamma,1)=f^0(\Gamma)\;,$$
$$\int c_i(\Gamma)f(\Gamma,a)\,\mathrm{d}\Gamma=\mathrm{const}\;,\quad \partial_a f(\Gamma,a)|_{a=0}\propto Q_0(\Gamma)\;. \tag{9.35}$$

In other words, as a varies from zero to one, the states $f(\Gamma,a)$ follow the solution $f(\Gamma,t)$ as t varies from zero to infinity. Since the entropy increases with time on the solution $f(\Gamma,t)$, the function $S_B(a)=S_B(f(a))$ is a monotonically increasing function of the variable a. This condition, as well as the conditions (9.35), must be met by any method of constructing an approximation to the trajectory $f(\Gamma,a)$ (see the conditions 1-6 in the Introduction).

The simplest approximation based on the function f^* of the preceding section can be constructed as follows:

$$f(\Gamma,a)=\begin{cases}(1-2a)f_0(\Gamma)+2af^*(\Gamma) & \text{for } 0\le a\le\frac{1}{2}\\ 2(1-a)f^*(\Gamma)+(2a-1)f^0(\Gamma) & \text{for } \frac{1}{2}\le a\le 1\end{cases}\;. \tag{9.36}$$

This approximation amounts to the *two-step* relaxation from the initial state f_0 to the equilibrium state f^0 through the intermediate state f^* (9.24). The first step (parameter a increases from 0 to 1/2) is the relaxation directed along Q_0 up to the state f^* (9.24). The second step (parameter a increases from 1/2 to 1) is the linear relaxation from f^* towards the equilibrium state. The last step can be viewed as the trajectory of a solution to the equation,

$$\partial_t f=-k_2(f-f^0)\;, \tag{9.37}$$

with the initial condition f^* (9.24). In kinetic theory, equation of the form (9.37) is known as the BGK-model (2.17). The entropy increase along the second step is due to the well known properties of the equation (9.37).

Expression (9.36) demonstrates the advantage of using the state f^* for the purpose of approximating the trajectory: all the conditions (9.35) are obviously satisfied, and also we do not worry about the entropy increase. Thus, all the conditions 1-6 mentioned in the Introduction are satisfied by the approximation (9.36) due to the features of the state f^*. For explicit expressions the estimate (9.32) can be used.

A disadvantage of the two-step approximation (9.36) is its non-smoothness at $a=1/2$. This can be improved as follows: Let us consider a *triangle* T formed by the three states, f_0, f^*, and f^0, i.e. a closed set of convex linear combinations of these functions[4]. This object allows to use a geometrical language. A simple consequence of the properties of the state f^* is that all the elements of the triangle T are non-negative functions, and if f belongs to T then $C_i(f)=C_i(f_0)$, where $i=1,\dots,k$ (all the conservation laws are fixed in the triangle). Therefore, a better approximation to the trajectory can be constructed as a smooth curve inscribed into the triangle T in such a way that:

[4] The state f belongs to T if $f=a_1f_0+a_2f^*+a_3f^0$, where $a_i\ge 0$, and $a_1+a_2+a_3=1$.

1. It begins in the state f_0 at $a = 0$;
2. It is tangent to the side $L_{f_0 f^*} = \{f | f = a_1 f_0 + a_2 f^*, a_1 \geq 0, a_2 \geq 0, a_1 + a_2 = 1\}$ in the state f_0;
3. It ends in the equilibrium state f^0 at $a = 1$.

Notice that the approximation (9.36) corresponds to the path from f_0 to f^0 over the two sides of the triangle T: firstly, over the segment between f_0 and f^*, and, secondly, over the segment between f^* and f^0.

The simplest form of such a smooth curve reads (the MDD spline):

$$f_g(\Gamma, a) = f^0 + (1 - a^2)\{ag(f^* - f_0) + f_0 - f^0\} , \tag{9.38}$$

where $g, 0 < g \leq 1$, is a parameter which has to be determined in a way that the entropy $S_B(a)$, calculated in the states (9.38), is monotonically increasing function of a. The explicit *sufficient* method to estimate the value of parameter g in (9.38) is rather non-trivial, and it is developed in Subsect. 9.3.5.

Finally, let us consider briefly a question of the time dependence for the approximation $f(\Gamma, a)$. Clearly, this question is relevant as soon as one looks for the approximate trajectories directly, rather than integrating (9.34) in time[5]. The answer assumes a dependence $a(t)$, and requires an ordinary differential equation for a. Such an equation should be obtained upon substitution of the expression $f(\Gamma, a)$ into the originating kinetic equation (9.34), and by a further projecting. Specifically, the equation for $a(t)$ has a form:

$$\frac{\mathrm{d}a}{\mathrm{d}t} \int \varphi(\Gamma, a) \frac{\partial f(\Gamma, a)}{\partial a} \, \mathrm{d}\Gamma = \int \varphi(\Gamma, a) Q(f(\Gamma, a)) \, \mathrm{d}\Gamma , \tag{9.39}$$

where integration with the function $\varphi(\Gamma, a)$ establishes the projection operation. Usually, this is achieved by some moment projecting (φ is independent of a), but this choice is arbitrary. Another possibility is to use the *thermodynamic projector* (Chap. 5). Then (9.39) becomes the entropy rate equation along the path (9.38):

$$\frac{\mathrm{d}a}{\mathrm{d}t} \frac{\mathrm{d}S_B(a)}{\mathrm{d}a} = \sigma_B(a) , \tag{9.40}$$

where $S_B(a) = -\int f(\Gamma, a) \ln f(\Gamma, a) \, \mathrm{d}\Gamma$
and $\sigma_B(a) = -\int Q(f(\Gamma, a)) \ln f(\Gamma, a) \, \mathrm{d}\Gamma$
are the entropy and the entropy production in the states $f(\Gamma, a)$ (9.38), respectively.

A further consideration of (9.40) is beyond the scope of this Example. Nevertheless, let us consider the asymptotics of (9.40) for the motion from f_0 towards f^*. As above, we take $f(\Gamma, a) = (1 - a) f_0 + a f^*$. Equation (9.40) for this function gives:

[5] This question is typical to various approximations used in the kinetic theory [9, 11].

$$a(t) \sim \frac{1}{a^*}t, \quad a \ll 1$$
$$a(t) \sim \frac{\sigma_B^*}{(a^*)^2 K_0}\sqrt{t}, \quad 1-a \ll 1\ ,$$

where σ_B^* is the entropy production in the state f^*, and $K_0 = \int \frac{Q_0^2}{f_0}\,\mathrm{d}\Gamma$. The slowing down at the final stage is due to the fact that $\mathrm{d}S_B(a)/\,\mathrm{d}a \to 0$, as $a \to 1$, and $\sigma_B^* > 0$.

9.3.4 Relaxation of the Boltzmann Gas

The direct and the simplest application of the approach is the space-independent Boltzmann equation. In what follows, Γ is the velocity $\mathbf{v}$, and $f(\Gamma)$ is the one-body distribution function, $f(\mathbf{v})$, which obeys the the equation:

$$\partial_t f(\mathbf{v},t) = Q(f)\ , \tag{9.41}$$

with $Q(f)$ the Boltzmann collision integral.

In the first example we consider the following form of the collision integral

$$Q(f) = \int d\mathbf{w} \int \mathrm{d}\hat{\mathbf{n}}\gamma(\hat{\mathbf{g}}\cdot\hat{\mathbf{n}})\left\{f(\mathbf{v}',t)f(\mathbf{w}',t) - f(\mathbf{v},t)f(\mathbf{w},t)\right\}\ , \tag{9.42}$$

where the function γ depends only on the scalar product of unit vectors $\hat{\mathbf{g}} = \frac{\mathbf{v}-\mathbf{w}}{|\mathbf{v}-\mathbf{w}|}$ and $\hat{\mathbf{n}} = \frac{\mathbf{v}'-\mathbf{w}'}{|\mathbf{v}-\mathbf{w}|}$, while $\mathbf{v}' = \frac{1}{2}(\mathbf{v}+\mathbf{w}+\hat{\mathbf{n}}|\mathbf{v}-\mathbf{w}|)$, and $\mathbf{w}' = \frac{1}{2}(\mathbf{v}+\mathbf{w}-\hat{\mathbf{n}}|\mathbf{v}-\mathbf{w}|)$. The Boltzmann equation (9.41) with the collision integral (9.42) corresponds to the power-law repelling potential inversly proportional to the fourth degree of the distance (the 3D Maxwell molecules, see e.g. [261]). The reason to consider this model is that it admits the exact solution, the famous BKW-mode discovered by Bobylev [262], and by Krook and Wu [255, 256]. The BKW-mode is the following one-parametric set of the distribution functions $f(c,\mathbf{v})$:

$$f(c,\mathbf{v}) = \frac{1}{2}\left(\frac{2\pi}{c}\right)^{-3/2}\exp\left\{-\frac{cv^2}{2}\right\}\left((5-3c)+c(c-1)v^2\right)\ , \tag{9.43}$$

where the parameter c spans the segment $[1, \frac{5}{3}[$, the value $c=1$ corresponds to the equilibrium Maxwell distribution

$$f^0(\mathbf{v}) = f(1,\mathbf{v}) = (2\pi)^{-3/2}\exp\{-v^2/2\}\ .$$

As c decays from a given value c_0, where $1 < c_0 < 5/3$, to the value $c=1$, the functions $f(c,\mathbf{v})$ (9.43) describe the trajectory of the BKW-mode (the time dependence of c is unimportant in the present context, see e.g. [286]).

Considering the states (9.43) as the initial states in the procedure described above, we can construct the upper limiting states, $f^*(c,\mathbf{v}) = f(c,\mathbf{v}) +$

$a^*(c)Q(c,\mathbf{v})$, for each value of c. First, we compute the collision integral (9.42) in the states (9.43) and obtain the functions $Q(c,\mathbf{v})$:

$$Q(c,\mathbf{v}) = \frac{\lambda}{2}(c-1)^2\left(\frac{2\pi}{c}\right)^{-3/2}\exp\left\{-\frac{cv^2}{2}\right\}\left(15-10cv^2+c^2(v^2)^2\right)\ , \quad (9.44)$$

where λ is a constant: $\lambda = \frac{1}{8}\int \mathrm{d}\hat{\mathbf{n}}\gamma(\hat{\mathbf{k}}\cdot\hat{\mathbf{n}})(1-(\hat{\mathbf{k}}\cdot\hat{\mathbf{n}})^2)$.

Expression (9.44) suggests a simple structure of the velocity space partition into the domains $V_+(c)$ and $V_-(c)$ (corresponding to the domains $\Gamma_\pm$ (9.31)). Namely, for a given c, the function (9.44) is positive inside a sphere of radius $v_-(c) = \sqrt{c^{-1}(5-\sqrt{10})}$, and outside a larger sphere of radius $v_+(c) = \sqrt{c^{-1}(5+\sqrt{10})}$ (both the spheres are centered in $\mathbf{v}=0$), while it is negative inside the spheric layer between these spheres:

$$\begin{aligned} V_-(c) &= \{\mathbf{v} \mid v_-(c) < |\mathbf{v}| < v_+(c)\}\ , \\ V_+(c) &= \{\mathbf{v} \mid v_-(c) > |\mathbf{v}|\} \cup \{\mathbf{v} \mid |\mathbf{v}| > v_+(c)\}\ . \end{aligned} \quad (9.45)$$

The limiting states $f^*(c,\mathbf{v})$ are given by the following expression:

$$\begin{aligned} f^*(c,\mathbf{v}) = \frac{1}{2}&\left(\frac{2\pi}{c}\right)^{-3/2}\exp\left\{-\frac{cv^2}{2}\right\} \\ &\times\left(5-3c+15a^*(c)+(c-1-10a^*(c))cv^2+a^*(c)c^2(v^2)^2\right)\ , \end{aligned} \quad (9.46)$$

where $a^*(c)$ is a solution to (9.26):

$$\int Q(c,\mathbf{v})\ln\left(f(c,\mathbf{v})+a^*(c)\frac{Q(c,\mathbf{v})}{\lambda(c-1)^2}\right)\mathrm{d}\mathbf{v} = 0\ . \quad (9.47)$$

Taking into account the partition (9.45), all the parameters (9.33) are expressed by definite one-dimensional integrals. Thus, we obtain the first approximate $a_1^*(c)$. Numerical results are presented in Table 9.3 (second column) for the three values of the parameter c taken on the BKW mode. It is interesting to compare $a_1^*(c)$ with $a_{\max}(c)$, for which the function, $f(c,\mathbf{v}) + a\frac{Q(c,\mathbf{v})}{\lambda(c-1)^2}$, looses positivity (i.e., this function becomes negative for some $\mathbf{v}$, as $a > a_{\max}(c)$). The ratio $a_1^*(c)/a_{\max}(c)$ is given in the third column of Table 9.3. The step in the direction $Q(c,\mathbf{v})$ which is allowed due to the entropy estimate reasons is never negligible in comparison to that determined by the positivity reasons, as seen in Table 9.3.

We now use (9.46) to get the approximations of trajectories (9.36) and (9.38). The estimation of the parameter g in the expression (9.38) according to Subsect. 9.3.5 gives the value $g=1$ for all the initial states (9.43).

In order to make a comparison with the exact result (9.43), we have considered the dependencies of the normalized moments $m_k(m_l)$, where

Table 9.3. The limiting states for the Maxwell molecules

c	a_1^*	$a_1^*/a_{\max}$
1.12	$3.1779 \cdot 10^{-3}$	0.2221
1.24	$1.1660 \cdot 10^{-2}$	0.4291
1.48	$3.8277 \cdot 10^{-2}$	0.7087

$$m_s(f) = \frac{\int (v^2)^s f \, \mathrm{d}\mathbf{v}}{\int (v^2)^s f^0 \, \mathrm{d}\mathbf{v}}, \quad s = 0, 1, 2, \dots \ . \tag{9.48}$$

Typical dependencies of the higher-order moments ($k \geq 3$) on the lowest-order non-trivial moment ($l = 2$) are presented in the Fig. 9.1 for a considerably nonequilibrium initial state (9.43) with $c = 1.42$.

The error of the approximation (9.38) was estimated as follows: In each moment plane (m_k, m_l), the approximation (9.38) and the BKW-mode (9.43) generate two sets (two curvilinear segments), X_{kl} and Y_{kl}, respectively. First, in order to eliminate the contribution from the difference in the total variation of the moments, we rescale the variables:

$$\hat{m}_i = m_i / \Delta_i \ , \quad i = k, l \ ,$$

where

$$\Delta_i = \max_{\mathbf{x}, \mathbf{x}' \in X_{kl} \bigcup Y_{kl}} |x_i - x_i'| \ .$$

Second, in the plane $(\hat{m}_k, \hat{m}_l)$, we compute the Hausdorff distance, d_{kl}, between the two corresponding sets, $\hat{X}_{kl}$ and $\hat{Y}_{kl}$:

$$\mathrm{d}_{kl} = \max \left\{ \max_{\mathbf{x} \in \hat{X}_{kl}} \min_{\mathbf{y} \in \hat{Y}_{kl}} \mathrm{d}(\mathbf{x}, \mathbf{y}), \quad \max_{\mathbf{y} \in \hat{Y}_{kl}} \min_{\mathbf{x} \in \hat{X}_{kl}} \mathrm{d}(\mathbf{x}, \mathbf{y}) \right\} \ , \tag{9.49}$$

where $\mathrm{d}(\mathbf{x}, \mathbf{y})$ is the standard Euclidian distance between two points. Finally, the error δ_{kl} was estimated as the normalized distance d_{kl}:

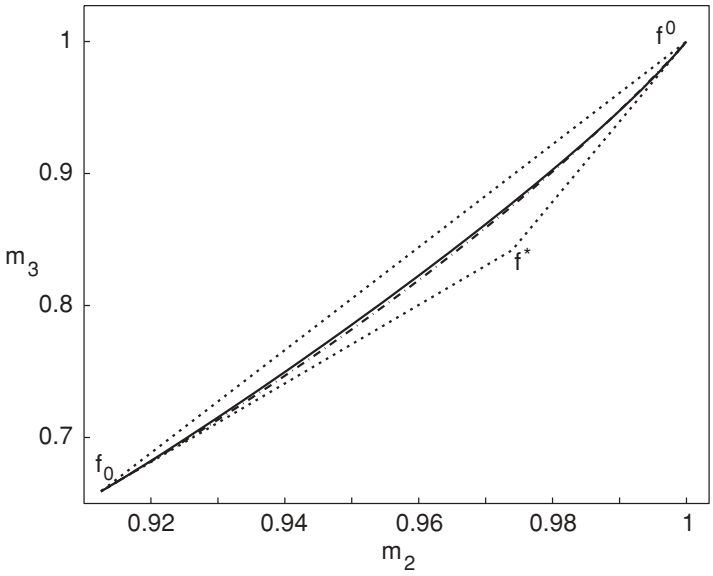
$$\delta_{kl} = \frac{\mathrm{d}_{kl}}{D_{kl}} \cdot 100\% \ , \tag{9.50}$$

where

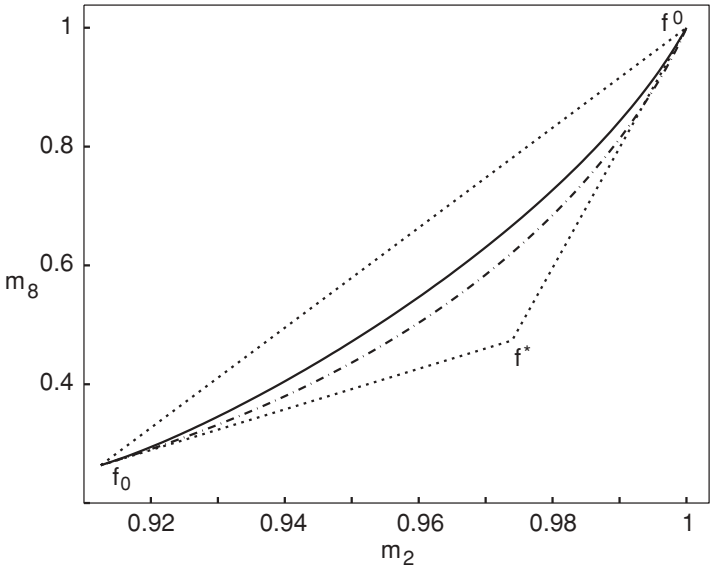
$$D_{kl} = \max_{\mathbf{x}, \mathbf{y} \in \hat{Y}_{kl} \bigcup \hat{X}_{kl}} \mathrm{d}(\mathbf{x}, \mathbf{y}) \ .$$

The error δ_{k2} of the plots like in Fig. 9.1 is presented in the Table 9.4 for several values of the parameter c.

The quality of the smooth approximation (9.38) is either good or reasonable up to the order of the moment $k \sim 10$, depending on the closeness of the initial state to the equilibrium. when either k increases, or the initial state is taken very far from the equilibria (i.e., when c is close to 5/3) the comparison



(a) m_3 vs. m_2,



(b) m_8 vs. m_2,

Fig. 9.1. Moment dependencies for the Maxwell molecules: The initial state f_0 is the function (9.43) with $c = 1.42$. Punctuated contour is the image of the triangle T. Punctuated dash line is the BKW-mode. *Solid* line is the smooth approximation (9.38). Punctuated path $f_0 \to f^* \to f^0$ is the non-smooth approximation (9.36)

Table 9.4. The error δ_{k2} (9.50) of the approximation (9.38) for the Maxwell molecules with the initial data (9.43)

k	$c = 1.12$	$c = 1.24$	$c = 1.36$	$c = 1.48$	$c = 1.59$
3	0.31	0.33	0.30	0.41	0.70
4	0.44	0.47	0.44	0.81	1.57
5	0.58	0.55	0.71	1.41	2.67
6	0.71	0.57	1.10	2.20	3.97
7	0.81	0.62	1.58	3.14	5.40
8	0.89	0.84	2.19	4.19	6.93
9	0.95	1.11	2.87	5.34	8.52
10	0.99	1.41	3.64	6.55	10.11
20	1.46	6.77	12.91	18.15	22.87
50	10.38	28.47	27.36	30.81	33.94
100	21.76	29.26	32.49	34.78	37.22

becomes worser. For the moments of a very high order, the approximation with the smooth function (9.38) is only qualitative. On the other hand, the two-step (non-smooth) approximation (9.36) provides a much better approximation for higher-order moments ($k \sim 40$ and higher). The explanation is as follows: the BKW-mode (9.43) demonstrates a very rapid relaxation of higher moments to their equilibrium values. Therefore, as expected, the relaxation in the direction Q_0 leads to the state where the higher-order moments are practically the same as in the equilibrium.

The second example is the very hard particles (VHP) model [257, 258]. The distribution function $F(x)$ depends on the phase variable x, where $0 \le x \le \infty$, and is governed by the following kinetic equation:

$$\partial_t F(x,t) = \int_x^\infty \mathrm{d}u \int_0^u \mathrm{d}y \left[F(y,t)F(u-y,t) - F(x,t)F(u-x,t)\right] \ . \quad (9.51)$$

This model has the two conservation laws:

$$N = \int_0^\infty F(x,t)\,\mathrm{d}x = 1 \ ,$$
$$E = \int_0^\infty xF(x,t)\,\mathrm{d}x = 1 \ ,$$

and has the entropy $S_B(F) = -\int_0^\infty F(x)\ln F(x)\,\mathrm{d}x$. The equilibrium distribution reads: $F^0(x) = \exp(-x)$. The general solution to this model is known [257, 258, 286].

The first set of initial conditions which was tested was as follows:

$$F_0(x,\beta) = \beta((2-\beta) + \beta(\beta-1)x)\exp(-\beta x) \ , \quad (9.52)$$

where $1 \le \beta < 2$, the value $\beta = 1$ corresponds to the equilibrium state $F_0(x,1) = F^0(x)$.

In accordance with [257, 258, 286], the exact solution solution to (9.51) with the initial data (9.52) reads:

$$F_{ex}(x,\beta,t) = \frac{Az_+ + C}{z_+ - z_-}\mathrm{e}^{xz_+} + \frac{Az_- + C}{z_- - z_+}\mathrm{e}^{xz_-} \ , \tag{9.53}$$

$$z_\pm = -\frac{t+2\beta}{2} \pm \sqrt{\left(\frac{t+2\beta}{2}\right)^2 - C} \ ,$$

$$A = 1-(\beta-1)^2\mathrm{e}^{-t}; \quad C = t+2\beta-1+\mathrm{e}^{-t}(\beta-1)^2 \ .$$

Comparison of the smooth approximation (9.38) with the exact solution (9.53) demonstrates the same quality as in the case of the Maxwell molecules. As above, the normalized moments m_k were compared, where

$$m_k = \frac{\int_0^\infty x^k F(x)\,\mathrm{d}x}{\int_0^\infty x^k F^0(x)\,\mathrm{d}x} \ .$$

In Table 9.5, the error δ_{k2} (9.50) is represented for several values of the parameter β, while Fig. 9.2 illustrate the typical moment behavior. We also represent in this figure the result of the *correction* to the approximation (9.38) due to the first iteration of the Newton method with incomplete linearization (Chap. 6).

Table 9.5. The error δ_{k2} (9.50) of the approximation (9.38) for the VHP model with the initial data (9.52)

k	4	6	8	10	20	100
$\beta = 1.2$	0.95	1.81	2.26	2.23	2.24	9.64
$\beta = 1.6$	0.88	1.89	2.59	2.77	6.14	24.29
$\beta = 1.9$	1.16	1.65	1.45	3.16	12.7	28.22

The second set of the initial conditions for the VHP model (9.51) was considered as follows:

$$F_0(x,\lambda) = \exp(-2x)\left\{1 + \frac{1}{2}\lambda + 2x^2(1-\lambda) + \frac{1}{3}\lambda x^4\right\} \ , \tag{9.54}$$

where $0 < \lambda < 1/5(7+\sqrt{19})$. The exact solution to (9.51) with the initial condition (9.54) was found in [258]. This solution demonstrates so-called Tjon's overshoot effect [264]. We remind that Tjon's effect takes place when the distribution function becomes overpopulated for some velocities in comparison to both the initial and the equilibrium states. This effect was intensively studied for solvable Boltzmann-like kinetic equations, such as the Maxwell molecules (9.42), the VHP model (9.51), and others (see [286], [265] and

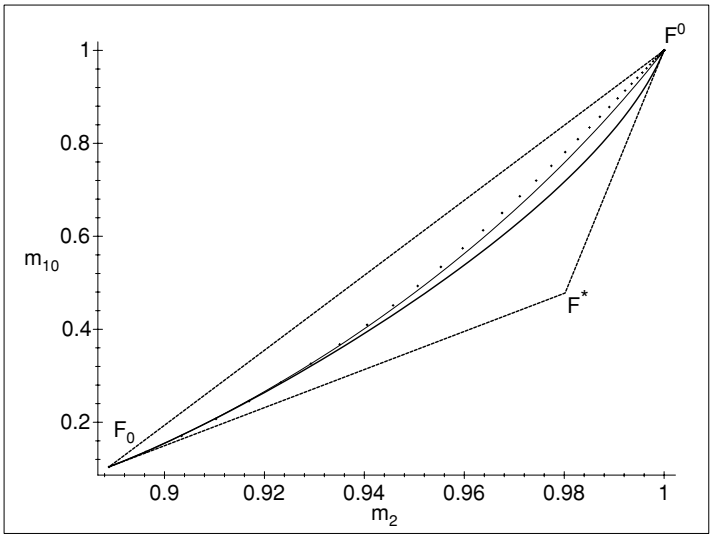


Fig. 9.2. Moment dependency m_{10} vs. m_2 for the VHP model with the initial condition (9.52), $\beta = 1.5$. *Dots* – the exact solution (9.53); *Bold* line is the smooth approximation (9.38); *Solid* line is the first correction to the approximation (9.38)

references therein; it is worthwhile to mention here extensive studies of the Tjon-like effects in chemical kinetics [81, 115]).

The approximation (9.38) for the VHP model (9.51) with the initial condition (9.54) also demonstrates the overshoot just mentioned. In the moment representation, the overshoot of the moments is clearly seen in Fig. 9.3. The quality of the approximation is the same as in the examples above.

9.3.5 Estimations

This is the technical subsection which contains estimations for the limiting state and for the smooth approximation of the trajectory.

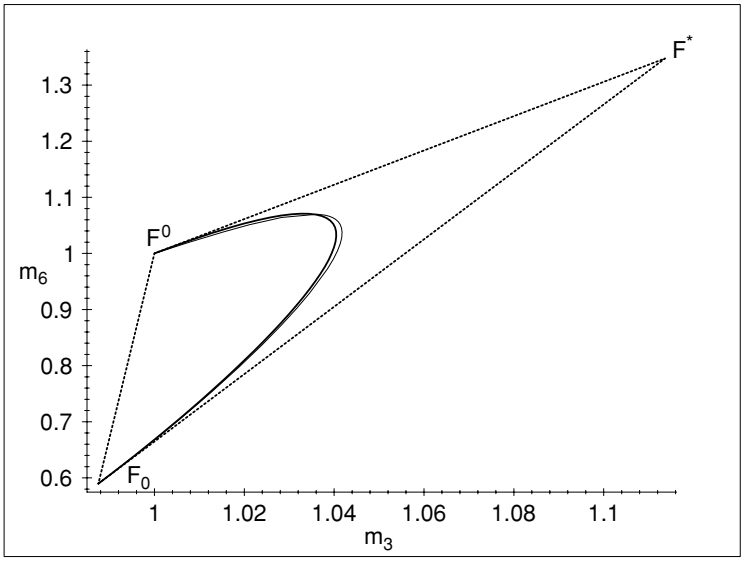
Evaluation of the Limiting State. Double-Space Newton Method

Let us introduce a normalization of the partition $Q_0^{\pm}(\Gamma)$:

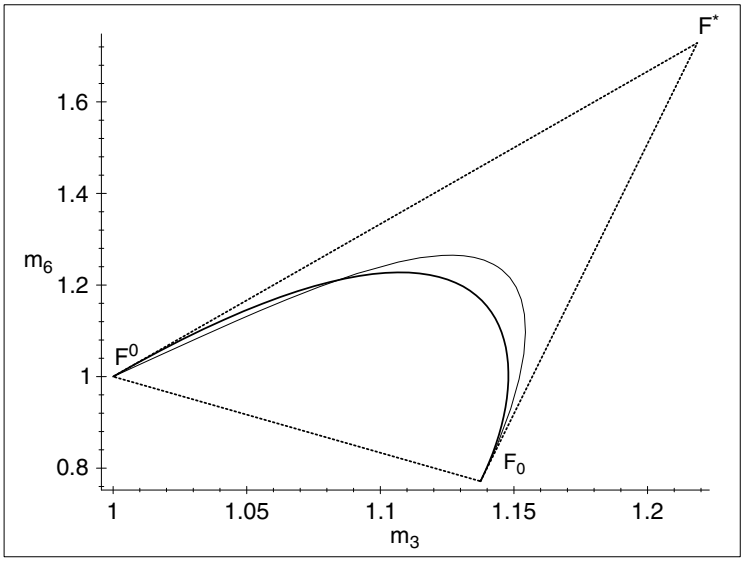
$$q_0^{\pm}(\Gamma) = q^{-1} Q_0^{\pm}(\Gamma) \,, \quad q = \int_{\Gamma_{\pm}} Q_0^{\pm}(\Gamma)\, \mathrm{d}\Gamma \,. \tag{9.55}$$

Switching to the variable $b = qa$, so that $f^* = f_0(\Gamma) + b^* q_0(\Gamma)$, where $q_0(\Gamma) = q^{-1} Q_0(\Gamma)$, equation (9.26) can be rewritten as follows:

$$A_+(b^*) = A_-(b^*) \,, \tag{9.56}$$



(a) $\lambda = 0.6$



(b) $\lambda = 0.9$

Fig. 9.3. Moment dependencies m_6 vs. m_3 for the VHP model with the initial condition (9.54). *Solid* line is the exact solution [258], *Bold* line is the smooth approximation (9.38)

where

$$A_{\pm}(b) = \int_{\Gamma_{\pm}} q_0^{\pm}(\Gamma) \ln(f_0(\Gamma) \pm b q_0^{\pm}(\Gamma))\, \mathrm{d}\Gamma \,. \tag{9.57}$$

It is easy to check the following properties of the functions $A_{\pm}$ (9.57):

1. The domain of A_+ is the open semi-axis $]b_+, +\infty[$, where $b_+ < 0$, and domain of A_- is the open semi-axis $]-\infty, b_-[$, where $b_- > 0$. The functions $A_{\pm}$ have logarithmic singularities at points $b_{\pm}$, respectively.
2. The functions $A_{\pm}$ are monotonic and concave inside their domains.
3. An inequality holds as: $A_+(0) - A_-(0) = -q^{-1}\sigma_0 < 0$, where $\sigma_0 = -\int Q_0(\Gamma) \ln f_0(\Gamma)\, \mathrm{d}\Gamma$ is the entropy production in the state f_0.

One has to solve (9.56) in order to obtain approximations $b_1^*, b_2^*, \ldots$ not greater than the unknown exact value b^*. To obtain a relevant lower estimate of b^*, it is convenient to use the concavity properties of the functions (9.57). Indeed, for positive b, the function A_- is estimated from below as:

$$A_-(b) \geq A_-(0) + \ln(1 - \alpha_1 b) \,. \tag{9.58}$$

Here α_1 is the inverse of b_-:

$$\alpha_1 = \sup_{\Gamma \in \Gamma_-} \frac{q_0^-(\Gamma)}{f_0(\Gamma)} = \sup_{\Gamma \in \Gamma_-} \frac{Q_0^-(\Gamma)}{q f_0(\Gamma)} = q^{-1}\alpha \,,$$

while α was introduced in (9.33).

On the contrary, the function A_+ should be estimated from above. Note that a function $\exp A_+$ is also monotonic and concave. We can write for positive b:

$$A_+(b) \leq A_+(0) + \ln\left(1 + b\frac{\mathrm{d}A_+(0)}{\mathrm{d}b}\right) \,, \tag{9.59}$$

where

$$\frac{dA_+(0)}{db} = \int_{\Gamma_+} \frac{(q_0^+(\Gamma))^2}{f_0(\Gamma)}\, \mathrm{d}\Gamma = q^{-1}\beta \,,$$

and β was introduced in (9.33).

Equating the right-hand side of (9.59) to the right-hand side of (9.58), and solving the linear equation obtained, we get the estimate $b_1^* \leq b^*$. Next, switching back to the variable a, we get the estimate a_1^* (9.32) and (9.33). One can readily recognize that the procedure just described is the first iterate of the Newton method for (9.56) (modified by making use of the concavity to guarantee positivity of the approximate solution, $a_1^* \leq a^*$). We call it the double-space Newton method. Next iterations are performed in the same manner.

Smooth Approximations of the Trajectories

The Triangle of Model Motions

Notation $\overline{\text{conv}}\{f_1, \dots, f_k\}$ stands for a closed convex linear hull of the functions $f_1, \dots, f_k$, and we drop the variable Γ. In particular, the triangle T introduced in the section "Approximate trajectories" reads:

$$T = \overline{\text{conv}}\{f_0, f^*, f^0\} \,. \tag{9.60}$$

A function from the triangle T (9.60) can be specified with two parameters, ξ and η, as $f(\xi, \eta)$:

$$f(\xi, \eta) = f^0 + \xi\{\eta(f^* - f_0) + f_0 - f^0\}, \quad 0 \le \xi, \eta \le 1 \,. \tag{9.61}$$

A shift of the function $f(\xi, \eta)$ under a variation of ξ and of η reads:

$$\begin{aligned} \Delta f(\xi, \eta) &= \partial_\xi f(\xi, \eta)\Delta\xi + \partial_\eta f(\xi, \eta)\Delta\eta + o(\Delta\xi, \Delta\eta) \\ &= (f(\xi, \eta) - f^0)\xi^{-1}\Delta\xi + a^* Q_0 \xi \Delta\eta + o(\Delta\xi, \Delta\eta) \,. \end{aligned}$$

This shift is a combination of the two: a shift towards f^0, and a shift in the direction Q_0. We further refer to these as to the BGK-motion and the Q_0-motion, respectively. The differential of the entropy $S_B(\xi, \eta) = S_B(f(\xi, \eta))$ is:

$$\mathrm{d}S_B(\xi, \eta) = -\sigma_1(\xi, \eta)\xi^{-1}\,\mathrm{d}\xi + \sigma_2(\xi, \eta)\xi\,\mathrm{d}\eta \,, \tag{9.62}$$

where

$$\begin{aligned} \sigma_1(\xi, \eta) &= \int (f(\xi, \eta) - f^0) \ln \frac{f(\xi, \eta)}{f^0}\,\mathrm{d}\Gamma \,, \\ \sigma_2(\xi, \eta) &= \int (f_0 - f^*) \ln f(\xi, \eta)\,\mathrm{d}\Gamma = -a^* \int Q_0 \ln f(\xi, \eta)\,\mathrm{d}\Gamma \,, \end{aligned} \tag{9.63}$$

are the entropy productions in the BGK-motion and in the Q_0-motion, respectively.

Introducing smooth dependencies, $\xi(a)$ and $\eta(a)$, where $0 \le a \le 1$, and requiring

$$\begin{gathered} 0 \le \xi(a), \eta(a) \le 1,\ \xi(0) = 1,\ \xi(1) = 0,\ \eta(0) = 0,\ \eta(1) < \infty \,, \\ \left.\frac{\mathrm{d}\xi(a)}{\mathrm{d}a}\right|_{a=0} = 0,\ \left.\frac{\mathrm{d}\eta(a)}{\mathrm{d}a}\right|_{a=0} = \gamma,\ 0 < \gamma \le 1 \,, \end{gathered} \tag{9.64}$$

we obtain a one-parametric set, $f(a) = f(\xi(a), \eta(a))$. Geometrically, $f(a)$ is a smooth curve located in T. This curve begins in f_0 at $a = 0$, ends up in f^0 at $a = 1$, and is tangent to the side of T, $L_{f_0 f^*} = \overline{\text{conv}}\{f_0, f^*\}$, at $a = 0$. Further, only monotonic functions $\xi(a)$ and $\eta(a)$ will be considered:

$$\frac{\mathrm{d}\xi(a)}{\mathrm{d}a} \le 0, \quad \frac{\mathrm{d}\eta(a)}{\mathrm{d}a} \ge 0 \,. \tag{9.65}$$

The crucial point is that the function $f(a)$ should have a correct entropy behavior. Specifically, we require that the entropy $S_B(a) = S_B(f(a)) = S_B(f(\xi(a), \eta(a)))$ is a monotonic function:

$$\frac{\mathrm{d}S_B(a)}{\mathrm{d}a} = -\sigma_1(\xi(a), \eta(a))\xi^{-1}(a)\frac{\mathrm{d}\xi(a)}{\mathrm{d}a} + \sigma_2(\xi(a), \eta(a))\xi(a)\frac{\mathrm{d}\eta(a)}{\mathrm{d}a} \geq 0 \,. \tag{9.66}$$

Since $\sigma_1(\xi, \eta)$ is non-negative everywhere in T, a sufficient condition for inequality (9.66) to be valid for any pair of functions $\xi(a)$ and $\eta(a)$ with the properties (9.64) and (9.65) is that $\sigma_2(\xi, \eta)$ is non-negative everywhere in T. However, this situation might not always be realized for arbitrary f_0 and Q_0. In order to take into account a general situation, we execute the following procedure:

1. We derive a subset of T, inside which σ_2 is non-negative. This subset includes f_0, and will be constructed as a triangle $T' \subseteq T$.
2. We tune the functions $\xi(a)$ and $\eta(a)$ in such a way that $\sigma_1(a)$ dominates $\sigma_2(a)$ outside T'.

The Triangle T'

Let us introduce a different specification of the functions in the triangle T. Denote

$$f_1(y) = (1-y)f_0 + yf^*, \quad f_2(y) = (1-y)f_0 + yf^0, \quad 0 \leq y \leq 1 \,. \tag{9.67}$$

The functions in T are labeled with two parameters, x and y:

$$f(x, y) = (1-x)f_1(y) + xf_2(y), \quad 0 \leq x, y \leq 1 \,. \tag{9.68}$$

Let us derive y', where $0 < y' \leq 1$, in such a way that σ_2 is non-negative everywhere in the triangle $T' = \overline{\mathrm{conv}}\{f_0, f_1(y'), f_2(y')\}$.

Introducing a representation $\sigma_2(x, y) = \sigma_2^+(x, y) - \sigma_2^-(x, y)$, where

$$\sigma_2^+(x, y) = \int f_0 \ln f(x, y)\, \mathrm{d}\Gamma, \quad \sigma_2^-(x, y) = \int f^* \ln f(x, y)\, \mathrm{d}\Gamma \,, \tag{9.69}$$

we notice that the functions $\sigma_2^{\pm}(x, y)$ are concave in the variable y on the segment $[0, 1]$, for any fixed x. Now we apply the standard estimations of a smooth concave function on $[0, 1]$ (if $\mathrm{d}^2\psi(t)/\,\mathrm{d}t^2 \leq 0$ on $[0, 1]$, then $\psi(t) \geq (1-t)\psi(0) + t\psi(1)$, and $\psi(t) \leq (\mathrm{d}\psi(t)/\,\mathrm{d}t|_{t=0})t + \psi(0)$) to the functions (9.69):

$$\begin{aligned} \sigma_2^+(x, y) &\geq (1-y)\sigma_2^+(x, 0) + y\sigma_2^+(x, 1) \,, \\ \sigma_2^-(x, y) &\leq (\partial_y \sigma_2^-(x, y)|_{y=0})y + \sigma_2^-(x, 0) \,. \end{aligned}$$

Furthermore, the function $\sigma_2^+(x, 1)$ is concave, hence

$$\sigma_2^+(x,1) \geq (1-x)\sigma_2^+(0,1) + x\sigma_2^+(1,1) \; .$$

Making use of the three inequalities just derived, and taking into account the explicit form of the function $f(x,y)$, we are led to the following estimate of σ_2 in T:

$$\sigma_2(x,y) \geq a^*\sigma_0 - y(xK_1 + K_2) \; , \tag{9.70}$$

where σ_0 is the entropy production in the initial state (9.33), and parameters K_1 and K_2 are:

$$\begin{aligned} K_1 &= \int \frac{f^*}{f_0}(f^0 - f^*)\,\mathrm{d}\Gamma + S_B(f^0) - S_B(f^*) \; , \\ K_2 &= \int \frac{f^*}{f_0}(f^* - f_0)\,\mathrm{d}\Gamma + S_B(f^*) - S_B(f_0) \; . \end{aligned} \tag{9.71}$$

Here $S_B(f_0)$, $S_B(f^*)$, and $S_B(f^0)$ are values of the entropy in the states f_0, f^*, and f^0, respectively.

Since σ_0 is positive, there always exists such y', where $0 < y' \leq 1$, that the right-hand side of (9.70) is non-negative for all x on the segment $[0,1]$. Specifically, let us introduce a function $\varphi(x) = a^*\sigma_0 - (xK_1 + K_2)$, and denote

$$z = a^*\sigma_0 \min\{K_2^{-1}, (K_1+K_2)^{-1}\} \; , \tag{9.72}$$

where $\min\{K_2^{-1}, (K_1+K_2)^{-1}\}$ stands for the minimal of the two numbers, K_2^{-1} and $(K_1+K_2)^{-1}$. Then y' is defined as:

$$y' = \begin{cases} 1 & \text{if} \quad \varphi(x) \geq 0 \quad \text{on} \quad [0,1], \quad \text{or} \quad z \geq 1 \\ z & \text{otherwise} \end{cases} \; . \tag{9.73}$$

Thus, σ_2 is non-negative inside the triangle $T' = \overline{\mathrm{conv}}\{f_0, f_1(y'), f_2(y')\}$, where $f_{1,2}(y')$ are given by (9.67), and y' is given by (9.73). If it happens that $y' = 1$, then $T' = T$, and σ_2 is non-negative everywhere in T. In this case any pair of the functions $\xi(a)$ and $\eta(a)$ with the properties (9.64) and (9.65) give the approximation $f(a)$ consistent with the inequality (9.66). Otherwise, we continue the procedure.

Near-Equilibrium Estimations of the Functions σ_1 and σ_2

Let us come back to the specification (9.61) in order to establish the following inequalities for the functions $\sigma_{1,2}(\xi,\eta)$ (9.63):

$$\begin{aligned} \sigma_1(\xi,\eta) &\geq M_1\xi^2 \; , \\ \sigma_2(\xi,\eta) &\geq M_2\xi \; . \end{aligned} \tag{9.74}$$

Inequalities (9.74) are motivated by the following consideration. Since

$$f(\xi,\eta) \to f^0, \text{ as } \xi \to 0 \; ,$$

parameter ξ controls a deviation of $f(\xi,\eta)$ from f^0 in T. Near the equilibrium state f^0, the function $\sigma_1(\xi,\eta)$ is quadratic in ξ, while the function $\sigma_2(\xi,\eta)$ is linear. Inequalities (9.74) extend these near-equilibrium estimations to other points of T, and they are intended to control dominance of σ_1 over σ_2 outside T' in the case $T' \neq T$.

Writing $\sigma_1(\xi,\eta) = \xi\lambda(\xi,\eta)$, and representing $\lambda(\xi,\eta)$ as a combination of the concave functions, and after making the estimations as above, we come to the following expression for M_1 in the first of the inequalities (9.74):

$$M_1 = S_B(f^0) - S_B(f^*) \; . \tag{9.75}$$

Since $S_B(f^0) > S_B(f^*)$, expression (9.75) is always positive. The estimate of M_2 is much the same. First, representing $\sigma_2(\xi,\eta)$ in the manner of (9.69), and again estimating the concave functions obtained, we come to the following inequality:

$$\sigma_2(\xi,\eta) \geq \xi(\eta N_1 + N_2) \; , \tag{9.76}$$

where constants N_1 and N_2 are:

$$\begin{aligned} N_1 &= \int \frac{f^*}{f^0}(f_0 - f^*)\,\mathrm{d}\Gamma + S_B(f_0) - S_B(f^*) \; , \\ N_2 &= \int \frac{f^*}{f^0}(f^0 - f_0)\,\mathrm{d}\Gamma + S_B(f_0) - S_B(f^0) \; . \end{aligned} \tag{9.77}$$

Second, denoting $\min\{N_2, N_1 + N_2\}$ as the minimal of the two numbers, N_2 and $N_1 + N_2$, we derive the constant in the second of the inequalities (9.74):

$$M_2 = \min\{N_2, N_1 + N_2\} \tag{9.78}$$

As above, there are two possibilities:

1. If $M_2 \geq 0$, then σ_2 is non-negative everywhere in T, and any pair of functions $\xi(a)$ and $\eta(a)$ with the properties (9.64) and (9.65) gives $f(a)$ with the correct entropy behavior.
2. If $M_2 < 0$, then we continue the procedure.

Adjustment of the Functions $\xi(a)$ and $\eta(a)$

Let $y' < 1$ and $M_2 < 0$. A further analysis requires an explicit form of the functions $\xi(a)$ and $\eta(a)$ with the properties (9.64) and (9.65), and can be done in any particular case. Consider the simplest choice:

$$\xi(a) = 1 - a^2, \quad \eta(a) = ga \; , \tag{9.79}$$

where g, $0 < g \leq 1$, is a parameter to be determined. The function (9.61) with the dependencies (9.79) has the form (9.38):

$$f_g(a) = f^0 + (1 - a^2)\{ga(f^* - f_0) + f_0 - f^0\} \; . \tag{9.80}$$

We should derive the parameter g in (9.79) in such a way that the states $f(a)$ (9.38) belong to T', when a varies from 0 to some a_1, and also that $\sigma_1(a)$ dominates $\sigma_2(a)$ when a varies from a_1 to 1. Under these conditions, the entropy inequality (9.66) is valid for all a on the segment $[0,1]$.

Substitute now (9.79) into (9.66) and apply the inequalities (9.74) to get:

$$\frac{\mathrm{d}S_B(a)}{\mathrm{d}a} \geq 2a(1-a^2)M_1 - g(1-a^2)^2|M_2| \,. \tag{9.81}$$

We require that $f(a_1) \in \overline{\mathrm{conv}}\{f_1(y'), f_2(y')\}$, and that the right-hand side of the inequality (9.81) is non-negative at a_1:

$$\begin{cases} f_g(a_1) = f(x_1, y') \\ 2a(1-a^2)M_1 - g(1-a^2)^2|M_2| \geq 0 \end{cases} . \tag{9.82}$$

Here $f(x_1, y')$ is the specification (9.68) of the function $f_g(a_1)$. Explicitly, condition (9.82) reads:

$$\begin{cases} a_1^2 = x_1 y' \\ a_1 g(1-a_1^2) = (1-x_1)y' \\ g(1-a_1^2) \leq \frac{2M_1}{|M_2|} a_1 \end{cases} . \tag{9.83}$$

Eliminating a_1 and x_1 in (9.83), we are left with the following estimate of the parameter g:

$$g \leq \lambda \frac{\sqrt{y'(1+\lambda)}}{1-y'+\lambda} \,, \tag{9.84}$$

where

$$\lambda = \frac{2M_1}{|M_2|} \,. \tag{9.85}$$

It may happen that the right-hand side of the inequality (9.84) is greater than 1. In this case we take $g = 1$ in (9.80). Thus, if $y' < 1$, and $M_2 < 0$, the parameter g in (9.80) and (9.38) is estimated as:

$$g = \min\left\{1, \lambda \frac{\sqrt{y'(1+\lambda)}}{1-y'+\lambda}\right\} \,. \tag{9.86}$$

Summary of the Algorithm

The choice of the parameter g in the smooth approximate to the trajectory (9.38) is done in the following four steps:

1. Evaluate K_1 and K_2 (9.71).
2. If $a^*\sigma_0 - (K_1 x + K_2) \geq 0$ on $[0,1]$, take $g = 1$. Otherwise, evaluate

$$y' = a^*\sigma_0 \min\{K_2^{-1}, (K_1+K_2)^{-1}\} \,.$$

3. If $y' \geq 1$, take $g = 1$. Otherwise evaluate N_1 and N_2 (9.77).

4. If $\min\{N_2, N_1 + N_2\} \geq 0$, take $g = 1$. Otherwise evaluate M_1 (9.75) and take

$$g = \min\left\{1, \lambda\frac{\sqrt{y'(1+\lambda)}}{1-y'+\lambda}\right\}, \quad \lambda = \frac{2M_1}{|M_2|}\ .$$

The function $f_g(a)$ (9.38) with g thus derived has the following properties:

1. It begins in f_0 at $a = 0$ and ends in f^0 at $a = 1$.
2. It is a non-negative function of Γ for each a.
3. It satisfies the conservation laws.
4. The entropy $S_B(f_g(a))$ is a monotonic function of a.
5. It is tangent to the exact trajectory at $a = 0$.

In practical computations, the approximation $f_1^* = f_0 + a_1^* Q_0$ with a_1^* (9.32) can be used in this algorithm instead of the exact f^*.

9.3.6 Discussion

Main results of this Example are:

1. The description of the Q_0-dominated kinetics, and of its equilibrium state f^*. The state f^* is explicitly evaluated.
2. The explicit construction of the approximate trajectory $f(\Gamma, a)$ for nonlinear space-independent kinetic equations equipped with the entropy (Lyapunov) function.

The approach used can be termed "geometric" since it avoids integration of kinetic equations in time. In the point 1, it stays at variance with many alternative approaches to the early-time evolution, which usually involve the time integration over the first few collisions. These methods encounter two general difficulties: the time of integration cannot be defined precisely, and approximations involved can violate the entropy increase and the positivity of distribution function. These difficulties are avoided in the present approach. On the other hand, the presentation of the Q_0-dominated relaxation is itself an ansatz, whose relevance to the actual process can be judged only a posteriori. As the examples show, we can indeed speak about such a dynamics. It is remarkable that the limiting state f^* differs significantly from both the initial and equilibrium states. In other words, irrespectively of how short in time the initial stage of the relaxation might be, the change of the state can be large.

Concerning the point 2, it is worthwhile to notice that, though the space-independent problem is too "refined", it nevertheless gives a good example of a problem without small parameters. It is rather remarkable that the global requirements to the trajectory (e.g., the entropy increase) are accomplished with the direct local analysis (Subsect. 9.3.5). Estimations in this part are sufficient, and can be enhanced.

Final comments concern a further treatment of the space-independent relaxation. The goal now is to develop a procedure of *corrections* to the approximate trajectory. In other words, what we need is a sequence of the functions $f_0(I, a), f_1(I, a), \ldots$, which converges to the exact trajectory, and where $f_0(I, a)$ is the initial (global) approximation to the trajectory. Again, a general obstacle is the absence of a small parameter in the problem. However, the method of invariant manifold (Chap. 6) appears to be appropriate (at least formally) since it is based on the Newton method and not on the small parameter expansions. It turns out that smoothness and all the requirements listed in the Introduction should be met by any initial approximation $f_0(I, a)$ chosen for this procedure. Thus, the approximation (9.38) can be used for this purpose. We have already annonsed this method with a result of the first Newton correction to the approximation (9.38) for the VHP model (see Fig. 9.2).

Finally, the present method recently became a part of the so-called Entropic lattice Boltzman method [136, 137, 140, 141] (see Sect. 2.7) because it enables to implement collision in a numerically stable fashion.