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Some examples of kinetic schemes whose diffusion limit is Il'in's exponential-fitting

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Abstract

This paper is concerned with diffusive approximations of some numerical schemes for several linear (or weakly nonlinear) kinetic models which are motivated by wide-range applications, including radiative transfer or neutron transport, run-and-tumble models of chemotaxis dynamics, and Vlasov–Fokker–Planck plasma modeling. The well-balanced method applied to such kinetic equations leads to time-marching schemes involving a "*scattering* S*-matrix*", itself derived from a normal modes decomposition of the stationary solution. One common feature these models share is the type of diffusive approximation: their macroscopic densities solve drift-diffusion systems, for which a distinguished numerical scheme is Il'in/Scharfetter–Gummel's "*exponential fitting*" discretization. We prove that these well-balanced schemes relax, within a parabolic rescaling, towards such type of discretization by means of an appropriate decomposition of the S-matrix, hence are *asymptotic preserving*.

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1 Introduction and contextualization

1.1 General setup

Drift-diffusion equations, like (1.9), arise naturally as diffusive approximations of numerous kinetic equations when time t and space x variables are conveniently rescaled. Such parabolic equations, in a context of semiconductor modeling, sparkled the development of so–called "uniformly accurate" [nowadays rephrased "asymptotic-preserving" (AP)] numerical methods: see e.g. [2,3,23,38,53,55]. A thorough survey of such algorithms is presented in the book [54]. The "exponential-fitting" Il'in/Scharfetter–Gummel algorithm realizes one of the first well-balanced (WB) schemes for a parabolic equation in divergence form, like drift-diffusion equations, and is uniformly accurate (or AP), too, in the vanishing viscosity limit (contrary to the more standard Crank–Nicolson method). Recently well-balanced numerical methods have been proposed in [27, Part II] to discretize kinetic equations, involving so-called scattering S-matrices. Accordingly, it is quite natural to wonder how this approach may be adapted to build well-balanced numerical methods which

1. are "asymptotic preserving" (AP) within a diffusive scaling of variables?
2. lead asymptotically to an "exponential-fitting" discretization?

In this paper, we intend to give a positive answer to both these questions for three examples of kinetic equations for which an explicit form of the S-matrix is known. Let $f(t, x, v)$ be a distribution function, depending on time $t > 0$, position $x \in \mathbb{R}$, and velocity $v \in V$: we shall consider,

– a first kinetic model, in parabolic scaling, which reads

$$\varepsilon \partial_t f^\varepsilon + v \partial_x f^\varepsilon = \frac{1}{\varepsilon} \left(\int_{-1}^{1} T_\varepsilon(t, x, v') f^\varepsilon(t, x, v') \, \frac{dv'}{2} - T_\varepsilon(t, x, v) f^\varepsilon(t, x, v) \right). \tag{1.1}$$

  When $T_\varepsilon \equiv 1$, the well-known conservative radiative transfer equation is recovered, which, as $\varepsilon \to 0$, approaches the heat equation. When modeling chemotactic motions of bacteria, Eq. (1.1) is the so-called Othmer–Alt model [49]. The tumbling rate T_ε describes the response to variations of chemical concentration along a bacteria's path. When the parameter $\varepsilon \to 0$, it is now well-established that the macroscopic density $\rho := \int_{-1}^{1} f(v)\, dv$ solves the Keller–Segel system [17].

– a related model, the Vlasov–Fokker–Planck system, where the integral collision term is reduced to a diffusion operator. It reads, in parabolic scaling,

$$\varepsilon \partial_t f^\varepsilon + v \partial_x f^\varepsilon + E \cdot \partial_v f^\varepsilon = \frac{1}{\varepsilon} \partial_v \left(v f^\varepsilon + \kappa \partial_v f^\varepsilon \right). \tag{1.2}$$

  It converges, as $\varepsilon \to 0$ towards the drift-diffusion equation [48,52,60].

1.2 General strategy for building AP and WB schemes

We first define a classical discrete-ordinates (DO) setup. A spatial domain is gridded with nodes $x_j = x_0 + j\Delta x$, $j \in \mathbb{Z}$ along with a velocity domain, V, symmetric with respect to 0, by

$$v_k : k \in \{-K, \dots, -1, 1, \dots, K\}, \quad 0 < v_1 < v_2 < \dots < v_K, \quad v_{-k} = -v_k.$$

We denote

$$\mathcal{V} = (v_1, \dots, v_K)^\top \in \mathbb{R}^K, \qquad \mathbb{V} := \mathrm{diag}(v_1, \dots, v_K, v_1, \dots, v_K) \in \mathcal{M}_{2K}(\mathbb{R}).$$

Corresponding weights $(\omega_k)_{k=1,\dots,K}$ may be given by a Gauss quadrature, so

$$\int_V \phi(v)dv \text{ is approximated by } \sum_{k=1}^{K} \omega_k(\phi(v_k) + \phi(-v_k)).$$

The time step will be denoted $\Delta t > 0$.

We consider a kinetic system in parabolic scaling

$$\varepsilon\partial_t f + v\partial_x f = \frac{1}{\varepsilon}\mathcal{L}(f), \qquad t, x, v, \in \mathbb{R}_*^+ \times \mathbb{R} \times V,$$

where $\mathcal{L}$ is a linear operator, depending on the nature of the given problem. We assume that when $\varepsilon \to 0$ the macroscopic density, defined by $\rho := \int_V f(v)\,dv$, converges to a solution of a drift-diffusion kind of Eq. (1.9).

Let a discretization of the distribution function at time t^n, be $(f_j^n(\pm v_k))_{j,k}$. Our general strategy for building AP and WB schemes follows these steps.

– *1st step. Determination of the* S-matrix To build a well-balanced scheme, i.e. which preserves equilibria, it is convenient to have at hand stationary solutions. Consider the following stationary problem with incoming boundary conditions on $(0, \Delta x)$ for each $j = 1, \dots, N_x$,

$$\varepsilon v\partial_x \bar{f} = \mathcal{L}_{j-\frac{1}{2}}(\bar{f}), \quad \bar{f}(0, \mathcal{V}) = f_{j-1}(\mathcal{V}), \quad \bar{f}(\Delta x, -\mathcal{V}) = f_j(-\mathcal{V}). \tag{1.3}$$

In this system $\mathcal{L}_{j-\frac{1}{2}}$ is a discretization of $\mathcal{L}$ on (x_{j-1}, x_j) such that $\mathcal{L}_{j-\frac{1}{2}}$ is a linear operator. Notice that it is enough to solve the problem with $\varepsilon = 1$ thanks to the change of variable $x \to x/\varepsilon$. The unknwon of the problem is the function $\bar{f}$ and we want to determine the outgoing flux $\begin{pmatrix} \bar{f}(\Delta x, \mathcal{V}) \\ \bar{f}(0, -\mathcal{V}) \end{pmatrix}$. Since (1.3) is linear, the computation of the outgoing flux involves a so-called scattering matrix $\mathcal{S}^\varepsilon_{j-\frac{1}{2}}$ defined by

$$\begin{pmatrix} \bar{f}_{j-\frac{1}{2}}(\mathcal{V}) \\ \bar{f}_{j-\frac{1}{2}}(-\mathcal{V}) \end{pmatrix} := \begin{pmatrix} \bar{f}(\Delta x, \mathcal{V}) \\ \bar{f}(0, -\mathcal{V}) \end{pmatrix} = \mathcal{S}^\varepsilon_{j-\frac{1}{2}} \begin{pmatrix} f_{j-1}(\mathcal{V}) \\ f_j(-\mathcal{V}) \end{pmatrix}. \tag{1.4}$$

Several S-matrices for various kinetic models are provided in [27, Part II], including the approach based on Case's elementary solutions [1].

- *2nd step. Well-balanced scheme* Once the scattering matrix is known, one may define the well-balanced scheme as (see [28])

$$\begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V}) \end{pmatrix} = \begin{pmatrix} f_j^{n}(\mathcal{V}) \\ f_{j-1}^{n}(-\mathcal{V}) \end{pmatrix} - \frac{\Delta t}{\varepsilon \Delta x} \mathbb{V} \begin{pmatrix} f_j(\mathcal{V}) - \bar{f}_{j-\frac{1}{2}}(\mathcal{V}) \\ f_{j-1}(-\mathcal{V}) - \bar{f}_{j-\frac{1}{2}}(-\mathcal{V}) \end{pmatrix} \tag{1.5}$$

It verifies the well-balanced property, i.e. stationary states are preserved.

- *3rd step. Asymptotic preserving scheme* In order to be able to pass to the limit as $\varepsilon \to 0$ (Asymptotic-Preserving property) in (1.5), we need to treat implicitly the terms in $\frac{1}{\varepsilon}$. To do so, a crucial step is the decomposition

$$\boxed{\mathcal{S}^{\varepsilon}_{j-\frac{1}{2}} = \mathcal{S}^{0}_{j-\frac{1}{2}} + \varepsilon \mathcal{S}^{1,\varepsilon}_{j-\frac{1}{2}}.} \tag{1.6}$$

Finally, the scheme (1.5)–(1.4) becomes

$$\begin{aligned} &\begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\varepsilon \Delta x} \mathbb{V} \left[\begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V}) \end{pmatrix} - \mathcal{S}^{0}_{j-\frac{1}{2}} \begin{pmatrix} f_{j-1}^{n+1}(\mathcal{V}) \\ f_{j}^{n+1}(-\mathcal{V}) \end{pmatrix} \right] \\ &\quad = \begin{pmatrix} f_j^{n}(\mathcal{V}) \\ f_{j-1}^{n}(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\Delta x} \mathbb{V} \mathcal{S}^{1,\varepsilon}_{j-\frac{1}{2}} \begin{pmatrix} f_{j-1}^{n}(\mathcal{V}) \\ f_{j}^{n}(-\mathcal{V}) \end{pmatrix}. \end{aligned} \tag{1.7}$$

An approximation of macroscopic density is recovered thanks to the quadrature by

$$\forall j, n, \qquad \rho_j^n := \sum_{k=1}^{K} \omega_k (f_j^n(v_k) + f_j^n(-v_k)). \tag{1.8}$$

1.3 Scope and plan of the paper

An object lying at the center of our matters is the so–called "exponential-fit" (Il'in [38], Scharfetter–Gummel [55], or Chang–Cooper [19]) numerical scheme for 1D drift-diffusion equations, that we briefly recall now. Consider,

$$\partial_t \rho - \partial_x (\mathbb{D} \partial_x \rho - E\rho) = 0. \qquad 0 \le \mathbb{D}, \quad E \in \mathbb{R}. \tag{1.9}$$

This equation is discretized by means of a conservative numerical flux:

$$\frac{\rho_j^{n+1} - \rho_j^n}{\Delta t} - \frac{F^n_{j+\frac{1}{2}} - F^n_{j-\frac{1}{2}}}{\Delta x} = 0, \tag{1.10}$$

where ρ_j^n is an approximation of $\rho(t^n, x_j)$. The flux $F^n_{j-\frac{1}{2}}$ is an approximation of $J := \mathbb{D}\partial_x\rho - E\rho$ at each interface of the grid $x_{j-\frac{1}{2}}$, which is derived by taking advantage of stationary solutions (characterized by a constant flux J).

$$J = \mathbb{D}\partial_x\bar{\rho}(x) - E\,\bar{\rho}(x), \qquad \bar{\rho}(0) = \rho^n_{j-1}, \quad \bar{\rho}(\Delta x) = \rho^n_j.$$

Then, elementary calculations lead to:

$$F^n_{j-\frac{1}{2}} := J = E\,\frac{\rho^n_{j-1} - \exp(-E\,\Delta x/\mathbb{D})\,\rho^n_j}{1 - \exp(-E\,\Delta x/\mathbb{D})} \tag{1.11}$$

Scheme (1.10), (1.11) constitutes the classical Il'in/Sharfetter Gummel scheme [4,23, 38,51,53,55]. Our main result may be formulated as:

Theorem 1.1 *Let* (1.5)–(1.4) *be a numerical scheme relying on a S-matrix for any of the linear* $1+1$ *kinetic Eqs.* (1.1) *and* (1.2) *in parabolic scaling. Then, for* $0 \leq \varepsilon \ll 1$*, and uniformly in* $\Delta x > 0$*,*

- *each one, among the three considered S-matrices acting in* (1.5)–(1.4)*, admits a decomposition of the type* (1.6)*; such a decomposition yields a Well-Balanced/ Asymptotic-Preserving IMEX scheme like* (1.7)*;*
- *when* $\varepsilon \to 0$ *in the numerical scheme, the corresponding macroscopic densities satisfy the Il'In/Sharfetter–Gummel scheme* (1.10)*,* (1.11)*.*

Obviously, such a general statement contains several former ones, among which the two-stream Goldstein–Taylor model relaxing to the heat equation [33], or the so–called "Cattaneo model of chemotaxis" [25]; some of these results were surveyed in [27, Part II]. Yet, as a guideline for more involved calculations, we first explain in Sect. 2 how the limiting process works for a simple two-stream approximation of (1.1), the so–called "Greenberg-Alt" model of chemotaxis [36]. We mention that for this simple two-velocity model, a numerical scheme formulated in terms of (1.5) with 2×2 S-matrices is provided in both [27, page 158] and [34, Lemma 4.1] (for the purpose of hydrodynamic limits, though).

Another type of closely related "diffusive limit" involving a 2×2 S-matrix was studied in [30]. This elementary calculation carried out on the two-stream "Greenberg-Alt" model (2.1) reveals why it is rather natural to expect that a well-balanced algorithm (2.7) (based on stationary solutions) may relax, within a parabolic scaling, toward the exponential-fit scheme (2.4), (2.5) for the corresponding asymptotic Keller–Segel model. However, as our Theorem 1.1 covers also continuous-velocity models discretized with general quadrature rules, we present in Sect. 1.4 our strategy of proof: in particular, the general scheme involving a scattering matrix is presented in (1.5) and the importance of the decomposition of the scattering matrix (1.6) is emphasized. In Sect. 4, such a strategy is applied to the simplest case of continuous equation, namely the "grey radiative transfer" model (3.1). For this system, it is shown in Theorem 3.1 that our numerical scheme relaxes to the finite-difference discretization of the heat Eq. (3.27). In Sect. 4, the case of the Othmer–Alt [49] model of chemotaxis dynamics (4.1), (4.2) is handled in a similar manner (at the price of more intricate computations, though), yielding asymptotically the scheme (4.4), this is Theorem 4.1. At last, in Sect. 5, the case of a Vlasov–Fokker–Planck model (5.1) is studied, and its asymptotic convergence towards (5.3) is studied.

An essential difference between Vlasov–Fokker–Planck kinetic models and the ones involving an integral collision operator (3.1), (4.1) is that, being exponential polynomials, stationary solutions of (5.1) may not constitute Chebyshev T-systems on $v \in (0, +\infty)$. This drawback has to be compensated by supplementary assumptions on the set of discrete velocities, like (5.11) and (5.12). Accordingly, general properties of eigenfunctions for each of the stationary kinetic models are stated in an Appendix, along with a new result on exponential monomials. Chebyshev T-systems are recalled in Sect. A, too.

Remark 1.1 (Notations) When $u \in \mathbb{R}^N$ and $v \in \mathbb{R}^M$, the matrix $u \otimes v$ is an element of $\mathcal{M}_{N\times M}$ whose coefficients are $(u_k v_\ell)$. We will also commonly use the notation

$$\frac{1}{1+u\otimes v} \in \mathcal{M}_{N\times M}, \text{ with coefficients } \left(\frac{1}{1+u_k v_\ell}\right)_{k,\ell}.$$

The present work somehow completes the former ones [29,34,35] where hydrodynamic limits, involving finite-time concentrations, were considered; hereafter, diffusive limits yielding smooth solutions are studied, and general conclusions are identical: the schemes proposed in [27, Part II], involving S-matrices based on stationary solutions, yield more accurate discretizations of the asymptotic regime. Namely, the upwind scheme for hydrodynamic limit (instead of Lax-Friedrichs [39]), and exponential-fitting in the diffusive one.

1.4 Strategy for the proof of the main result

The aim of this paper is to prove that, at least for the kinetic systems (1.1) and (1.2) for which scattering matrices are well established, the limit as $\varepsilon \to 0$ of scheme (1.7) leads to the Il'In/Sharfetter Gummel scheme (1.10), (1.11) for the macroscopic density defined in (1.8). A first ingredient in the proof will be to establish that actually the leading order term in the decomposition (1.6) writes with $K \times K$ block matrices

$$\mathcal{S}^0_{j-\frac12} = \begin{pmatrix} \mathbf{0}_K & \mathcal{S}^0_{1,j-\frac12} \\ \mathcal{S}^0_{1,j-\frac12} & \mathbf{0}_K \end{pmatrix} \quad \text{and} \quad \mathcal{S}^{1,\varepsilon}_{j-\frac12} = \begin{pmatrix} \mathcal{S}^{1,\varepsilon}_{1,j-\frac12} & \mathcal{S}^{1,\varepsilon}_{2,j-\frac12} \\ \mathcal{S}^{1,\varepsilon}_{3,j-\frac12} & \mathcal{S}^{1,\varepsilon}_{4,j-\frac12} \end{pmatrix}.$$

Accordingly, (1.7) is recast in IMEX (IMplicit–EXplicit [9,50]) form,

$$\mathcal{R}_\varepsilon \begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_j^{n+1}(-\mathcal{V}) \end{pmatrix} = \begin{pmatrix} \varepsilon f_j^n(\mathcal{V}) \\ \varepsilon f_j^n(-\mathcal{V}) \end{pmatrix} + \frac{\varepsilon \Delta t}{\Delta x} \mathbb{V} \begin{pmatrix} S^{1,\varepsilon}_{1,j-\frac12} f^n_{j-1}(\mathcal{V}) + S^{1,\varepsilon}_{2,j-\frac12} f^n_j(-\mathcal{V}) \\ S^{1,\varepsilon}_{3,j+\frac12} f^n_j(\mathcal{V}) + S^{1,\varepsilon}_{4,j+\frac12} f^n_{j+1}(-\mathcal{V}) \end{pmatrix}, \tag{1.12}$$

for a matrix $\mathcal{R}_\varepsilon$ (which details depend on each kinetic model) given by,

$$\mathcal{R}_\varepsilon = \varepsilon \mathbf{I}_{\mathbb{R}^{2K}} + \frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} \mathbf{I}_K & -\mathcal{S}^0_{1,j-\frac{1}{2}} \\ -\mathcal{S}^0_{1,j+\frac{1}{2}} & \mathbf{I}_K \end{pmatrix} \underset{\varepsilon\to 0}{\longrightarrow} \mathcal{R}_0 := \frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} \mathbf{I}_K & -\mathcal{S}^0_{1,j-\frac{1}{2}} \\ -\mathcal{S}^0_{1,j+\frac{1}{2}} & \mathbf{I}_K \end{pmatrix}.$$

To ensure global solvability of such a scheme in the diffusive limit, we shall argue according to the analysis performed for continuous equations, see for instance [40, Chap. 5], namely by proving that:

- $\mathrm{Ker}(\mathcal{R}_0)$ is a vectorial line, closely related to Maxwellian distributions;
- its range is an hyperplane which contains all kinetic distributions with vanishing macroscopic densities (i.e. null moments of order zero).

These conditions are discrete analogues of the Fredholm alternative holding for continuous limits. Yet, we write that kinetic densities have a Hilbert expansion, $f = f^0 + \varepsilon f^1 + \cdots$. Injecting into (1.12), we first deduce by identifying the term at order 0 in ε that $f^0 \in \mathrm{Ker}(\mathcal{R}_0)$. Identifying the terms at order 1 in ε,

$$\mathcal{R}_0 \begin{pmatrix} \{f^1\}^{n+1}_j(\mathcal{V}) \\ \{f^1\}^{n+1}_j(\mathcal{V}) \end{pmatrix} = \begin{pmatrix} (\{f^0\}^n_j - \{f^0\}^{n+1}_j)(\mathcal{V}) \\ (\{f^0\}^n_j - \{f^0\}^{n+1}_j)(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} S^{1,0}_{1,j-\frac{1}{2}}\{f^0\}^n_{j-1}(\mathcal{V}) + S^{1,0}_{2,j-\frac{1}{2}}\{f^0\}^n_j(-\mathcal{V}) \\ S^{1,0}_{3,j+\frac{1}{2}}\{f^0\}^n_j(-\mathcal{V}) + S^{1,0}_{4,j+\frac{1}{2}}\{f^0\}^n_{j+1}(-\mathcal{V}) \end{pmatrix}. \tag{1.13}$$

This equation admits a solution iff the right hand side belongs to the range of $\mathcal{R}_0$. Taking moments of order zero allows us to deduce the asymptotic discretization governing the numerical macroscopic density.

To summarize, the main issues are:

- to compute the scattering matrix $\mathcal{S}$ and determine its decomposition (1.6);
- to study the kernel and the range of $\mathcal{R}_0$;
- to establish that taking the moment of order zero of (1.13) leads to Il'In/Sharfetter Gummel scheme for macroscopic density.

Finally, for future use, we recall the following result:

Lemma 1.1 (Lemma 3.1 in [13], Prop. 1 in [28]) *Let Γ be the diagonal matrix,*

$$\Gamma = \begin{pmatrix} diag(\omega_k v_k)_{k=1,\dots,K} & 0_K \\ 0_K & diag(\omega_k v_k)_{k=1,\dots,K} \end{pmatrix},$$

then, being given a nonnegative initial data $f^0_j(\pm\mathcal{V})_j$, the scheme (1.5) preserves both non-negativity and the (discrete) L^1 norm of $f^n_j(\pm\mathcal{V})$ as soon as

$$\max(\mathbb{V})\Delta t \le \varepsilon \Delta x, \quad \textit{CFL condition,} \tag{1.14}$$

$$\forall\, j, \quad \Gamma \mathcal{S}^n_{j-\frac{1}{2}} \Gamma^{-1} \text{ is left-stochastic (each column summing to 1).} \tag{1.15}$$

Moreover, it preserves its L^∞ norm as well if $\mathcal{S}^n_{j-\frac{1}{2}}$ is right-stochastic (each row summing to 1).

2 The two-stream Greenberg–Alt kinetic model

For the sake of simplicity, we first start our exposition by a very simple model consisting in a two-velocity kinetic model.

2.1 Diffusive limit of the continuous system

The simplest two-velocity kinetic model describing the motion of bacteria by chemotaxis was given in [36]. Let f^+ (f^-) be the distribution function of right-moving (left-moving) bacteria, the following system describes their motion governed by a *run and tumble* process (see also e.g. [17,20])

$$\varepsilon \partial_t f^\pm \pm \partial_x f^\pm = \pm \frac{1}{2\varepsilon}\Big(\big(1 + \varepsilon\phi(\partial_x S)\big) f^- - \big(1 - \varepsilon\phi(\partial_x S)\big) f^+ \Big). \tag{2.1}$$

The quantity S is the chemoattractant concentration, and solves

$$-\partial_{xx} S + S = \rho. \tag{2.2}$$

Macroscopic quantities being $\rho = f^+ + f^-$ (density) and $J = \frac{1}{\varepsilon}(f^+ - f^-)$ (current), adding and subtracting former equations yields,

$$\partial_t \rho + \partial_x J = 0, \qquad \varepsilon^2 \partial_t J + \partial_x \rho = \phi(\partial_x S)\rho - J.$$

Letting formally $\varepsilon \to 0$ in the second equation,

$$J = \phi(\partial_x S)\rho - \partial_x \rho,$$

and yields the well-known Keller–Segel system when coupled with (2.2),

$$\partial_t \rho - \partial_{xx}\rho + \partial_x\big(\phi(\partial_x S)\rho\big) = 0. \tag{2.3}$$

2.2 Exponential-fit scheme for Keller–Segel equation

We first recall the Il'in/Sharfetter Gummel scheme for system (2.3), which writes under the form (1.9) with $\mathbb{D} = 1$ and $E = \phi(\partial_x S)$. Assuming that approximations $(\rho_j^n)_j$ of $\rho(t^n, x_j)$ and $(S_j^n)_j$ of $S(t^n, x_j)$ are available, we denote

$$\forall j, \qquad \phi^n_{j-\frac{1}{2}} = \phi\Big(\frac{S^n_j - S^n_{j-1}}{\Delta x}\Big).$$

Then, Il'In/Sharfetter Gummel scheme (1.10), (1.11) reads, in this framework,

$$\bar{\mathcal{J}}^n_{j-\frac{1}{2}} = \frac{\phi^n_{j-\frac{1}{2}}}{1 - e^{-\phi^n_{j-\frac{1}{2}}\Delta x}}\big(\rho^n_{j-1} - e^{-\phi^n_{j-\frac{1}{2}}\Delta x}\rho^n_j\big), \tag{2.4}$$

which gives (constant) currents. Then densities are updated by,

$$\rho^{n+1}_j = \rho^n_j + \frac{\Delta t}{\Delta x}\big(\bar{\mathcal{J}}^n_{j-\frac{1}{2}} - \bar{\mathcal{J}}^n_{j+\frac{1}{2}}\big). \tag{2.5}$$

2.3 Asymptotic preserving and well-balanced scheme

We follow the strategy proposed in Sect. 1.2: assume that $(f^{n,+}_j, f^{n,-}_j)_j$ are known at time t^n, with an approximation S^n_j of $S(t^n, x_j)$, giving $\phi^n_{j-\frac{1}{2}} = \phi(\frac{S^n_j - S^n_{j-1}}{\Delta x})$.

– *1st step. Scattering matrix* It is computed by solving the stationary system in (x_{j-1}, x_j) with incoming boundary conditions,

$$\begin{cases} \partial_x \bar{f}^{\pm} = \dfrac{1}{2\varepsilon}\big((1 + \varepsilon\phi^n_{j-\frac{1}{2}})\bar{f}^- - (1 - \varepsilon\phi^n_{j-\frac{1}{2}})\bar{f}^+\big) \\ \bar{f}^+(x_{j-1}) = f^+_{j-1}; \qquad \bar{f}^-(x_j) = f^-_j. \end{cases} \tag{2.6}$$

The unknowns are interface values $\bar{f}^+_{j-\frac{1}{2}} := \bar{f}^+(x_j)$ and $\bar{f}^-_{j-\frac{1}{2}} := \bar{f}^-(x_{j-1})$. System (2.6) may be solved exactly by, first, subtracting both equations,

$$\partial_x(\bar{f}^+ - \bar{f}^-) = 0, \qquad \bar{J} := \frac{1}{\varepsilon}(\bar{f}^+ - \bar{f}^-) \text{ is constant in } (x_{j-1}, x_j).$$

and then, adding them, so that by denoting $\bar{\rho} = \bar{f}^+ + \bar{f}^-$,

$$\partial_x \bar{\rho} = \phi^n_{j-\frac{1}{2}}\bar{\rho} - \bar{J}, \qquad e^{-\phi^n_{j-\frac{1}{2}}\Delta x}\bar{\rho}_j - \bar{\rho}_{j-1} = \bar{J}\,\frac{e^{-\phi^n_{j-\frac{1}{2}}\Delta x} - 1}{\phi^n_{j-\frac{1}{2}}}.$$

Thus the system to be solved is

$$f^+_{j-1} - \bar{f}^-_{j-\frac{1}{2}} = \bar{f}^+_{j-\frac{1}{2}} - f^-_j$$

$$e^{-\phi^n_{j-\frac{1}{2}}\Delta x}(f^-_j + \bar{f}^+_{j-\frac{1}{2}}) - (f^+_{j-1} + \bar{f}^-_{j-\frac{1}{2}}) = \frac{e^{-\phi^n_{j-\frac{1}{2}}\Delta x} - 1}{\varepsilon\phi^n_{j-\frac{1}{2}}}(f^+_{j-1} - \bar{f}^-_{j-\frac{1}{2}}).$$

After easy computations,

$$\bar f^-_{j-\frac12} = f^+_{j-1} + \frac{2\varepsilon\phi^n_{j-\frac12}\left(f^+_{j-1} - e^{-\phi^n_{j-\frac12}\Delta x} f^-_j\right)}{e^{-\phi^n_{j-\frac12}\Delta x} - 1 - \varepsilon\phi^n_{j-\frac12}(1 + e^{-\phi^n_{j-\frac12}\Delta x})},$$

$$\bar f^+_{j-\frac12} = f^-_j - \frac{2\varepsilon\phi^n_{j-\frac12}\left(f^+_{j-1} - e^{-\phi^n_{j-\frac12}\Delta x} f^-_j\right)}{e^{-\phi^n_{j-\frac12}\Delta x} - 1 - \varepsilon\phi^n_{j-\frac12}(1 + e^{-\phi^n_{j-\frac12}\Delta x})}.$$

Like in [27, pp. 157–58], or [29], the latter system rewrites with an S-matrix,

$$\begin{pmatrix} \bar f^+_{j-\frac12} \\ \bar f^-_{j-\frac12} \end{pmatrix} = \mathcal{S}^n_{j-\frac12} \begin{pmatrix} f^+_{j-1} \\ f^-_j \end{pmatrix},$$

which (with shorthand notation $\mathcal{E} = e^{-\phi^n_{j-\frac12}\Delta x}$) reads

$$\mathcal{S}^n_{j-\frac12} = \begin{pmatrix} \frac{-2\varepsilon\phi^n_{j-\frac12}}{\mathcal{E}-1-\varepsilon\phi^n_{j-\frac12}(1+\mathcal{E})} & 1 + \frac{2\varepsilon\phi^n_{j-\frac12}\mathcal{E}}{\mathcal{E}-1-\varepsilon\phi^n_{j-\frac12}(1+\mathcal{E})} \\ 1 + \frac{2\varepsilon\phi^n_{j-\frac12}}{\mathcal{E}-1-\varepsilon\phi^n_{j-\frac12}(1+\mathcal{E})} & \frac{-2\varepsilon\phi^n_{j-\frac12}\mathcal{E}}{\mathcal{E}-1-\varepsilon\phi^n_{j-\frac12}(1+\mathcal{E})} \end{pmatrix}.$$

Notice that it is clearly left-stochastic.

– *2nd step. WB scheme* Following [33], we consider

$$\begin{cases} f^{+,n+1}_j = f^{+,n}_j - \frac{\Delta t}{\varepsilon\Delta x}(f^{+,n+1}_j - \bar f^+_{j-\frac12}) \\ f^{-,n+1}_{j-1} = f^{-,n}_{j-1} - \frac{\Delta t}{\varepsilon\Delta x}(f^{-,n+1}_{j-1} - \bar f^-_{j-\frac12}). \end{cases} \tag{2.7}$$

– *3rd step. AP scheme* In such a simple case, the decomposition (1.6) is:

$$\mathcal{S}^n_{j-\frac12} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + 2\varepsilon \cdot \frac{\phi^n_{j-\frac12}}{\mathcal{E} - 1 - \varepsilon\phi^n_{j-\frac12}(1 + \mathcal{E})} \begin{pmatrix} -1 & \mathcal{E} \\ 1 & -\mathcal{E} \end{pmatrix}. \tag{2.8}$$

By treating implicitly the first (stiff) term and plugging into (1.5),

$$\begin{cases} f^{+,n+1}_j = f^{+,n}_j - \frac{\Delta t}{\varepsilon\Delta x}\left(f^{+,n+1}_j - f^{-,n+1}_j\right) + \frac{\Delta t}{\Delta x}\bar J^n_{j-\frac12} \\ f^{-,n+1}_j = f^{-,n}_j - \frac{\Delta t}{\varepsilon\Delta x}\left(f^{-,n+1}_j - f^{+,n+1}_j\right) - \frac{\Delta t}{\Delta x}\bar J^n_{j+\frac12} \\ \bar J^n_{j-\frac12} = \frac{-2\phi^n_{j-\frac12}\left(f^{n,+}_{j-1} - e^{-\phi^n_{j-\frac12}\Delta x} f^{n,-}_j\right)}{e^{-\phi^n_{j-\frac12}\Delta x} - 1 - \varepsilon\phi^n_{j-\frac12}(1 + e^{-\phi^n_{j-\frac12}\Delta x})}. \end{cases} \tag{2.9}$$

The limit $\varepsilon \to 0$ is done easily by adding the first two equations in (2.9),

$$\rho_j^n = f_j^{+,n} + f_j^{-,n}, \qquad \rho_j^{n+1} = \rho_j^n - \frac{\Delta t}{\Delta x}\left(\bar{J}_{j+\frac{1}{2}}^n - \bar{J}_{j-\frac{1}{2}}^n\right). \tag{2.10}$$

Letting then $\varepsilon \to 0$, we deduce easily from (2.9) that

$$\bar{J}_{j-\frac{1}{2}}^n \to \frac{-2\phi_{j-\frac{1}{2}}^n}{e^{-\phi_{j-\frac{1}{2}}^n \Delta x} - 1}\left(f_{j-1}^{n,+} - e^{-\phi_{j-\frac{1}{2}}^n \Delta x} f_j^{n,-}\right).$$

Yet, multiplying the first equations of (2.9) by ε and letting $\varepsilon \to 0$, at the limit the relation $f_j^{+,n+1} = f_j^{-,n+1}$ is enforced. Accordingly, the current rewrites

$$\bar{J}_{j-\frac{1}{2}}^n \to \frac{-\phi_{j-\frac{1}{2}}^n}{e^{-\phi_{j-\frac{1}{2}}^n \Delta x} - 1}\left(\rho_{j-1}^n - e^{-\phi_{j-\frac{1}{2}}^n \Delta x} \rho_j^n\right). \tag{2.11}$$

Injecting (2.11) into (2.10), Il'in scheme for Keller–Segel system (2.3) is found.

Remark 2.1 All computations are explicit, so there is no real need of $\mathcal{R}_\varepsilon$ when passing to the limit. From (2.9), we get the matrix already met in [33, §3],

$$\mathcal{R}_\varepsilon = \begin{pmatrix} \varepsilon + \frac{\Delta t}{\Delta x} & -\frac{\Delta t}{\Delta x} \\ -\frac{\Delta t}{\Delta x} & \varepsilon + \frac{\Delta t}{\Delta x} \end{pmatrix} \underset{\varepsilon \to 0}{\longrightarrow} \mathcal{R}_0 = \frac{\Delta t}{\Delta x}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}.$$

Thus, $\mathrm{Ker}(\mathcal{R}_0) = \mathrm{Vect}\{(1,1)^\top\}$ and $(u,v)^\top \in \mathrm{Im}(\mathcal{R}_0)$ iff $u + v = 0$.

3 Heat equation as a diffusive limit of radiative transfer

Let us consider the kinetic model (1.1) in the simple case $T_\varepsilon \equiv 1$:

$$\varepsilon \partial_t f + v \partial_x f = \frac{1}{\varepsilon}\left(\int_{-1}^{1} f(t,x,v')\frac{dv'}{2} - f\right). \tag{3.1}$$

The macroscopic density, at the limit $\varepsilon \to 0$, satisfies the heat equation

$$\partial_t \rho - \frac{1}{3}\partial_{xx}\rho = 0, \qquad \rho(t,x) = \int_{-1}^{1} f(t,x,v)dv. \tag{3.2}$$

Equation (3.1) is usually referred to as to "gray radiative transfer"; more specific models can be drawn by replacing the uniform integral kernel $\frac{1}{2}$ by an even, nonnegative, function of the velocity variable, $0 \le \mathcal{K}(v) = \mathcal{K}(-v)$,

$$\varepsilon \partial_t f + v \partial_x f = \frac{1}{\varepsilon}\left(\mathcal{K}(v)\int_{-1}^{1} f(t,x,v')dv' - f\right), \qquad \int_{-1}^{1} \mathcal{K}(v) = 1.$$

For this system, the velocity domain being $V = (-1, 1)$, we assume that the set (ω_k, v_k) introduced in Sect. 1.2 satisfies the mild restrictions,

$$\sum_{k=1}^{K} \omega_k = 1, \qquad \sum_{k=1}^{K} \omega_k v_k^2 = \frac{1}{3}, \qquad v_{-k} = -v_k. \tag{3.3}$$

3.1 Separation of variables and the stationary problem

Let us review stationary solutions for a general nonnegative kernel T:

Proposition 3.1 *Let $\bar{f}(x, v) = \exp(-\lambda x)\phi_\lambda(v)$ be a separated-variables solution of the stationary equation*

$$v\,\partial_x \bar{f} = \int_{-1}^{1} T(v')\,\bar{f}(x, v')d\nu(v') - T(v)\,\bar{f}, \qquad v \in (-1, 1), \tag{3.4}$$

where ν is a probability measure on $(-1, 1)$. Then, we have

$$\phi_\lambda(v) = \frac{1}{T(v) - \lambda v}, \qquad \int_{-1}^{1} \frac{T(v)}{T(v) - \lambda v} d\nu(v) = 1. \tag{3.5}$$

Moreover, the following orthogonality relation holds

$$\forall \lambda \neq \mu, \quad \int_{-1}^{1} v\,\phi_\lambda(v)\phi_\mu(v)\,T(v)\,d\nu(v) = 0. \tag{3.6}$$

In particular, for $\lambda = 0$,

$$\phi_0(v) = \frac{1}{T(v)}, \qquad \forall \mu \neq 0, \quad J_\mu = \int_{-1}^{1} v\,\phi_\mu(v)\,d\nu(v) = 0.$$

The λ are usually called "eigenvalues" and corresponding ϕ_λ are "Case's eigenfunctions": see e.g. [41] for more precise definitions and functional spaces.

Remark 3.1 Under assumption (3.3) on the discrete velocity set, we may choose the measure $\nu = \frac{1}{2}\sum_{k=-K}^{K} \omega_k \delta(v - v_k)$ in this proposition. Thus, (3.6) becomes

$$\forall \lambda \neq \mu, \qquad \sum_{k=-K}^{K} \omega_k v_k \phi_\lambda(v_k)\phi_\mu(v_k)T(v_k) = 0. \tag{3.7}$$

In particular, for $\lambda = 0$,

$$\forall \mu \neq 0, \qquad \sum_{k=1}^{K} \omega_k v_k (\phi_\mu(v_k) - \phi_\mu(-v_k)) = 0. \tag{3.8}$$

Proof Inserting the ansatz $\bar{f}(x, v) = \exp(-\lambda x)\phi_\lambda(v)$ into (3.4) implies

$$(T(v) - \lambda v)\phi_\lambda(v) = \int_{-1}^{1} T(v)\phi_\lambda(v)\,d\nu(v).$$

By linearity, ϕ_λ is defined up to a constant, which is fixed by imposing

$$\int_{-1}^{1} T(v)\phi_\lambda(v)\,d\nu(v) = 1.$$

It gives the relations (3.5). Then, for two eigenvalues $\lambda \neq \mu$, we have

$$(T(v) - \lambda v)\phi_\lambda(v) = 1; \qquad (T(v) - \mu v)\phi_\mu(v) = 1.$$

We multiply the first identity by $T(v)\phi_\mu(v)$, the second by $T(v)\phi_\lambda(v)$, and integrate over $d\nu(v)$, we obtain after subtracting the resulting identities

$$(\lambda - \mu)\int_{-1}^{1} v\phi_\lambda(v)\phi_\mu(v)T(v)\,d\nu(v) = 0.$$

We deduce the orthogonality relation in (3.6). □

3.2 The scattering matrix and its decomposition (1.6)

Following the strategy proposed in Sect. 1.2, we first determine the scattering matrix and its expansion (1.6). The stationary problem with incoming boundary data reads,

$$\varepsilon v \partial_x \bar{f} = \frac{1}{2}\int_{-1}^{1} \bar{f}(v')dv' - \bar{f}, \qquad \text{on } (0, \Delta x), \tag{3.9}$$

$$\bar{f}(0, v) = f_{j-1}(v), \qquad \bar{f}(\Delta x, -v) = f_j(-v), \tag{3.10}$$

where $\big(f_{j-1}(|v|), f_j(-|v|)\big)$ are "incoming values", and outgoing ones read:

$$\bar{f}_{j-\frac{1}{2}}(|v|) = \bar{f}(\Delta x, |v|), \quad \bar{f}_{j-\frac{1}{2}}(-|v|) = \bar{f}(0, -|v|).$$

In view of Proposition 3.1, Eq. (3.5) in the particular case $T = 1$, the discrete eigenelements are given by

$$\frac{1}{2}\sum_{k=1}^{K}\omega_k\left(\frac{1}{1-\lambda v_k} + \frac{1}{1+\lambda v_k}\right) = 1, \qquad \phi_\lambda(v) = \frac{1}{1-\lambda v}.$$

Clearly, we have that if λ is an eigenvalue, then $-\lambda$ is also an eigenvalue and $\phi_{-\lambda}(v) = \phi_\lambda(-v)$. We observe also that the eigenvalue $\lambda = 0$ is double; the eigenvectors are

1 and $x - \varepsilon v$. [Indeed we verify easily that such functions solve (3.9)]. Therefore, a quite general stationary solution is obtained by truncating to the first $2K$ eigenmodes, (see e.g. [1,14,27])

$$\bar{f}(x,v) = a_0 + b_0(x - \varepsilon v) + \sum_{\ell=1}^{K-1} \left(\frac{a_\ell\, e^{-\lambda_\ell x/\varepsilon}}{1 - \lambda_\ell\, v} + \frac{b_\ell\, e^{\lambda_\ell (x-\Delta x)/\varepsilon}}{1 + \lambda_\ell\, v} \right), \quad \lambda_\ell \geq 0.$$

We denote the vector of so–called "normal modes", $0 \leq \lambda := (\lambda_1, \ldots, \lambda_{K-1})^\top$, and the matrix of "Case's eigenfunction"

$$\Phi^\pm(x) = \left(\frac{e^{-\lambda\, x/\varepsilon}}{1 \mp \mathcal{V} \otimes \lambda}\ \mathbf{1}_{\mathbb{R}^K}\ \frac{e^{\lambda\,(x-\Delta x)/\varepsilon}}{1 \pm \mathcal{V} \otimes \lambda}\ x\mathbf{1}_{\mathbb{R}^K} \mp \varepsilon\mathcal{V} \right) \in \mathcal{M}_{K\times 2K}(\mathbb{R}),$$

such that $\bar{f}(x, \pm\mathcal{V}) = \Phi^\pm(x) \begin{pmatrix} a \\ b \end{pmatrix}$, with the notations $a = (a_1, \ldots, a_{K-1}, a_0)^\top$ and $b = (b_1, \ldots, b_{K-1}, b_0)^\top$. (We recall that the notation $\frac{1}{1+\mathcal{V}\otimes\lambda}$ denotes the matrix in $\mathcal{M}_K(\mathbb{R})$ whose coefficients are $(\frac{1}{1+v_k\lambda_\ell})_{k,\ell}$). Thanks to the boundary conditions (3.10)

$$\begin{pmatrix} \bar{f}(0,\mathcal{V}) \\ \bar{f}(\Delta x, -\mathcal{V}) \end{pmatrix} = \begin{pmatrix} \Phi^+(0) \\ \Phi^-(\Delta x) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}, \qquad \begin{pmatrix} \bar{f}(\Delta x,\mathcal{V}) \\ \bar{f}(0, -\mathcal{V}) \end{pmatrix} = \begin{pmatrix} \Phi^+(\Delta x) \\ \Phi^-(0) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}.$$

Thus, (see also [27, Chap. 9 pp. 175–176]), the solution of (3.9), (3.10) is,

$$\begin{pmatrix} \bar{f}_{j-\frac{1}{2}}(\mathcal{V}) \\ \bar{f}_{j-\frac{1}{2}}(-\mathcal{V}) \end{pmatrix} = \widetilde{M}_\varepsilon M_\varepsilon^{-1} \begin{pmatrix} f_{j-1}(\mathcal{V}) \\ f_j(-\mathcal{V}) \end{pmatrix},$$

where

$$\widetilde{M}_\varepsilon := \begin{pmatrix} \Phi^+(\Delta x) \\ \Phi^-(0) \end{pmatrix} = \begin{pmatrix} \frac{e^{-\lambda\,\Delta x/\varepsilon}}{1-\mathcal{V}\otimes\lambda} & \mathbf{1}_{\mathbb{R}^K} & \frac{1}{1+\mathcal{V}\otimes\lambda} & \Delta x\mathbf{1}_{\mathbb{R}^K} - \varepsilon\mathcal{V} \\ \frac{1}{1+\mathcal{V}\otimes\lambda} & \mathbf{1}_{\mathbb{R}^K} & \frac{e^{-\lambda\,\Delta x/\varepsilon}}{1-\mathcal{V}\otimes\lambda} & \varepsilon\mathcal{V} \end{pmatrix}, \tag{3.11}$$

$$M_\varepsilon := \begin{pmatrix} \Phi^+(0) \\ \Phi^-(\Delta x) \end{pmatrix} = \begin{pmatrix} \frac{1}{1-\mathcal{V}\otimes\lambda} & \mathbf{1}_{\mathbb{R}^K} & \frac{e^{-\lambda\,\Delta x/\varepsilon}}{1+\mathcal{V}\otimes\lambda} & -\varepsilon\mathcal{V} \\ \frac{e^{-\lambda\,\Delta x/\varepsilon}}{1+\mathcal{V}\otimes\lambda} & \mathbf{1}_{\mathbb{R}^K} & \frac{1}{1-\mathcal{V}\otimes\lambda} & \Delta x\mathbf{1}_{\mathbb{R}^K} + \varepsilon\mathcal{V} \end{pmatrix}. \tag{3.12}$$

Thus we have obtained the first statement of the following Proposition:

Proposition 3.2 *The scattering matrix for radiative transfer system is:*

$$\mathcal{S}^\varepsilon = \widetilde{M}_\varepsilon M_\varepsilon^{-1}, \qquad \textit{(independent of } j\textit{)} \tag{3.13}$$

where $\widetilde{M}_\varepsilon$ *and* M_ε *are given in* (3.11), (3.12). *It admits the decomposition*

$$\boxed{\mathcal{S}^\varepsilon = \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K - \zeta\gamma \\ \mathbf{I}_K - \zeta\gamma & \mathbf{0}_K \end{pmatrix} + \varepsilon B_\varepsilon, \ \textit{where}\ B_\varepsilon := \frac{1}{\varepsilon}(A_\varepsilon M_\varepsilon^{-1} - A_0 M_0^{-1}),} \tag{3.14}$$

with $A_\varepsilon = \widetilde{M}_\varepsilon - \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K \\ \mathbf{I}_K & \mathbf{0}_K \end{pmatrix} M_\varepsilon$, *(where* $\mathbf{I}_K, \mathbf{0}_K$ *are* $K \times K$ *identity and null matrices, respectively, and* $\mathbf{0}_{\mathbb{R}^K}, \mathbf{1}_{\mathbb{R}^K}$ *are* $\mathbb{R}^K$ *vectors of zeros and ones)*

$$\zeta = \left(\frac{1}{1 - \mathcal{V} \otimes \lambda}\right) - \left(\frac{1}{1 + \mathcal{V} \otimes \lambda}\right) \in \mathcal{M}_{K \times K-1}(\mathbb{R}),$$

and $\gamma \in \mathcal{M}_{K-1 \times K}(\mathbb{R})$, $\beta^\top \in \mathbb{R}^K$ *are such that*

$$\gamma \left(\frac{1}{1 - \mathcal{V} \otimes \lambda}\right) = \mathbf{I}_{K-1}, \qquad \gamma \mathbf{1}_{\mathbb{R}^K} = \mathbf{0}_{\mathbb{R}^{K-1}}, \tag{3.15}$$

$$\beta^\top \left(\frac{1}{1 - \mathcal{V} \otimes \lambda}\right) = \mathbf{0}^\top_{\mathbb{R}^{K-1}}, \qquad \beta^\top \mathbf{1}_{\mathbb{R}^K} = 1. \tag{3.16}$$

Remark 3.2 The existence of γ and β is provided by Proposition B.1 (iii) in Appendix. It's good to have an "intuitive idea" of the nature of ζ, γ and β:

- First, $\zeta : \mathbb{R}^{K-1} \to \mathbb{R}^K$ converts a set of $K - 1$ spectral coefficients into the restriction to $v \in \mathcal{V}$ of a kinetic density $F(v)$ having a specific property,

$$\forall v_k \in \mathcal{V}, \qquad F(v_k) = -F(-v_k), \quad \text{so} \quad \sum_{k=1}^{K} \omega_k (F(v_k) + F(-v_k)) = 0.$$

- Then, $\gamma : \mathbb{R}^K \to \mathbb{R}^{K-1}$ recovers $K - 1$ spectral coefficients corresponding to "damped modes" (Knudsen layers) out of K samples of any kinetic density $F(v_k)$. More precisely, if we consider a given steady kinetic density,

$$\forall v_k \in \mathcal{V}, \qquad G(v_k) = a_0 + \sum_{\ell=1}^{K-1} \frac{a_\ell}{1 - v_k \lambda_\ell},$$

  then $\gamma\,[G(\mathcal{V})] = (a_1, a_2, \ldots, a_{K-1})$: this is meaningful for $\varepsilon \ll 1$.
- Oppositely, β detects the "Maxwellian part" in the decomposition of G, that is, the a_0 coefficient, so that $\beta^\top\,[G(\mathcal{V})] = a_0$.

Yet, consider the product $\zeta\gamma : \mathbb{R}^K \to \mathbb{R}^K$, applied to $G(\mathcal{V})$. It produces,

$$(\zeta\gamma[G])(v_k) = \sum_{\ell=1}^{K-1} a_\ell \left(\frac{1}{1 - v_k \lambda_\ell} - \frac{1}{1 + v_k \lambda_\ell}\right), \qquad k = 1, \ldots, K,$$

so that,

$$\forall v_k \in \mathcal{V}, \qquad \big(\mathbf{I}_K - (\zeta\gamma)\big)[G](v_k) = a_0 + \sum_{\ell=1}^{K-1} \frac{a_\ell}{1 + v_k \lambda_\ell}.$$

Proof 1. Based on the simple case (2.8), we define A^ε such that,

$$\forall \varepsilon > 0, \qquad \mathcal{S}^\varepsilon = \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K \\ \mathbf{I}_K & \mathbf{0}_K \end{pmatrix} + A_\varepsilon M_\varepsilon^{-1},$$

which clearly yields:

$$A_\varepsilon = \widetilde{M}_\varepsilon - \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K \\ \mathbf{I}_K & \mathbf{0}_K \end{pmatrix} M_\varepsilon = \begin{pmatrix} \zeta e^{-\lambda\,\Delta x/\varepsilon} & \mathbf{0}_{\mathbb{R}^K} & -\zeta & -2\mathcal{V}\varepsilon \\ -\zeta & \mathbf{0}_{\mathbb{R}^K} & \zeta e^{-\lambda\,\Delta x/\varepsilon} & 2\mathcal{V}\varepsilon \end{pmatrix},$$

As $\varepsilon \to 0$,

$$A_\varepsilon \to A_0 = \begin{pmatrix} \mathbf{0}_K & (-\zeta \quad \mathbf{0}_{\mathbb{R}^K}) \\ (-\zeta \quad \mathbf{0}_{\mathbb{R}^K}) & \mathbf{0}_K \end{pmatrix}, \tag{3.17}$$

along with,

$$\begin{aligned} M_\varepsilon \to M_0 &= \begin{pmatrix} \frac{1}{1-\mathcal{V}\otimes\lambda} & \mathbf{1}_{\mathbb{R}^K} & \mathbf{0}_{K\times(K-1)} & \mathbf{0}_K \\ \mathbf{0}_{K\times(K-1)} & \mathbf{1}_{\mathbb{R}^K} & \frac{1}{1-\mathcal{V}\otimes\lambda} & \Delta x \mathbf{1}_{\mathbb{R}^K} \end{pmatrix} \\ &:= \begin{pmatrix} M_{01} & \mathbf{0}_K \\ (\mathbf{0}_{K\times(K-1)} \quad \mathbf{1}_{\mathbb{R}^K}) & M_{02} \end{pmatrix}, \end{aligned}$$

with the notation

$$M_{01} = \begin{pmatrix} \frac{1}{1-\mathcal{V}\otimes\lambda} & \mathbf{1}_{\mathbb{R}^K} \end{pmatrix}, \qquad M_{02} = \begin{pmatrix} \frac{1}{1-\mathcal{V}\otimes\lambda} & \Delta x\, \mathbf{1}_{\mathbb{R}^K} \end{pmatrix}.$$

2. We now intend to compute the following inverse,

$$M_0^{-1} = \begin{pmatrix} M_{01}^{-1} & \mathbf{0}_K \\ -M_{02}^{-1}(\mathbf{0}_{K\times(K-1)} \quad \mathbf{1}_{\mathbb{R}^K})M_{01}^{-1} & M_{02}^{-1} \end{pmatrix}, \tag{3.18}$$

where

$$M_{01}^{-1} = \begin{pmatrix} \gamma \\ \beta^\top \end{pmatrix} \in \mathcal{M}_K(\mathbb{R}), \qquad M_{02}^{-1} = \begin{pmatrix} \gamma \\ \frac{1}{\Delta x}\beta^\top \end{pmatrix} \in \mathcal{M}_K(\mathbb{R}),$$

being γ a matrix of size $(K-1) \times K$ and β an element in $\mathbb{R}^K$, such that (3.15) and (3.16) hold. From the expression (3.17) and (3.18), it comes:

$$A_0 M_0^{-1} = \begin{pmatrix} (-\zeta \quad \mathbf{0}_{\mathbb{R}^K})M_{02}^{-1}(\mathbf{0}_{K\times(K-1)} \quad \mathbf{1}_{\mathbb{R}^K})M_{01}^{-1} & (-\zeta \quad \mathbf{0}_{\mathbb{R}^K})M_{02}^{-1} \\ (-\zeta \quad \mathbf{0}_{\mathbb{R}^K})M_{01}^{-1} & \mathbf{0}_K \end{pmatrix}$$

– We first observe that

$$(-\zeta \quad \mathbf{0}_{\mathbb{R}^K})\begin{pmatrix} \gamma \\ \beta^\top \end{pmatrix} = (-\zeta \quad \mathbf{0}_{\mathbb{R}^K})\begin{pmatrix} \gamma \\ \frac{1}{\Delta x}\beta^\top \end{pmatrix} = -\zeta\gamma.$$

– Then, using the second identity in (3.15),

$$A_0 M_0^{-1} = \begin{pmatrix} \mathbf{0}_K & -\zeta\gamma \\ -\zeta\gamma & \mathbf{0}_K \end{pmatrix}.$$

Finally, we reach the decomposition (3.14). □

Lemma 3.1 *With identical notation as Proposition 3.2, as $\varepsilon \to 0$,*

$$B_\varepsilon = \frac{1}{\Delta x} \begin{pmatrix} (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top & -(2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \\ -(2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top & (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \end{pmatrix} + o(1). \tag{3.19}$$

Proof From (3.14), and using the form,

$$M_\varepsilon = M_0 + \begin{pmatrix} \mathbf{0}_{K\times(K-1)} & \mathbf{0}_{\mathbb{R}^K} & \frac{e^{-\lambda\,\Delta x/\varepsilon}}{1+\mathcal{V}\otimes\lambda} & -\varepsilon\mathcal{V} \\ \frac{e^{-\lambda\,\Delta x/\varepsilon}}{1+\mathcal{V}\otimes\lambda} & \mathbf{0}_{\mathbb{R}^K} & \mathbf{0}_{K\times(K-1)} & \varepsilon\mathcal{V} \end{pmatrix},$$

we get

$$\begin{aligned} B_\varepsilon &= \frac{1}{\varepsilon}(A_\varepsilon - A_0 M_0^{-1} M_\varepsilon) M_\varepsilon^{-1} \\ &= \frac{1}{\varepsilon}(A_\varepsilon - A_0) M_\varepsilon^{-1} \\ &\quad + \begin{pmatrix} \zeta\gamma(\frac{1}{1+\mathcal{V}\otimes\lambda})\delta_\varepsilon & \mathbf{0}_{\mathbb{R}^K} & \mathbf{0}_{K\times(K-1)} & \zeta\gamma\mathcal{V} \\ \mathbf{0}_K & & \zeta\gamma(\frac{1}{1+\mathcal{V}\otimes\lambda})\delta_\varepsilon & -\zeta\gamma\mathcal{V} \end{pmatrix} M_\varepsilon^{-1}, \end{aligned}$$

where $\delta_\varepsilon = \frac{1}{\varepsilon} e^{-\lambda\,\Delta x/\varepsilon} \to 0$ as $\varepsilon \to 0$. Then,

$$B_\varepsilon = \begin{pmatrix} \zeta\delta_\varepsilon + \zeta\gamma(\frac{1}{1+\mathcal{V}\otimes\lambda})\delta_\varepsilon & \mathbf{0}_{\mathbb{R}^K} & \mathbf{0}_{K\times(K-1)} & (-2\mathbf{I}_K + \zeta\gamma)\mathcal{V} \\ \mathbf{0}_{K\times(K-1)} & \mathbf{0}_{\mathbb{R}^K} & \zeta\delta_\varepsilon + \zeta\gamma(\frac{1}{1+\mathcal{V}\otimes\lambda})\delta_\varepsilon & (2\mathbf{I}_K - \zeta\gamma)\mathcal{V} \end{pmatrix} M_\varepsilon^{-1}. \tag{3.20}$$

As $\varepsilon \to 0$, we get from (3.20)

$$B_\varepsilon = \frac{1}{\varepsilon}(A_\varepsilon M_\varepsilon^{-1} - A_0 M_0^{-1}) \underset{\varepsilon\to 0}{\longrightarrow} B_0 := \begin{pmatrix} \mathbf{0}_{K\times(2K-1)} & (-2\mathbf{I}_K + \zeta\gamma)\mathcal{V} \\ \mathbf{0}_{K\times(2K-1)} & (2\mathbf{I}_K - \zeta\gamma)\mathcal{V} \end{pmatrix} M_0^{-1}.$$

With the expression of the inverse of M_0 in (3.18), we get

$$B_0 = \frac{1}{\Delta x} \begin{pmatrix} (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \mathbf{1}_{\mathbb{R}^K}\beta^\top & -(2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \\ -(2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \mathbf{1}_{\mathbb{R}^K}\beta^\top & (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \end{pmatrix}.$$

Thanks to (3.16), we have $\beta^\top \mathbf{1}_{\mathbb{R}^K} = 1$ and we are done. □

3.3 Emergence of the macroscopic discretization

Thanks to Proposition 3.2, we have at hand the expansion of the scattering matrix with respect to ε; then, the final scheme (1.7) for the radiative transfer equation is,

$$\begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\varepsilon \Delta x} \mathbb{V} \begin{pmatrix} f_j^{n+1}(\mathcal{V}) - (\mathbf{I}_K - \zeta\gamma) f_j^{n+1}(-\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V}) - (\mathbf{I}_K - \zeta\gamma) f_{j-1}^{n+1}(\mathcal{V}) \end{pmatrix}$$
$$= \begin{pmatrix} f_j^{n}(\mathcal{V}) \\ f_{j-1}^{n}(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\Delta x} \mathbb{V} B_\varepsilon \begin{pmatrix} f_{j-1}^{n}(\mathcal{V}) \\ f_{j}^{n}(-\mathcal{V}) \end{pmatrix}. \tag{3.21}$$

We are now in position to state our main result for the radiative transfer equation, whose proof is postponed to the next subsection.

Theorem 3.1 *The scheme (3.21) for the radiative transfer Eq. (3.1) is well-balanced and asymptotic-preserving (AP) with respect to ε. Moreover, assuming (3.3) holds, when $\varepsilon \to 0$, the macroscopic density $\rho_j^n := \sum_{k=-K}^{K} \omega_k f_j^n(v_k)$ solves the centered finite difference scheme for the heat Eq. (3.2).*

As noticed in Sect. 1.4, we may rewrite (3.21) in IMEX form [see (1.12)],

$$\frac{1}{\varepsilon}\mathcal{R}_\varepsilon \begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_j^{n+1}(-\mathcal{V}) \end{pmatrix} = \begin{pmatrix} f_j^{n}(\mathcal{V}) \\ f_j^{n}(-\mathcal{V})) \end{pmatrix} + \frac{\Delta t}{\Delta x} \mathbb{V} \begin{pmatrix} B_{1\varepsilon} f_{j-1}^n(\mathcal{V}) + B_{2\varepsilon} f_j^n(-\mathcal{V}) \\ B_{3\varepsilon} f_j^n(\mathcal{V}) + B_{4\varepsilon} f_{j+1}^n(-\mathcal{V}) \end{pmatrix}, \tag{3.22}$$

where we use the notation $B_\varepsilon = \begin{pmatrix} B_{1\varepsilon} & B_{2\varepsilon} \\ B_{3\varepsilon} & B_{4\varepsilon} \end{pmatrix}$, and

$$\mathcal{R}_\varepsilon = \varepsilon \mathbf{I}_{2K} + \frac{\Delta t}{\Delta x} \mathbb{V} \begin{pmatrix} \mathbf{I}_K & \zeta\gamma - \mathbf{I}_K \\ \zeta\gamma - \mathbf{I}_K & \mathbf{I}_K \end{pmatrix}. \tag{3.23}$$

Solving this system amounts to the inversion of matrix $\mathcal{R}_\varepsilon$. By construction, this scheme satisfies the well-balanced property and is asymptotic preserving.

Proposition 3.3 *Assume that for all discrete eigenvalues λ_i, $i = 1, \dots, K-1$, identity (3.8) holds, i.e.*

$$\sum_{k=1}^{K} \omega_k v_k \left(\frac{1}{1 - v_k \lambda_i} - \frac{1}{1 + v_k \lambda_i} \right) = 0.$$

Then the scheme (3.22) is mass-preserving, uniformly when $\varepsilon \ll 1$.

Proof It is mostly a consequence of Lemma 1.1 and Proposition 3.2. Indeed, by Lemma 1.1, $\Gamma \mathcal{S}^\varepsilon \Gamma^{-1}$ needs to be left stochastic for any $\varepsilon > 0$, which implies (by Proposition 3.2) that, for $\varepsilon \ll 1$, the matrix

$$\Gamma \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K - \zeta\gamma \\ \mathbf{I}_K - \zeta\gamma & \mathbf{0}_K \end{pmatrix} \Gamma^{-1} \quad \text{is left stochastic.}$$

Hence, for all $j = 1, \dots, K$, the sum of the jth column is equal to 1, that is $\sum_{k=1}^{K} \omega_k v_k (\zeta\gamma)_{kj} = 0$. Accordingly, it comes (by general assumptions) that,

$$\sum_{k=1}^{K} \omega_k v_k (\zeta\gamma)_{kj} = \sum_{k=1}^{K} \sum_{i=1}^{K-1} \omega_k v_k \left(\frac{1}{1 - v_k \lambda_i} - \frac{1}{1 + v_k \lambda_i} \right) \gamma_{ij} = 0. \qquad \square$$

3.4 Consistency with the diffusive limit

This subsection is devoted to the proof of Theorem 3.1.

Proof of Theorem 3.1 When $\varepsilon \to 0$, we get from (3.20)

$$B_\varepsilon \longrightarrow B_0 = \frac{1}{\Delta x} \begin{pmatrix} (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top & -(2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \\ -(2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top & (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top \end{pmatrix}.$$

Moreover, with (3.23),

$$\mathcal{R}_\varepsilon = \mathcal{R}_0 + \varepsilon \mathbf{I}_{2K}, \quad \text{where } \mathcal{R}_0 := \frac{\Delta t}{\Delta x} \mathbb{V} \begin{pmatrix} \mathbf{I}_K & \zeta\gamma - \mathbf{I}_K \\ \zeta\gamma - \mathbf{I}_K & \mathbf{I}_K \end{pmatrix}.$$

Assuming that f admits a Hilbert expansion $f = f^0 + \varepsilon f^1 + o(\varepsilon)$. We inject into scheme (3.22). Then by identifying the term in power of ε, we get

$$\mathcal{R}_0 \begin{pmatrix} \{f^0\}_j^{n+1}(\mathcal{V}) \\ \{f^0\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} = 0, \tag{3.24}$$

and at order 0 in ε,

$$\begin{aligned} \mathcal{R}_0 \begin{pmatrix} \{f^1\}_j^{n+1}(\mathcal{V}) \\ \{f^1\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} &= \begin{pmatrix} \{f^0\}_j^{n}(\mathcal{V}) - \{f^0\}_j^{n+1}(\mathcal{V}) \\ \{f^0\}_j^{n}(-\mathcal{V}) - \{f^0\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} \\ &\quad + \frac{\Delta t}{\Delta x^2} \mathbb{V} \begin{pmatrix} (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top (\{f^0\}_{j-1}^{n}(\mathcal{V}) - \{f^0\}_j^{n}(-\mathcal{V})) \\ (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}\beta^\top (\{f^0\}_{j+1}^{n}(\mathcal{V}) - \{f^0\}_j^{n}(-\mathcal{V})) \end{pmatrix}. \end{aligned} \tag{3.25}$$

We will make use of Lemma B.1 in the Appendix, which may be applied with $\mu = \lambda$ since (3.8) holds, it gives:

- $\mathrm{Ker}(\mathcal{R}_0) = \mathrm{Span}(\mathbf{1}_{\mathbb{R}^{2K}})$,
- $\mathrm{Im}(\mathcal{R}_0) = \left\{ Z = (Z_1\ Z_2)^\top,\ Z_i \in \mathbb{R}^K \text{ such that } \sum_{k=1}^{K} \omega_k (Z_{1k} + Z_{2k}) = 0 \right\}$.

Roughly speaking, the range of $\mathcal{R}_0$ is an hyperplane containing kinetic densities which moment of order zero vanishes. Its kernel is the (one-dimensional) vectorial line of constant kinetic densities, which are the Maxwellians for (3.1). We deduce from (3.24)

$$\{f^0\}_j^{n+1}(\pm\mathcal{V}) = \frac{\rho_j^{n+1}}{2}\mathbf{1}_{\mathbb{R}^K}, \qquad \rho_j^n = \sum_{k=1}^{K}\omega_k(f_j^n(v_k) + f_j^n(-v_k)). \tag{3.26}$$

Then, injecting (3.26) into (3.25) and using (3.16), we obtain

$$\mathcal{R}_0\begin{pmatrix}\{f^1\}_j^{n+1}(\mathcal{V})\\ \{f^1\}_j^{n+1}(-\mathcal{V})\end{pmatrix} = \frac{1}{2}\begin{pmatrix}(\rho_j^n - \rho_j^{n+1})\mathbf{1}_{\mathbb{R}^K}\\ (\rho_j^n - \rho_j^{n+1})\mathbf{1}_{\mathbb{R}^K}\end{pmatrix} + \frac{\Delta t}{2\Delta x^2}\mathbb{V}\begin{pmatrix}(2\mathbf{I}_K - \zeta\gamma)\mathcal{V}(\rho_{j-1}^n - \rho_j^n)\\ (2\mathbf{I}_K - \zeta\gamma)\mathcal{V}(\rho_{j+1}^n - \rho_j^n)\end{pmatrix}.$$

Moreover, by definition of $\mathcal{R}_0$, we have

$$\frac{1}{2\Delta x}\mathcal{R}_0\begin{pmatrix}\mathcal{V}(\rho_{j+1}^n - \rho_j^n)\\ \mathcal{V}(\rho_{j-1}^n - \rho_j^n)\end{pmatrix} = \frac{\Delta t}{2\Delta x^2}\mathbb{V}\begin{pmatrix}\mathcal{V}(\rho_{j+1}^n - \rho_j^n) + (\zeta\gamma - \mathbf{I}_K)\mathcal{V}(\rho_{j-1}^n - \rho_j^n)\\ (\zeta\gamma - \mathbf{I}_K)\mathcal{V}(\rho_{j+1}^n - \rho_j^n) + \mathcal{V}(\rho_{j-1}^n - \rho_j^n)\end{pmatrix}.$$

Therefore, adding the last two equalities, we deduce that

$$\mathcal{R}_0\begin{pmatrix}\{f^1\}_j^{n+1}(\mathcal{V}) + \frac{1}{2\Delta x}\mathcal{V}(\rho_{j+1}^n - \rho_j^n)\\ \{f^1\}_j^{n+1}(-\mathcal{V}) + \frac{1}{2\Delta x}\mathcal{V}(\rho_{j-1}^n - \rho_j^n)\end{pmatrix} = \frac{1}{2}(\rho_j^n - \rho_j^{n+1})\mathbf{1}_{\mathbb{R}^{2K}} + \frac{\Delta t}{2\Delta x^2}\mathbb{V}^2(\rho_{j+1}^n + \rho_{j-1}^n - 2\rho_j^n).$$

A solution exists iff the right hand side belongs to $\mathrm{Im}(\mathcal{R}_0)$, so by Lemma B.1,

$$\boxed{0 = \rho_j^n - \rho_j^{n+1} + \frac{\Delta t}{\Delta x^2}(\rho_{j-1}^n - 2\rho_j^n + \rho_{j+1}^n)\sum_{k=1}^{K}\omega_k v_k^2.} \tag{3.27}$$

We conclude the proof thanks to (3.3). □

3.5 A preliminary numerical validation

The IMEX scheme (1.7) was implemented on the following simple practical problem for various values of the relaxation parameter $\varepsilon > 0$, along with a fixed meshsize of $\Delta x = 8/2^8 = 2^{-5}$, a time-step obeying a parabolic CFL restriction $\Delta t = \Delta x^2$, and a Gaussian quadrature for which $K = 4$. The initial data was chosen to be a sum of two Gaussian distributions,

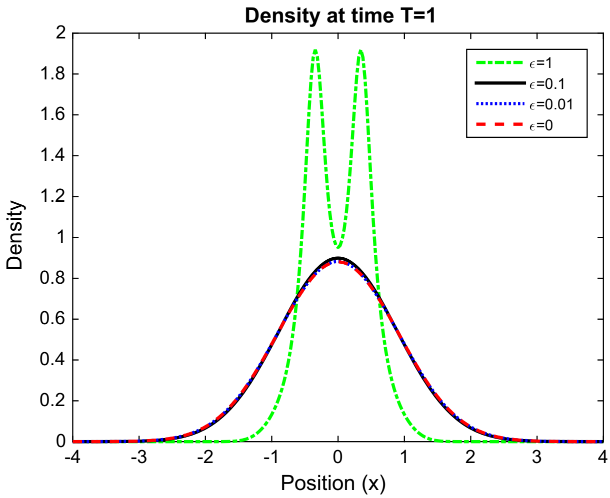

Fig. 1 Comparison between (1.7) and a centered discretization (3.27) of the heat equation

$$\partial_t f^\varepsilon + \frac{v}{\varepsilon}\partial_x f^\varepsilon = \frac{1}{\varepsilon^2}\left(\frac{1}{2}\int_{-1}^{1} f^\varepsilon(t,x,v')dv' - f^\varepsilon\right), \quad v \in (-1,1),$$
$$f^\varepsilon(t=0,x,v) = 10\,e^{-20v^2}\left(e^{-50(x+0.35)^2} + e^{-50(x-0.35)^2}\right).$$

Numerical results on its macroscopic density variable, $\rho^\varepsilon(t,x)$ are displayed on Fig. 1. In this figure, the limiting system (for $\varepsilon = 0$) is solved directly with the scheme (3.27). The IMEX scheme (1.7) is shown to be reliable by producing a non-oscillatory approximation of the moment of order zero of the kinetic density f, which moreover is asymptotically consistent with its diffusion limit.

4 Othmer–Alt model for one-dimensional chemotaxis

4.1 Continuous diffusive limit toward Keller–Segel

We consider now a model of chemotaxis in parabolic scaling, (see also [21])

$$\varepsilon\partial_t f + v\partial_x f = \frac{1}{\varepsilon}\left(\int_V T_\varepsilon(t,x,v')f(t,x,v')\,\frac{dv'}{2} - T_\varepsilon(t,x,v)f(t,x,v)\right). \quad (4.1)$$

The tumbling rate T_ε describes the response to variations of chemical concentration along the path of bacteria. Among several choices [13,49], we choose, (see [27, sect 10.4])

$$T_\varepsilon(t,x,v) = 1 + \varepsilon\phi\big(v\partial_x S(t,x)\big), \quad \phi \text{ an odd function.} \quad (4.2)$$

In applications, the quantity S models the concentration of the chemoattractant which is released by bacteria themselves. It is then computed thanks to an elliptic/parabolic equation depending on the density of bacteria. Since we only focus on the diffusive limit of the kinetic system, we will consider that S is given, which boils down, from a numerical point of view, to treat explicitely in time the equation for S.

Formally, the limit $\varepsilon \to 0$ may be obtained easily by performing a Hilbert expansion, $f = f^0 + \varepsilon f^1 + \cdots$, equating each term in power of ε in (4.1),

$$f^0 = \frac{1}{2}\rho^0, \qquad \rho^0 = \int_V f^0(v)\,dv;$$
$$f^1 - \frac{1}{2}\int_V f^1(v')\,dv' = \frac{1}{2}\int_V \phi(v'\partial_x S) f_0(v')\,dv' - \phi(v\partial_x S) f_0 - v\partial_x f^0.$$

Since ϕ is odd, $V = (-1, 1)$ is symmetric and f^0 is independent of v, the first term of the right hand side vanishes. By conservation, we have

$$\partial_t \int_V f^0(v)\,dv + \partial_x \int_V v f^1(v)\,dv = 0.$$

Along with the expressions of f^0 and f^1,

$$\partial_t \rho^0 - \partial_x \left(\frac{1}{3}\partial_x \rho^0 + E\rho^0\right) = 0, \qquad E = \frac{1}{2}\int_V v\phi(v\partial_x S)\,dv. \tag{4.3}$$

Sharfetter–Gummel scheme

The Il'in/Sharfetter–Gummel scheme (1.10), (1.11) for this latter equation is

$$\rho_j^{n+1} = \rho_j^n + \frac{\Delta t}{\Delta x}\left(\bar{\mathcal{J}}_{j-\frac{1}{2}}^n - \bar{\mathcal{J}}_{j+\frac{1}{2}}^n\right), \quad \bar{\mathcal{J}}_{j-\frac{1}{2}}^n = E_{j-\frac{1}{2}} \frac{e^{3E_{j-\frac{1}{2}}\Delta x}\rho_j^n - \rho_{j-1}^n}{1 - e^{3E_{j-\frac{1}{2}}\Delta x}}, \tag{4.4}$$

where $E_{j-\frac{1}{2}}$ is a discretization of E at each interface of the mesh.

Remark 4.1 Clearly, if $\phi \equiv 0$, the former model (3.1) is recovered out of (4.1), along with its limit (3.2), being a particular case of (4.3). Accordingly, (3.27) appears as a restriction of (4.4) when $E_{j-\frac{1}{2}} \equiv 0$. However, the situation $\phi \not\equiv 0$ gives rise to sufficiently strong peculiarities so that we choose, in this paper, to neatly distinguish between both cases.

As previously, $V = (-1, 1)$, the set $\{\omega_k, v_k\}_k$ is assumed to verify (3.3).

4.2 Asymptotic expansion of eigenvalues

Let us focus on the eigenvalues of the discrete problem, computed thanks to the condition in (3.5), which, for $\nu = \frac{1}{2}\sum_{k=-K}^{K} \omega_k \delta(v - v_k)$, reads

$$1 = \frac{1}{2}\sum_{k=-K}^{K} \frac{\omega_k T_\varepsilon(v_k)}{T_\varepsilon(v_k) - \lambda^\varepsilon v_k}. \tag{4.5}$$

Clearly, $\lambda = 0$ is a solution. Thanks to (3.3), we deduce from the latter equality that nonzero eigenvalues verify

$$\sum_{k=-K}^{K} \frac{\omega_k}{\frac{T_\varepsilon(v_k)}{v_k} - \lambda^\varepsilon} = 0, \quad \text{for } \lambda^\varepsilon \neq 0.$$

By studying the variations of the left-hand side with respect to λ^ε, one deduces the existence of exactly $2K-1$ distinct solutions which are interlaced as follows

$$\frac{T_\varepsilon(v_{-1})}{v_{-1}} < \lambda^\varepsilon_{-K+1} < \frac{T_\varepsilon(v_{-2})}{v_{-2}} < \cdots < \frac{T_\varepsilon(v_{-K})}{v_{-K}} < \lambda^\varepsilon_0$$
$$< \frac{T_\varepsilon(v_K)}{v_K} < \lambda^\varepsilon_1 < \frac{T_\varepsilon(v_{K-1})}{v_{K-1}} < \lambda^\varepsilon_2 < \cdots < \lambda^\varepsilon_{K-1} < \frac{T_\varepsilon(v_1)}{v_1}.$$

The sign of λ^ε_0 is given by the sign of $\sum_{k=-K}^{K} \omega_k \dfrac{v_k}{T_\varepsilon(v_k)}$.

In the following, we always assume that $\lambda^\varepsilon_0 < 0$, the opposite case can be treated in the same way. Then, vectors of negative/positive eigenvalues are,

$$\lambda^\varepsilon_- = (\lambda^\varepsilon_{-K+1}, \ldots, \lambda^\varepsilon_{-1})^\top, \qquad \lambda^\varepsilon_+ = (\lambda^\varepsilon_1, \ldots, \lambda^\varepsilon_{K-1})^\top.$$

Lemma 4.1 *When $\varepsilon \to 0$, we have $\lambda_\ell = \lambda^0_\ell + \varepsilon \lambda^1_\ell + o(\varepsilon)$ where*

$$\lambda^0_0 = 0, \quad \lambda^1_0 = 3\sum_{k=1}^{K} \omega_k v_k \phi(v_k \partial_x S).$$

For $\ell \neq 0$, λ^0_ℓ are the symmetric ($\lambda^0_{-\ell} = -\lambda^0_\ell$) eigenvalues of

$$1 = \frac{1}{2}\sum_{k=-K}^{K} \frac{\omega_k}{1 - \lambda^0_\ell v_k},$$

and

$$\lambda^1_\ell \sum_{k=-K}^{K} \frac{\omega_k v_k}{(1 - \lambda^0_\ell v_k)^2} = \lambda^0_\ell \sum_{k=-K}^{K} \frac{\omega_k v_k \phi(v_k \partial_x S)}{(1 - \lambda^0_\ell v_k)^2}.$$

We denote by

$$\lambda^0 = (\lambda_1^0, \ldots, \lambda_{K-1}^0)^\top$$

the vector of positive eigenvalues at the limit $\varepsilon \to 0$.

Proof Letting $\varepsilon \to 0$ in (4.5), eigenvalues λ^0 are solutions of

$$1 = \frac{1}{2} \sum_{k=-K}^{K} \frac{\omega_k}{1 - \lambda^0 v_k}.$$

Symmetry of the set $\{\omega_k, v_k\}_k$ implies that if λ^0 is solution, then $-\lambda^0$ is, too. As a consequence $\lambda_+^0 = -\lambda_-^0$, and $\lambda_0^0 = 0$. Assuming an asymptotic expansion $\lambda_k^\varepsilon = \lambda_k^0 + \varepsilon\lambda_k^1 + o(\varepsilon)$, and expanding the relation (4.5) with (4.2), we get

$$\begin{aligned}
1 &= \frac{1}{2} \sum_{k=-K}^{K} \frac{\omega_k}{1 - \lambda^0 v_k - \varepsilon v_k(\lambda^1 - \phi(v_k \partial_x S)\lambda^0) + o(\varepsilon)} \\
&= \frac{1}{2} \sum_{k=-K}^{K} \frac{\omega_k}{1 - \lambda^0 v_k} \left(1 + \varepsilon \frac{v_k(\lambda^1 - \phi(v_k \partial_x S)\lambda^0)}{1 - \lambda^0 v_k} + o(\varepsilon)\right).
\end{aligned}$$

Thus, for $\ell \neq 0$,

$$\lambda_\ell^1 \sum_{k=-K}^{K} \frac{\omega_k v_k}{(1 - \lambda_\ell^0 v_k)^2} = \lambda_\ell^0 \sum_{k=-K}^{K} \frac{\omega_k v_k \phi(v_k \partial_x S)}{(1 - \lambda_\ell^0 v_k)^2}.$$

For $\ell = 0$, this relation gives $\lambda_0^0 = 0$, forcing us to go at the second order in ε to compute λ_0^1: postulating that $\lambda_0^\varepsilon = \varepsilon\lambda_0^1 + \varepsilon^2\lambda_0^2 + \cdots$, it comes

$$\begin{aligned}
1 &= \frac{1}{2} \sum_{k=-K}^{K} \frac{\omega_k}{1 - \varepsilon v_k(\lambda_0^1 + \varepsilon\lambda_0^2)/(1 + \varepsilon\phi(v_k \partial_x S))} \\
&= \frac{1}{2} \sum_{k=-K}^{K} \omega_k \left(1 + \varepsilon v_k \frac{\lambda_0^1 + \varepsilon\lambda_0^2}{1 + \varepsilon\phi(v_k \partial_x S)} + \varepsilon^2 v_k^2 (\lambda_0^1)^2 + o(\varepsilon^2)\right).
\end{aligned}$$

We get

$$0 = \sum_{k=-K}^{K} \omega_k v_k \lambda_0^1 + \varepsilon \sum_{k=-K}^{K} \omega_k \Big(- v_k \phi(v_k \partial_x S)\lambda_0^1 + v_k \lambda_0^2 + v_k^2 (\lambda_0^1)^2 \Big) + o(\varepsilon).$$

By symmetry of the set $\{\omega_k, v_k\}$, we have $\sum_{k=-K}^{K} \omega_k v_k = 0$. Then, assumptions (3.3) yield two solutions, among which we discard the null one, it gives

$$\lambda_0^1 = \frac{3}{2} \sum_{k=-K}^{K} \omega_k v_k \phi(v_k \partial_x S).$$

Being ϕ an odd function and by symmetry of $\{\omega_k, v_k\}_k$, the claim is proved. □

4.3 Corresponding scattering S-matrix

A general stationary solution reads, (see the separation of variables in [12])

$$\begin{aligned}\bar{f}^\varepsilon(x,v) = &\sum_{\ell=1}^{K-1} \frac{a_\ell e^{-\lambda_\ell^\varepsilon x/\varepsilon}}{T_\varepsilon(v) - \lambda_\ell^\varepsilon v} + \frac{\bar{a}}{T_\varepsilon(v)} \\ &+ \sum_{\ell=-K+1}^{-1} \frac{a_\ell e^{-\lambda_\ell^\varepsilon (x-\Delta x)/\varepsilon}}{T_\varepsilon(v) - \lambda_\ell^\varepsilon v} + a_0 \left(\frac{e^{-\lambda_0^\varepsilon \frac{x}{\varepsilon}}}{T_\varepsilon(v) - \lambda_0^\varepsilon v} - \frac{1}{T_\varepsilon(v)} \right).\end{aligned}$$

The spectral component of the "zero-eigenfunction" $1/T_\varepsilon(v)$ was split between $\bar{a}$ and a_0. Like for radiative transfer in Sect. 3.2, where $\phi \equiv 0$, the S-matrix is,

$$\mathcal{S}^\varepsilon = \widetilde{N^\varepsilon}(N^\varepsilon)^{-1}, \qquad \text{(dependent of } j - \frac{1}{2}) \tag{4.6}$$

where the $j - \frac{1}{2}$ index was dropped for the sake of simplicity of the scripture,

$$N^\varepsilon = \begin{pmatrix} \frac{1}{T_\varepsilon(\mathcal{V}) - \mathcal{V}\otimes\lambda_+} & \frac{1}{T_\varepsilon(\mathcal{V})} & \frac{e^{\lambda_- \Delta x/\varepsilon}}{T_\varepsilon(\mathcal{V}) - \mathcal{V}\otimes\lambda_-} & \frac{1}{T_\varepsilon(\mathcal{V}) - \lambda_0^\varepsilon \mathcal{V}} - \frac{1}{T_\varepsilon(\mathcal{V})} \\ \frac{e^{-\lambda_+ \Delta x/\varepsilon}}{T_\varepsilon(-\mathcal{V}) + \mathcal{V}\otimes\lambda_+} & \frac{1}{T_\varepsilon(-\mathcal{V})} & \frac{1}{T_\varepsilon(-\mathcal{V}) + \mathcal{V}\otimes\lambda_-} & \frac{e^{-\lambda_0^\varepsilon \Delta x/\varepsilon}}{T_\varepsilon(-\mathcal{V}) + \lambda_0^\varepsilon \mathcal{V}} - \frac{1}{T_\varepsilon(-\mathcal{V})} \end{pmatrix},$$

$$\widetilde{N^\varepsilon} = \begin{pmatrix} \frac{e^{-\lambda_+ \Delta x/\varepsilon}}{T_\varepsilon(\mathcal{V}) - \mathcal{V}\otimes\lambda_+} & \frac{1}{T_\varepsilon(\mathcal{V})} & \frac{1}{T_\varepsilon(\mathcal{V}) - \mathcal{V}\otimes\lambda_-} & \frac{e^{-\lambda_0^\varepsilon \Delta x/\varepsilon}}{T_\varepsilon(\mathcal{V}) - \lambda_0^\varepsilon \mathcal{V}} - \frac{1}{T_\varepsilon(\mathcal{V})} \\ \frac{1}{T_\varepsilon(-\mathcal{V}) + \mathcal{V}\otimes\lambda_+} & \frac{1}{T_\varepsilon(-\mathcal{V})} & \frac{e^{\lambda_- \Delta x/\varepsilon}}{T_\varepsilon(-\mathcal{V}) + \mathcal{V}\otimes\lambda_-} & \frac{1}{T_\varepsilon(-\mathcal{V}) + \lambda_0^\varepsilon \mathcal{V}} - \frac{1}{T_\varepsilon(-\mathcal{V})} \end{pmatrix}.$$

The main differences with radiative transfer, as in Sect. 3, are that 0 is a simple eigenvalue but becomes a double eigenvalue when $\varepsilon \to 0$, and that all above quantities depend on the index j, which lead to more intricate computations.

4.4 Decomposition of the scattering matrix

We want to compute the expansion (1.6) for this scattering matrix.

Lemma 4.2 *The scattering matrix for the kinetic model for chemotaxis, defined in (4.6) admits the following asymptotic expansion in ε,*

$$\boxed{\mathcal{S}^\varepsilon = \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K - \zeta^0\gamma \\ \mathbf{I}_K - \zeta^0\gamma & \mathbf{0}_K \end{pmatrix} + \varepsilon B^\varepsilon, \quad B^\varepsilon = \frac{1}{\varepsilon}(A^\varepsilon (N^\varepsilon)^{-1} - A^0 (N^0)^{-1}),} \tag{4.7}$$

where $A^\varepsilon = \widetilde{N^\varepsilon} - \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K \\ \mathbf{I}_K & \mathbf{0}_K \end{pmatrix} N^\varepsilon$, and where the matrices $\gamma \in \mathcal{M}_{K-1\times K}(\mathbb{R})$ and $\zeta^0 \in \mathcal{M}_{K\times K-1}(\mathbb{R})$ satisfy,

$$\gamma \frac{1}{1-\mathcal{V}\otimes\lambda^0} = \mathbf{I}_{K-1}, \qquad \gamma \mathbf{1}_{\mathbb{R}^K} = \mathbf{0}_{\mathbb{R}^{K-1}}, \tag{4.8}$$

$$\zeta^0 = \frac{1}{1-\mathcal{V}\otimes\lambda^0} - \frac{1}{1+\mathcal{V}\otimes\lambda^0}. \tag{4.9}$$

Remark 4.2 Lemma 4.2 is the equivalent of Lemma 3.2 in the case of the radiative transfert equation. The existence of γ is also provided by Proposition B.1 (iii).

Proof The index $j - \frac{1}{2}$ is again dropped since there is no possible confusion.

1. When $\varepsilon \to 0$, being T_ε given in (4.2) and using Lemma 4.1

$$\frac{1}{T_\varepsilon(\mathcal{V}) - \lambda_0^\varepsilon \mathcal{V}} - \frac{1}{T_\varepsilon(\mathcal{V})} \to 0, \qquad \frac{e^{-\lambda_0^\varepsilon \Delta x/\varepsilon}}{T_\varepsilon(\mathcal{V}) - \lambda_0^\varepsilon \mathcal{V}} - \frac{1}{T_\varepsilon(\mathcal{V})} \to e^{-\lambda_0^1 \Delta x} - 1.$$

so that $\mathcal{S}^\varepsilon \to \mathcal{S}^0$, where $\mathcal{S}^0 = \widetilde{N^0}(N^0)^{-1}$. Since $\lambda^0 := \lambda_+^0 = -\lambda_-^0$,

$$N^0 = \begin{pmatrix} \frac{1}{1-\mathcal{V}\otimes\lambda^0} & \mathbf{1}_{\mathbb{R}^K} & \mathbf{0}_K \\ \mathbf{0}_{K\times K-1} & \mathbf{1}_{\mathbb{R}^K} & \left(\frac{1}{1-\lambda^0\otimes\mathcal{V}} \quad (e^{-\lambda_0^1\Delta x} - 1)\mathbf{1}_{\mathbb{R}^K}\right) \end{pmatrix},$$

$$\widetilde{N^0} = \begin{pmatrix} \mathbf{0}_{K\times K-1} & \mathbf{1}_{\mathbb{R}^K} & \left(\frac{1}{1+\mathcal{V}\otimes\lambda^0} \quad (e^{-\lambda_0^1\Delta x} - 1)\mathbf{1}_{\mathbb{R}^K}\right) \\ \frac{1}{1+\lambda^0\otimes\mathcal{V}} & \mathbf{1}_{\mathbb{R}^K} & \mathbf{0}_K \end{pmatrix}.$$

2. Using γ defined in (4.8), we define also $\beta \in \mathbb{R}^K$ such that

$$\beta^\top \frac{1}{1-\mathcal{V}\otimes\lambda^0} = \mathbf{0}_{\mathbb{R}^K}^\top, \qquad \beta^\top \mathbf{1}_{\mathbb{R}^K} = 1. \tag{4.10}$$

Then, we may write

$$(N^0)^{-1} = \begin{pmatrix} \begin{pmatrix} \gamma \\ \beta^\top \end{pmatrix} & \mathbf{0}_K \\ -\begin{pmatrix} \gamma \\ \frac{1}{e^{-\lambda_0^1\Delta x}-1}\beta^\top \end{pmatrix} \begin{pmatrix} \mathbf{0}_{K\times K-1} & \mathbf{1}_{\mathbb{R}^K} \end{pmatrix} \begin{pmatrix} \gamma \\ \beta^\top \end{pmatrix} & \begin{pmatrix} \gamma \\ \frac{1}{e^{-\lambda_0^1\Delta x}-1}\beta^\top \end{pmatrix} \end{pmatrix}$$

$$= \begin{pmatrix} \begin{pmatrix} \gamma \\ \beta^\top \end{pmatrix} & \mathbf{0}_K \\ -\begin{pmatrix} \mathbf{0}_{K-1\times K} \\ \frac{1}{e^{-\lambda_0^1 \Delta x}-1}\beta^\top \end{pmatrix} & \begin{pmatrix} \gamma \\ \frac{1}{e^{-\lambda_0^1 \Delta x}-1}\beta^\top \end{pmatrix} \end{pmatrix}.$$

By definition,

$$A^\varepsilon = \widetilde{N^\varepsilon} - \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K \\ \mathbf{I}_K & \mathbf{0}_K \end{pmatrix} N^\varepsilon, \quad \text{and so} \quad \mathcal{S}^\varepsilon = \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K \\ \mathbf{I}_K & \mathbf{0}_K \end{pmatrix} + A^\varepsilon (N^\varepsilon)^{-1}.$$

3. Let us denote

$$\zeta_\pm^\varepsilon = \frac{\pm 1}{T_\varepsilon(\mathcal{V}) - \mathcal{V}\otimes\lambda_\pm^\varepsilon} - \frac{\pm 1}{T_\varepsilon(-\mathcal{V}) + \mathcal{V}\otimes\lambda_\pm^\varepsilon} \in \mathcal{M}_{K\times K-1}(\mathbb{R}),$$
$$\zeta_0^\varepsilon = \frac{1}{T_\varepsilon(\mathcal{V}) - \lambda_0^\varepsilon\mathcal{V}} - \frac{1}{T_\varepsilon(-\mathcal{V}) + \lambda_0^\varepsilon\mathcal{V}} \in \mathbb{R}^K.$$

As $\varepsilon \to 0$, we obtain the limit

$$\zeta_\pm^\varepsilon \to \zeta^0 = \frac{1}{1 - \mathcal{V}\otimes\lambda^0} - \frac{1}{1 + \mathcal{V}\otimes\lambda^0}, \quad \text{and} \quad \zeta_0^\varepsilon \to 0.$$

From the expression,

$$A^\varepsilon = \begin{pmatrix} e^{-\lambda_+\Delta x/\varepsilon}\zeta_+^\varepsilon & \frac{1}{T_\varepsilon(\mathcal{V})} - \frac{1}{T_\varepsilon(-\mathcal{V})} & -\zeta_-^\varepsilon & e^{-\lambda_0^\varepsilon\Delta x/\varepsilon}\zeta_0^\varepsilon - \frac{1}{T_\varepsilon(\mathcal{V})} + \frac{1}{T_\varepsilon(-\mathcal{V})} \\ -\zeta_+^\varepsilon & \frac{1}{T_\varepsilon(-\mathcal{V})} - \frac{1}{T_\varepsilon(\mathcal{V})} & e^{\lambda_-\Delta x/\varepsilon}\zeta_-^\varepsilon & -\zeta_0^\varepsilon + \frac{1}{T_\varepsilon(\mathcal{V})} - \frac{1}{T_\varepsilon(-\mathcal{V})} \end{pmatrix}. \tag{4.11}$$

in the limit $\varepsilon \to 0$, we get

$$A^0 = \begin{pmatrix} \mathbf{0}_K & \begin{pmatrix} -\zeta^0 & \mathbf{0}_{\mathbb{R}^K} \end{pmatrix} \\ \begin{pmatrix} -\zeta^0 & \mathbf{0}_{\mathbb{R}^K} \end{pmatrix} & \mathbf{0}_K \end{pmatrix}, \qquad A^0(N^0)^{-1} = \begin{pmatrix} \mathbf{0}_K & -\zeta^0\gamma \\ -\zeta^0\gamma & \mathbf{0}_K \end{pmatrix}. \tag{4.12}$$

Thus we reach decomposition (4.7). □

4.5 Emergence of an asymptotic scheme

We deduce the final scheme from (1.7), which mostly reads as (3.21),

$$\begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\varepsilon\Delta x}\mathbb{V}\begin{pmatrix} f_j^{n+1}(\mathcal{V}) - (\mathbf{I}_K - \zeta^0_{j-\frac12}\gamma_{j-\frac12}) f_j^{n+1}(-\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V}) - (\mathbf{I}_K - \zeta^0_{j-\frac12}\gamma_{j-\frac12}) f_{j-1}^{n+1}(\mathcal{V}) \end{pmatrix}$$
$$= \begin{pmatrix} f_j^n(\mathcal{V}) \\ f_{j-1}^n(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\Delta x}\mathbb{V}B^\varepsilon_{j-\frac12}\begin{pmatrix} f_{j-1}^n(\mathcal{V}) \\ f_j^n(-\mathcal{V}) \end{pmatrix}. \tag{4.13}$$

Denoting $B^\varepsilon = \begin{pmatrix} B^{1\varepsilon} & B^{2\varepsilon} \\ B^{3\varepsilon} & B^{4\varepsilon} \end{pmatrix}$, we may rewrite (4.13) as

$$\frac{1}{\varepsilon}\mathcal{R}_j^\varepsilon \begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_j^{n+1}(-\mathcal{V}) \end{pmatrix} = \begin{pmatrix} f_j^n(\mathcal{V}) \\ f_j^n(-\mathcal{V})) \end{pmatrix} + \frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} B^{1\varepsilon}_{j-\frac12} f^n_{j-1}(\mathcal{V}) + B^{2\varepsilon}_{j-\frac12} f^n_j(-\mathcal{V}) \\ B^{3\varepsilon}_{j+\frac12} f^n_j(\mathcal{V}) + B^{4\varepsilon}_{j+\frac12} f^n_{j+1}(-\mathcal{V}) \end{pmatrix}, \tag{4.14}$$

where

$$\mathcal{R}_j^\varepsilon = \varepsilon \mathbf{I}_{2K} + \frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} \mathbf{I}_K & \zeta^0_{j-\frac12}\gamma_{j-\frac12} - \mathbf{I}_K \\ \zeta^0_{j+\frac12}\gamma_{j+\frac12} - \mathbf{I}_K & \mathbf{I}_K \end{pmatrix}. \tag{4.15}$$

After inversion of the matrix $\mathcal{R}_\varepsilon$, by construction, this scheme satisfies both the well-balanced property and is asymptotic preserving.

Our main result for the Othmer–Alt model for chemotaxis (4.1) reads:

Theorem 4.1 *The scheme* (4.14) *for the chemotaxis model* (4.1) *is well-balanced and asymptotic-preserving (AP) with respect to* ε. *Moreover, when* $\varepsilon \to 0$, *the macroscopic density* $\rho_j^n := \sum_{k=-K}^{K} \omega_k f_j^n(v_k)$ *satisfies the Sharfetter–Gummel discretization* (4.4), *where* $E_{j-\frac12} := \sum_{k=1}^{K} \omega_k v_k \phi(v_k \partial_x S_{j-\frac12})$.

The proof of this Theorem is done in the next subsection.

4.6 Consistency with the limit $\varepsilon \to 0$

We first state the following technical Lemma (dropping the subscript $j - \frac12$ since there is no possible confusion):

Lemma 4.3 *When* ε *goes to* 0,

$$B^\varepsilon = \begin{pmatrix} B^{1\varepsilon} & B^{2\varepsilon} \\ B^{3\varepsilon} & B^{4\varepsilon} \end{pmatrix} \to B^0 = \begin{pmatrix} B^{10} & B^{20} \\ B^{30} & B^{40} \end{pmatrix},$$

where

$$\begin{cases} B^{10} = -\dfrac{e^{-\lambda_0^1 \Delta x}}{e^{-\lambda_0^1 \Delta x}-1}(2-\zeta^0\gamma)\phi(\mathcal{V}\partial_x S)\beta^\top; \\ B^{20} = \left((\zeta^0\gamma-1)\dfrac{\phi(\mathcal{V}\partial_x S)-\mathcal{V}\otimes\lambda_-^1}{(1-\mathcal{V}\otimes\lambda^0)^2}+\dfrac{\phi(\mathcal{V}\partial_x S)-\mathcal{V}\otimes\lambda_-^1}{(1+\mathcal{V}\otimes\lambda^0)^2}\right)\gamma \\ \qquad +\dfrac{1}{e^{-\lambda_0^1 \Delta x}-1}(2-\zeta^0\gamma)\phi(\mathcal{V}\partial_x S)\beta^\top; \\ B^{30} = \left((\zeta^0\gamma-1)\dfrac{-\phi(\mathcal{V}\partial_x S)+\mathcal{V}\otimes\lambda_+^1}{(1-\mathcal{V}\otimes\lambda^0)^2}+\dfrac{-\phi(\mathcal{V}\partial_x S)+\mathcal{V}\otimes\lambda_+^1}{(1+\mathcal{V}\otimes\lambda^0)^2}\right)\gamma \\ \qquad +(2-\zeta^0\gamma)\phi(\mathcal{V}\partial_x S)\beta^\top+\dfrac{1}{e^{-\lambda_0^1 \Delta x}-1}(2-\zeta^0\gamma)\lambda_0^1\mathcal{V}\beta^\top; \\ B^{40} = -\dfrac{1}{e^{-\lambda_0^1 \Delta x}-1}(2-\zeta^0\gamma)\lambda_0^1\mathcal{V}\beta^\top; \end{cases}$$

with γ, ζ^0, and β defined in (4.8)–(4.10) *respectively.*

Proof 1. First, rewrite

$$B^\varepsilon = \frac{1}{\varepsilon}(A_\varepsilon - A_0)N_\varepsilon^{-1} + \frac{1}{\varepsilon}(A_0 - A_0 N_0^{-1} N_\varepsilon)N_\varepsilon^{-1}.$$

From (4.11) and (4.12), we have

$$\frac{A_\varepsilon - A_0}{\varepsilon} = \begin{pmatrix} \frac{1}{\varepsilon}e^{-\lambda_+\Delta x/\varepsilon}\zeta_+^\varepsilon & \frac{1}{\varepsilon}\left(\frac{1}{T_\varepsilon(\mathcal{V})}-\frac{1}{T_\varepsilon(-\mathcal{V})}\right) & -\frac{1}{\varepsilon}(\zeta_-^\varepsilon-\zeta^0) \\ -\frac{1}{\varepsilon}(\zeta_+^\varepsilon-\zeta^0) & \frac{1}{\varepsilon}\left(\frac{1}{T_\varepsilon(-\mathcal{V})}-\frac{1}{T_\varepsilon(\mathcal{V})}\right) & \frac{1}{\varepsilon}e^{\lambda_-\Delta x/\varepsilon}\zeta_-^\varepsilon \end{pmatrix.$$
$$\qquad \begin{matrix} \frac{1}{\varepsilon}\left(e^{-\lambda_0^\varepsilon\Delta x/\varepsilon}\zeta_0^\varepsilon-\frac{1}{T_\varepsilon(\mathcal{V})}+\frac{1}{T_\varepsilon(-\mathcal{V})}\right) \\ \frac{1}{\varepsilon}\left(-\zeta_0^\varepsilon+\frac{1}{T_\varepsilon(\mathcal{V})}-\frac{1}{T_\varepsilon(-\mathcal{V})}\right) \end{matrix} \Bigg),$$

where, from (4.2),

$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\frac{1}{T_\varepsilon(\mathcal{V})}-\frac{1}{T_\varepsilon(-\mathcal{V})}\right) = -2\phi(\mathcal{V}\partial_x S).$$

2. Denoting $\lambda_\pm^1 = \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(\lambda_\pm^\varepsilon - \lambda^0)$ (as in Lemma 4.1), we get

$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(\zeta_\pm^\varepsilon-\zeta^0) = \frac{\mathcal{V}\otimes\lambda_\pm^1-\phi(\mathcal{V}\partial_x S)}{(1\mp\mathcal{V}\otimes\lambda^0)^2} - \frac{\mathcal{V}\otimes\lambda_\pm^1-\phi(\mathcal{V}\partial_x S)}{(1\pm\mathcal{V}\otimes\lambda^0)^2}.$$

Also,

$$\frac{1}{\varepsilon}\zeta_0^\varepsilon \to -2\phi(\mathcal{V}\partial_x S)+2\lambda_0^1\mathcal{V}.$$

Thus, when $\varepsilon \to 0$,

$$\lim_{\varepsilon\to 0}\frac{A_\varepsilon - A_0}{\varepsilon} = \begin{pmatrix} \mathbf{0}_{K\times K-1} & -2\phi(\mathcal{V}\partial_x S) \\ \frac{\phi(\mathcal{V}\partial_x S)-\mathcal{V}\otimes\lambda_+^1}{(1-\mathcal{V}\otimes\lambda^0)^2} - \frac{\phi(\mathcal{V}\partial_x S)-\mathcal{V}\otimes\lambda_+^1}{(1+\mathcal{V}\otimes\lambda^0)^2} & 2\phi(\mathcal{V}\partial_x S) \\ \frac{\phi(\mathcal{V}\partial_x S)-\mathcal{V}\otimes\lambda_-^1}{(1+\mathcal{V}\otimes\lambda^0)^2} - \frac{\phi(\mathcal{V}\partial_x S)-\mathcal{V}\otimes\lambda_-^1}{(1-\mathcal{V}\otimes\lambda^0)^2} & 2\phi(\mathcal{V}\partial_x S) \\ \mathbf{0}_{K\times K-1} & -2\lambda_0^1\mathcal{V} \end{pmatrix}.$$

3. Thanks to the fact that $\gamma\frac{1}{1-\mathcal{V}\otimes\lambda^0} = \mathbf{I}_{K-1}$, it comes

$$\frac{1}{\varepsilon}(A_0 - A_0 N_0^{-1}N_\varepsilon) = \begin{pmatrix} \zeta^0\frac{\gamma}{\varepsilon}\left(\frac{e^{-\lambda_+\Delta x/\varepsilon}}{T_\varepsilon(-\mathcal{V})+\mathcal{V}\otimes\lambda_+} \quad \frac{1}{T_\varepsilon(-\mathcal{V})}\right) \\ \zeta^0\frac{\gamma}{\varepsilon}\left(\frac{1}{T_\varepsilon(\mathcal{V})-\mathcal{V}\otimes\lambda_+} - \frac{1}{1-\mathcal{V}\otimes\lambda^0} \quad \frac{1}{T_\varepsilon(\mathcal{V})}\right) \\ \zeta^0\frac{\gamma}{\varepsilon}\left(\frac{1}{T_\varepsilon(-\mathcal{V})+\mathcal{V}\otimes\lambda_-} - \frac{1}{1-\mathcal{V}\otimes\lambda^0} \quad \frac{e^{-\lambda_0^\varepsilon\Delta x/\varepsilon}}{T_\varepsilon(-\mathcal{V})+\lambda_0^\varepsilon\mathcal{V}} - \frac{1}{T_\varepsilon(-\mathcal{V})}\right) \\ \zeta^0\frac{\gamma}{\varepsilon}\left(\frac{e^{\lambda_-\Delta x/\varepsilon}}{T_\varepsilon(\mathcal{V})-\mathcal{V}\otimes\lambda_-} \quad \frac{1}{T_\varepsilon(\mathcal{V})-\lambda_0^\varepsilon\mathcal{V}} - \frac{1}{T_\varepsilon(\mathcal{V})}\right) \end{pmatrix}.$$

Since $\gamma\mathbf{1}_{\mathbb{R}^K} = \mathbf{0}_{\mathbb{R}^{K-1}}$, we have

$$\gamma\frac{1}{\varepsilon T_\varepsilon(\mathcal{V})} = \frac{\gamma}{\varepsilon}\left(\frac{1}{T_\varepsilon(\mathcal{V})} - \mathbf{1}_{\mathbb{R}^K}\right) = \gamma\frac{-\phi(\mathcal{V}\partial_x S)}{1+\varepsilon\phi(\mathcal{V}\partial_x S)} \underset{\varepsilon\to 0}{\longrightarrow} -\gamma\phi(\mathcal{V}\partial_x S).$$

We have also

$$\frac{\gamma}{\varepsilon}\left(\frac{1}{T_\varepsilon(\mathcal{V})-\mathcal{V}\otimes\lambda_+} - \frac{1}{1-\mathcal{V}\otimes\lambda^0}\right) \underset{\varepsilon\to 0}{\longrightarrow} \gamma\frac{-\phi(\mathcal{V}\partial_x S)+\mathcal{V}\otimes\lambda_+^1}{(1-\lambda^0\otimes\mathcal{V})^2}.$$

Then,

$$\begin{aligned} &\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(A_0 - A_0 N_0^{-1}N_\varepsilon) \\ &= \begin{pmatrix} \zeta^0\gamma\left(\mathbf{0}_{K\times K-1} \quad \phi(\mathcal{V}\partial_x S)\right) & \zeta^0\gamma\left(\frac{\phi(\mathcal{V}\partial_x S)-\mathcal{V}\otimes\lambda_-^1}{(1-\lambda^0\otimes\mathcal{V})^2} \quad -\phi(\mathcal{V}\partial_x S)\right) \\ \zeta^0\gamma\left(\frac{-\phi(\mathcal{V}\partial_x S)+\mathcal{V}\otimes\lambda_+^1}{(1-\lambda^0\otimes\mathcal{V})^2} \quad -\phi(\mathcal{V}\partial_x S)\right) & \zeta^0\gamma\left(\mathbf{0}_{K\times K-1} \quad \lambda_0^1\mathcal{V}\right) \end{pmatrix}. \end{aligned}$$

4. Gathering these computations, we reach

$$\begin{aligned} B^0 &:= \lim_{\varepsilon\to 0} B^\varepsilon \\ &= \lim_{\varepsilon\to 0}\frac{A^\varepsilon - A^0}{\varepsilon}(N^0)^{-1} + \lim_{\varepsilon\to 0}\frac{1}{\varepsilon}(A^0 - A^0(N^0)^{-1}N^\varepsilon)(N^0)^{-1} \\ &= \begin{pmatrix} B^{10} & B^{20} \\ B^{30} & B^{40} \end{pmatrix}, \end{aligned}$$

where B^{10}, B^{20}, B^{30}, and B^{40} are expressed in Lemma 4.3. $\square$

Proof of Theorem 4.1 We proceed as in Sect. 3.4. First, we have obviously from (4.15) $\mathcal{R}_j^\varepsilon = \varepsilon \mathbf{I}_{2K} + \mathcal{R}_j^0$ where

$$\mathcal{R}_j^0 := \frac{\Delta t}{\Delta x} \mathbb{V} \begin{pmatrix} \mathbf{I}_K & \zeta^0_{j-\frac{1}{2}} \gamma_{j-\frac{1}{2}} - \mathbf{I}_K \\ \zeta^0_{j+\frac{1}{2}} \gamma_{j+\frac{1}{2}} - \mathbf{I}_K & \mathbf{I}_K \end{pmatrix}$$

Assuming that f admits an Hilbert expansion $f = f^0 + \varepsilon f^1 + \cdots$, we get, by injecting this expansion into (4.14) and identifying the term in power of ε,

$$\mathcal{R}_j^0 \begin{pmatrix} \{f^0\}_j^{n+1}(\mathcal{V}) \\ \{f^0\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} = 0, \tag{4.16}$$

and

$$\begin{aligned} \mathcal{R}_j^0 \begin{pmatrix} \{f^1\}_j^{n+1}(\mathcal{V}) \\ \{f^1\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} &= \begin{pmatrix} \{f^0\}_j^n - \{f^0\}_j^{n+1} \\ \{f^0\}_j^n - \{f^0\}_j^{n+1} \end{pmatrix} \\ &\quad + \frac{\Delta t}{\Delta x} \mathbb{V} \begin{pmatrix} B^{10}_{j-\frac{1}{2}} \{f^0\}_{j-1}^n + B^{20}_{j-\frac{1}{2}} \{f^0\}_j^n \\ B^{30}_{j+\frac{1}{2}} \{f^0\}_j^n + B^{40}_{j+\frac{1}{2}} \{f^0\}_{j+1}^n \end{pmatrix}. \end{aligned} \tag{4.17}$$

Since from (3.8),

$$\forall \ell \in \{1, \dots, K\}, \qquad \sum_{k=1}^K \omega_k v_k (\zeta^0 \gamma)_{k\ell} = 0,$$

we may apply Lemma B.1 and deduce

- $\mathrm{Ker}(\mathcal{R}_j^0) = \mathrm{Span}\{\mathbf{1}_{\mathbb{R}^K}\}$,
- $\mathrm{Im}(\mathcal{R}_j^0) = \{Z = (Z_1 \quad Z_2)^\top,\ Z_i \in \mathbb{R}^K \text{ such that } \sum_{k=1}^K \omega_k (Z_{1k} + Z_{2k}) = 0\}$.

Thus Eq. (4.16) implies

$$\{f^0\}_j^{n+1}(\pm \mathcal{V}) = \frac{\rho_j^{n+1}}{2} \mathbf{1}_{\mathbb{R}^K},$$

which can be inserted into (4.17) in order to get:

$$\begin{aligned} \mathcal{R}_j^0 \begin{pmatrix} \{f^1\}_j^{n+1}(\mathcal{V}) \\ \{f^1\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} &= \frac{1}{2} \begin{pmatrix} (\rho_j^n - \rho_j^{n+1}) \mathbf{1}_{\mathbb{R}^K} \\ (\rho_j^n - \rho_j^{n+1}) \mathbf{1}_{\mathbb{R}^K} \end{pmatrix} \\ &\quad + \frac{\Delta t}{2\Delta x} \mathbb{V} \begin{pmatrix} B^{10}_{j-\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} \rho_{j-1}^n + B^{20}_{j-\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} \rho_j^n \\ B^{30}_{j+\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} \rho_j^n + B^{40}_{j+\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} \rho_{j+1}^n \end{pmatrix}. \end{aligned} \tag{4.18}$$

Thanks to the relations,

$$\gamma \mathbf{1}_{\mathbb{R}^K} = \mathbf{0}_{\mathbb{R}^{K-1}}. \qquad \beta^\top \mathbf{1}_{\mathbb{R}^K} = 1,$$

we deduce from the expression of B^0 in Lemma 4.3,

$$\begin{aligned}
B^{10}_{j-\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} &= -\frac{e^{-\lambda^1_{0,j-\frac{1}{2}}\Delta x}}{e^{-\lambda^1_{0,j-\frac{1}{2}}\Delta x} - 1} (2 - \zeta^0 \gamma) \phi(\mathcal{V} \partial_x S_{j-\frac{1}{2}});\\
B^{20}_{j-\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} &= \frac{1}{e^{-\lambda^1_{0,j-\frac{1}{2}}\Delta x} - 1} (2 - \zeta^0 \gamma) \phi(\mathcal{V} \partial_x S_{j-\frac{1}{2}});\\
B^{30}_{j+\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} &= (2 - \zeta^0 \gamma) \phi(\mathcal{V} \partial_x S_{j+\frac{1}{2}}) + \frac{\lambda^1_{0,j+\frac{1}{2}}}{e^{-\lambda^1_{0,j+\frac{1}{2}}\Delta x} - 1} (2 - \zeta^0 \gamma) \mathcal{V};\\
B^{40}_{j+\frac{1}{2}} \mathbf{1}_{\mathbb{R}^K} &= \frac{-\lambda^1_{0,j+\frac{1}{2}}}{e^{-\lambda^1_{0,j+\frac{1}{2}}\Delta x} - 1} (2 - \zeta^0 \gamma) \mathcal{V}.
\end{aligned}$$

The solvability condition for (4.18) is that its right hand side belongs to $\mathrm{Im}(\mathcal{R}^0_j)$. Then, we multiply each line by ω_k and add over k to obtain

$$\begin{aligned}
0 = \rho^n_j - \rho^{n+1}_j + \frac{\Delta t}{\Delta x} &\left(\frac{-e^{-\lambda^1_{0,j-\frac{1}{2}}\Delta x} \rho^n_{j-1} + \rho^n_j}{e^{-\lambda^1_{0,j-\frac{1}{2}}\Delta x} - 1} \sum_{k=1}^K \omega_k v_k \phi(v_k \partial_x S_{j-\frac{1}{2}}) \right.\\
&\left. + \rho^n_j \sum_{k=1}^K \omega_k v_k \phi(v_k \partial_x S_{j+\frac{1}{2}}) + \frac{\lambda^1_{0,j+\frac{1}{2}} (\rho^n_j - \rho^n_{j+1})}{e^{-\lambda^1_{0,j+\frac{1}{2}}\Delta x} - 1} \sum_{k=1}^K \omega_k v_k^2 \right),
\end{aligned}$$

where we have used also $\forall \ell$, $\sum_{k=1}^K \omega_k v_k (\zeta^0 \gamma)_{k\ell} = 0$. From Lemma 4.1 and assumptions (3.3), it comes

$$\frac{1}{3} \lambda^1_0 = \sum_{k=1}^K \omega_k v_k \phi(v_k \partial_x S).$$

Denoting $E_{j-\frac{1}{2}} := \sum_{k=1}^K \omega_k v_k \phi(v_k \partial_x S_{j-\frac{1}{2}})$, the above scheme rewrites as

$$\rho^{n+1}_j = \rho^n_j + \frac{\Delta t}{\Delta x} \left(-E_{j-\frac{1}{2}} \frac{e^{-3E_{j-\frac{1}{2}}\Delta x} \rho^n_{j-1} - \rho^n_j}{e^{-3E_{j-\frac{1}{2}}\Delta x} - 1} + E_{j+\frac{1}{2}} \frac{e^{-3E_{j+\frac{1}{2}}\Delta x} \rho^n_j - \rho^n_{j+1}}{e^{-3E_{j+\frac{1}{2}}\Delta x} - 1} \right),$$

in which we recognize the Sharfetter–Gummel scheme (4.4). □

5 Diffusive limit of Vlasov–Fokker–Planck kinetic equations

5.1 Presentation of the continuous model

This kinetic model reads, see [48,52,60], in parabolic scaling,

$$\varepsilon \partial_t f^\varepsilon + v\partial_x f^\varepsilon + E \cdot \partial_v f^\varepsilon = \frac{1}{\varepsilon}\partial_v \left(v f^\varepsilon + \kappa \partial_v f^\varepsilon \right), \qquad 0 < \varepsilon \ll 1. \tag{5.1}$$

The electric field, denoted E, derives from a potential ϕ by the relation $E = \pm\, \partial_x \phi$. When such a potential ϕ depends self-consistently on the macroscopic density of electrons (through the Poisson equation), one speaks about the Vlasov–Poisson–Fokker–Planck system. To keep the exposition simple, we shall assume that both a steady potential $\phi(x)$ and its electric field $E(x)$ are given. When $\varepsilon \to 0$, the kinetic distribution in (5.1) relaxes to a Maxwellian,

$$f^\varepsilon \to \rho^0 \frac{1}{\sqrt{2\pi\kappa}} e^{-v^2/2\kappa},$$

where the macroscopic density ρ^0 solves a drift-diffusion (continuity) equation,

$$\boxed{\partial_t \rho^0 + \kappa \partial_x \left(\frac{E}{\kappa}\rho^0 - \partial_x \rho^0 \right) = 0.} \tag{5.2}$$

The Sharfetter–Gummel scheme associated to this system reads

$$\begin{aligned} \rho_j^{n+1} &= \rho_j^n + \frac{\Delta t}{\Delta x}\big(\bar{\mathcal{J}}^n_{j-\frac{1}{2}} - \bar{\mathcal{J}}^n_{j+\frac{1}{2}}\big), \\ \bar{\mathcal{J}}^n_{j-\frac{1}{2}} &= E_{j-\frac{1}{2}} \frac{\rho^n_{j-1} - e^{-E_{j-\frac{1}{2}}\Delta x/\kappa}\rho^n_j}{1 - e^{-E_{j-\frac{1}{2}}\Delta x/\kappa}}. \end{aligned} \tag{5.3}$$

5.2 Spectral decomposition of stationary solutions

Consider the Fokker–Planck stationary problem with inflow boundaries,

$$v\partial_x \bar{f} = \frac{1}{\varepsilon}\partial_v \Big((v - \varepsilon E)\bar{f} + \kappa \partial_v \bar{f} \Big), \qquad \varepsilon, \kappa > 0. \tag{5.4}$$

A convenient "separated variables" ansatz reads now, (see e.g. [11])

$$\bar{f}(x, v) = \exp(-\lambda x - \mu v)\psi_\lambda(v),$$

so that one recovers a standard Sturm–Liouville eigenvalue problem (see [5] and [27, Chapter 12.3]) with a discrete spectrum. The null eigenvalue $\lambda = 0$ is double, its two associated non-damped modes are denoted $\Psi^{\varepsilon}_{\pm 0}$ ("diffusion solutions" in [22]) among which appears a space-homogeneous mode:

$$\Psi^{\varepsilon}_{\pm 0}(x, v) = \exp\left(-\frac{\mu^{\varepsilon}_{\pm 0} x}{\varepsilon}\right) \psi^{\varepsilon}_{\pm \ell}(v),$$

where

- when $E > 0$,

$$\mu^{\varepsilon}_{0} = 0; \quad \psi^{\varepsilon}_{0}(v) = \exp\left(-\frac{(v - |\varepsilon E|)^2}{2\kappa}\right);$$
$$\mu^{\varepsilon}_{-0} = -\frac{\varepsilon E}{\kappa}; \quad \psi^{\varepsilon}_{-0}(v) = \exp\left(-\frac{|\varepsilon E|^2}{2\kappa}\right) \exp\left(-\frac{v^2}{2\kappa}\right);$$

- when $E < 0$,

$$\mu^{\varepsilon}_{0} = -\frac{\varepsilon E}{\kappa}; \quad \psi^{\varepsilon}_{0}(v) = \exp\left(-\frac{|\varepsilon E|^2}{2\kappa}\right) \exp\left(-\frac{v^2}{2\kappa}\right);$$
$$\mu^{\varepsilon}_{-0} = 0; \quad \psi^{\varepsilon}_{-0}(v) = \exp\left(-\frac{(v + |\varepsilon E|)^2}{2\kappa}\right).$$

Other eigenfunctions $\Psi^{\varepsilon}_{\pm \ell}$, for $\ell \in \mathbb{N}^*$, are explicitly given in [27, p. 251]:

$$\Psi^{\varepsilon}_{\pm \ell}(x, v) = \exp\left(-\frac{\mu^{\varepsilon}_{\pm \ell} x}{\varepsilon}\right) \psi^{\varepsilon}_{\pm \ell}(v) \tag{5.5}$$

$$\psi^{\varepsilon}_{\pm \ell}(v) = \exp(-\mu^{\varepsilon}_{\pm \ell} v) H_{\ell}(\tilde{v}^{\varepsilon}_{\pm \ell}) \exp(-(\tilde{v}^{\varepsilon}_{\pm \ell})^2) \tag{5.6}$$

where H_{ℓ} is the ℓth Hermite polynomial and

$$\mu^{\varepsilon}_{\pm \ell} = \frac{-\varepsilon E \pm \sqrt{(\varepsilon E)^2 + 4\kappa \ell}}{2\kappa}, \qquad \tilde{v}^{\varepsilon}_{\pm \ell} = \frac{v - 2\mu^{\varepsilon}_{\pm \ell}\kappa - \varepsilon E}{\sqrt{2\kappa}}.$$

Hermite's polynomials are such that $\deg(H_{\ell}) = \ell$ and $H_{\ell}(-X) = (-1)^{\ell} H_{\ell}(X)$. They are orthogonal with respect to a strongly-growing (indefinite) weight:

$$\int_{\mathbb{R}} v\, \psi^{\varepsilon}_{\pm k}(v) \psi^{\varepsilon}_{\pm \ell}(v) \exp\left(\frac{(v - \varepsilon E)^2}{2\kappa}\right) dv = 0, \qquad \text{if } k \neq \ell. \tag{5.7}$$

A spectral decomposition follows, for smooth enough functions $\bar{f}(x, v)$ [6,16],

$$\boxed{\bar{f}(x, v) = \alpha_{+0} \Psi^{\varepsilon}_{0}(x, v) + \alpha_{-0} \Psi^{\varepsilon}_{-0}(x, v) + \sum_{\ell \geq 1} \left(\alpha_{\ell} \Psi^{\varepsilon}_{\ell}(x, v) + \alpha_{-\ell} \Psi^{\varepsilon}_{-\ell}(x, v)\right).} \tag{5.8}$$

By inserting the space-homogeneous eigenfunction associated to $k = 0$, one sees from (5.7) that none in all the set of $\Psi^{\varepsilon}_{\pm\ell}$, $\ell > 0$, can carry any net macroscopic flux:

$$\forall \ell \neq 0, \quad \int_{\mathbb{R}} v\psi^{\varepsilon}_{\pm\ell}(v)\psi^{\varepsilon}_{\pm 0}(v)\exp\left(\frac{(v-\varepsilon E)^2}{2\kappa}\right)dv = \int_{\mathbb{R}} v\psi^{\varepsilon}_{\pm\ell}(v)dv = 0. \quad (5.9)$$

For future use, we compute the limit as $\varepsilon \to 0$ of the above expressions. We obtain straightforwardly, as $\varepsilon \to 0$,

$$\psi^0_{\pm 0}(v) = \exp\Big(-\frac{v^2}{2\kappa}\Big); \quad (5.10a)$$

$$\psi^0_{\pm\ell}(v) = H_\ell\Big(\frac{v \mp 2\sqrt{\ell\kappa}}{\sqrt{2\kappa}}\Big)\exp\left(-\frac{v^2}{2\kappa} \pm v\sqrt{\frac{\ell}{\kappa}} - 2\ell\right), \quad \text{for } \ell \in \mathbb{N}^*. \quad (5.10b)$$

We deduce from the symmetry of Hermite polynomials that we have the identity $\psi^0_{-\ell}(-v) = (-1)^\ell \psi^0_\ell(v)$. These expressions do not depend on $E \in \mathbb{R}$.

5.3 Assumptions on the set of discrete velocities and weights.

As mentioned in the introduction, and contrary to the Case's functions, being exponential polynomials, solutions of the stationary Vlasov–Fokker–Planck equation, do not constitute a Chebyshev T-system on $(0, +\infty)$.

Indeed, if we assume that the family $\{\psi^0_0, \dots, \psi^0_{K-1}\}$ is endowed with the Haar property, then any non-zero linear combination of these functions will have no more than $K-1$ roots on $(0, +\infty)$; otherwise, denoting $v_0, \dots, v_{K-1}$ these roots, $\det(\psi^0_\ell(v_k))_{k,\ell} = 0$ (see Proposition A.1). However, it is not difficult to find ad-hoc coefficients $a_0, \dots, a_{K-1}$, for which the function

$$\mathbb{R}^+ \ni v \mapsto a_0\,\psi^0_0(v) + \sum_{\ell=1}^{K-1} a_\ell\,\psi^0_\ell(v)$$

admits more than $K-1$ roots on $(0, +\infty)$. For instance,

- for $K = 2$, the function (after simplification by $\exp(-v^2/2\kappa)$),

$$v \mapsto \frac{3}{2} + \frac{v-2}{\sqrt{2}}e^v$$

  has two positive roots, approximately given by 0.1216 and 1.5495;
- For $K = 3$, the function

$$v \mapsto -2.75 + 0.2e^v(v-2) + e^{\sqrt{2}v}\left(\frac{v^2}{2} - 2\sqrt{2}v + 3\right)$$

admits three positive roots, approximately given by 0.132, 0.796 and 4.192.

The number of real roots for exponential polynomials admits the Pólya–Szegö estimate as an upper bound, see Appendix D.1. However, exponential monomials do satisfy the Haar property on $(0, +\infty)$ as shown in Theorem D.1.

Accordingly, we must prescribe some assumptions on the set of discrete velocities. More precisely, we assume that $v_1, \ldots, v_K$ are chosen such that,

$$\text{given } K \in \mathbb{N}, \qquad \det\Big(\psi_0^0(\mathcal{V}) \quad \psi_1^0(\mathcal{V}) \quad \cdots \quad \psi_{K-1}^0(\mathcal{V})\Big) \neq 0, \tag{5.11}$$

and such that the family

$$\begin{aligned}&\left\{ \begin{pmatrix} \psi_0^0(\mathcal{V}) \\ \psi_0^0(-\mathcal{V}) \end{pmatrix}, \begin{pmatrix} \psi_1^0(\mathcal{V}) \\ \psi_1^0(-\mathcal{V}) \end{pmatrix}, \ldots, \begin{pmatrix} \psi_{K-1}^0(\mathcal{V}) \\ \psi_{K-1}^0(-\mathcal{V}) \end{pmatrix}, \right.\\ &\left. \times \begin{pmatrix} \psi_1^0(-\mathcal{V}) \\ \psi_1^0(\mathcal{V}) \end{pmatrix}, \ldots, \begin{pmatrix} \psi_{K-1}^0(-\mathcal{V}) \\ \psi_{K-1}^0(\mathcal{V}) \end{pmatrix} \right\} \quad \text{is linearly independent in } \mathbb{R}^{2K}.\end{aligned} \tag{5.12}$$

We assume moreover that the corresponding weights ω_k are such that the orthogonality relation (5.9) holds true at the discrete level, i.e.

$$\forall \ell = 1, \ldots, K-1, \qquad \sum_{k=1}^{K} \omega_k v_k (\psi_{\pm\ell}^0(v_k) - \psi_{\pm\ell}^0(-v_k)) = 0. \tag{5.13}$$

Thanks to the relation $\psi_{-\ell}^0(-v_k) = (-1)^\ell \psi_\ell^0(v_k)$, it suffices to get the above identity only for positive ℓ. Quadrature issues for Vlasov–Fokker–Planck were already raised in [27, Remark 12.5, page 253]. Yet, the following Lemma shows that actually assumptions (5.11) and (5.12) hold at the continuous level.

Lemma 5.1 *For any $N \in \mathbb{N}$, the family $(\psi_0^0, \psi_1^0, \ldots, \psi_{N-1}^0)$ given by (5.6) is linearly independent on $v \in (0, +\infty)$, and also on $v \in \mathbb{R}$.*

Proof Given N, we have to show the linear independence on $\mathbb{R}$ and on $(0, +\infty)$. The result on $\mathbb{R}$ is a direct consequence of the orthogonality relation (5.7). Thus we are left to prove the result on $(0, +\infty)$. After expanding the Gaussian term in (5.6) and normalizing coefficients, any linear combination with $\varepsilon = 0$ rewrites,

$$\forall v \in (0, +\infty), \qquad \sum_{i=0}^{N-1} \lambda_i \exp(\mu_i\, v) H_i(\tilde{v}_i) = 0.$$

Since $H_{N-1} \neq 0$ for v big enough, it suffices to let $v \to +\infty$ in

$$\lambda_{N-1} + \sum_{i=0}^{N-2} \lambda_i \exp((\mu_i - \mu_{N-1})\, v) \frac{H_i(\tilde{v}_i)}{H_{N-1}(\tilde{v}_{N-1})} = 0,$$

in order to get $\lambda_{N-1} = 0$ because $\mu_i - \mu_{N-1} \leq C < 0$. Successive coefficients vanish for the same reason. So for any N, the family $(\psi_i^0)_{i<N}$ is linearly independent on $\mathbb{R}_*^+$. $\square$

5.4 Corresponding scattering *S*-matrix

The stationary problem with incoming boundary condition reads

$$v\partial_x \bar{f} = \frac{1}{\varepsilon}\partial_v\big((v - \varepsilon E_{j-\frac{1}{2}})\bar{f} + \kappa\partial_v \bar{f}\big), \qquad \text{on } (0, \Delta x), \tag{5.14}$$

$$\bar{f}(0, v) = f_{j-1}^n(v), \quad \bar{f}(\Delta x, -v) = f_j^n(-v). \tag{5.15}$$

Based on (5.8) and (5.5), we seek spectral approximations obtained by truncating (5.8) to the first $2K$ modes,

$$\boxed{\bar{f}(x, v) = \alpha_{+0}\psi_0^\varepsilon(v)e^{-\mu_0^\varepsilon x/\varepsilon} + \alpha_{-0}\psi_{-0}^\varepsilon(v)e^{-\mu_{-0}^\varepsilon x/\varepsilon} + \sum_{\ell=1}^{K-1}\alpha_{\pm\ell}\psi_{\pm\ell}^\varepsilon(v)e^{-\mu_{\pm\ell}^\varepsilon x/\varepsilon}.} \tag{5.16}$$

Coefficients $\alpha_{\pm\ell}$ in this full-range expansion follow from incoming boundary conditions (5.15), according to a linear system: for $k = 1, \dots, K$,

$$\begin{aligned}
\bar{f}(0, v_k) &= f_{j-1}^n(v_k) = \alpha_0\psi_0^\varepsilon(v_k) + \alpha_{-0}\psi_{-0}^\varepsilon(v_k) + \sum_{\ell=1}^{K-1}\alpha_{\pm\ell}\psi_{\pm\ell}^\varepsilon(v_k),\\
\bar{f}(\Delta x, -v_k) &= f_{i+1}^n(-v_k) = \alpha_0\psi_0^\varepsilon(-v_k)e^{-\frac{\mu_0}{\varepsilon}\Delta x} + \alpha_{-0}\psi_{-0}^\varepsilon(-v_k)e^{-\frac{\mu_{-0}^\varepsilon}{\varepsilon}\Delta x}\\
&\quad + \sum_{\ell=1}^{K-1}\alpha_{\pm\ell}\psi_{\pm\ell}^\varepsilon(-v_k)e^{-\frac{\mu_{\pm\ell}^\varepsilon}{\varepsilon}\Delta x}.
\end{aligned}$$

The $K \times (K-1)$ matrix of eigenvectors associated to nonzero eigenvalues is

$$\psi_\pm^\varepsilon(\mathcal{V}) = \left(\psi_{\pm1}^\varepsilon(\mathcal{V}) \dots \psi_{\pm K-1}^\varepsilon(\mathcal{V})\right),$$

so that,

$$\begin{pmatrix}\alpha_+\\ \alpha_-\end{pmatrix} = (\mathcal{M}^\varepsilon)^{-1}\begin{pmatrix}f_{j-1}^n(\mathcal{V})\\ f_j^n(-\mathcal{V})\end{pmatrix},$$

where $\mathcal{M}^\varepsilon$ is the $2K \times 2K$ matrix defined by

$$\mathcal{M}^\varepsilon = \begin{pmatrix}\psi_+^\varepsilon(\mathcal{V}) & \psi_0^\varepsilon(\mathcal{V}) & \psi_-^\varepsilon(\mathcal{V}) & \psi_{-0}^\varepsilon(\mathcal{V})\\ \psi_+^\varepsilon(-\mathcal{V})e^{-\mu_+^\varepsilon\Delta x/\varepsilon} & \psi_0^\varepsilon(-\mathcal{V})e^{-\mu_0^\varepsilon\Delta x/\varepsilon} & \psi_-^\varepsilon(-\mathcal{V})e^{-\mu_-^\varepsilon\Delta x/\varepsilon} & \psi_{-0}^\varepsilon(-\mathcal{V})e^{-\mu_{-0}^\varepsilon\Delta x/\varepsilon}\end{pmatrix}.$$

Outgoing values of $\bar{f}$ follow thanks to (5.16),

$$\begin{aligned}\bar{f}(\Delta x, \mathcal{V}) &= \alpha_0 \psi_0^\varepsilon(\mathcal{V}) e^{-\mu_0^\varepsilon \Delta x/\varepsilon} + \alpha_{-0} \psi_{-0}^\varepsilon(\mathcal{V}) e^{-\mu_{-0}^\varepsilon \Delta x/\varepsilon} \\ &\quad + \sum_{\ell=1}^{K-1} \alpha_{\pm\ell} \psi_{\pm\ell}^\varepsilon(\mathcal{V}) e^{-\mu_{\pm\ell}^\varepsilon \Delta x/\varepsilon}, \\ \bar{f}(0, -\mathcal{V}) &= \alpha_0 \psi_0^\varepsilon(-\mathcal{V}) + \alpha_{-0} \psi_{-0}^\varepsilon(-\mathcal{V}) + \sum_{\ell=1}^{K-1} \alpha_{\pm\ell} \psi_{\pm\ell}^\varepsilon(-\mathcal{V}).\end{aligned}$$

Then, denoting

$$\widetilde{\mathcal{M}^\varepsilon} = \begin{pmatrix} \psi_+^\varepsilon(\mathcal{V}) e^{-\mu_+^\varepsilon \Delta x/\varepsilon} & \psi_0^\varepsilon(\mathcal{V}) e^{-\mu_0^\varepsilon \Delta x/\varepsilon} & \psi_-^\varepsilon(\mathcal{V}) e^{-\mu_-^\varepsilon \Delta x/\varepsilon} & \psi_{-0}^\varepsilon(\mathcal{V}) e^{-\mu_{-0}^\varepsilon \Delta x/\varepsilon} \\ \psi_+^\varepsilon(-\mathcal{V}) & \psi_0^\varepsilon(-\mathcal{V}) & \psi_-^\varepsilon(-\mathcal{V}) & \psi_{-0}^\varepsilon(-\mathcal{V}) \end{pmatrix},$$

we get

$$\begin{pmatrix} \widetilde{f}(\Delta x, \mathcal{V}) \\ \widetilde{f}(0, -\mathcal{V}) \end{pmatrix} = \widetilde{\mathcal{M}^\varepsilon} (\mathcal{M}^\varepsilon)^{-1} \begin{pmatrix} f_{j-1}^n(\mathcal{V}) \\ f_j^n(-\mathcal{V}) \end{pmatrix}.$$

Accordingly, the scattering matrix is defined by,

$$\mathcal{S}_{j-\frac{1}{2}}^\varepsilon = \widetilde{\mathcal{M}^\varepsilon} (\mathcal{M}^\varepsilon)^{-1}. \qquad \text{(dependent on } j - \frac{1}{2}\text{)}$$

5.5 Decomposition of the scattering matrix

We perform the computation in the case $E > 0$. Computations in the case $E < 0$ are similar. We start from the expression,

$$\mathcal{S}^\varepsilon = \widetilde{\mathcal{M}^\varepsilon} (\mathcal{M}^\varepsilon)^{-1} = \widetilde{N^\varepsilon} (N^\varepsilon)^{-1},$$

where (expressions of $\mu_{\pm 0}^\varepsilon$ are used),

$$\begin{aligned} N^\varepsilon &= \begin{pmatrix} \psi_+^\varepsilon(\mathcal{V}) & \psi_0^\varepsilon(\mathcal{V}) & \psi_-^\varepsilon(\mathcal{V}) e^{\mu_-^\varepsilon \Delta x/\varepsilon} & \psi_{-0}^\varepsilon(\mathcal{V}) e^{-E\Delta x/\kappa} \\ \psi_+^\varepsilon(-\mathcal{V}) e^{-\mu_+^\varepsilon \Delta x/\varepsilon} & \psi_0^\varepsilon(-\mathcal{V}) & \psi_-^\varepsilon(-\mathcal{V}) & \psi_{-0}^\varepsilon(-\mathcal{V}) \end{pmatrix}, \\ \widetilde{N^\varepsilon} &= \begin{pmatrix} \psi_+^\varepsilon(\mathcal{V}) e^{-\mu_+^\varepsilon \Delta x/\varepsilon} & \psi_0^\varepsilon(\mathcal{V}) & \psi_-^\varepsilon(\mathcal{V}) & \psi_{-0}^\varepsilon(\mathcal{V}) \\ \psi_+^\varepsilon(-\mathcal{V}) & \psi_0^\varepsilon(-\mathcal{V}) & \psi_-^\varepsilon(-\mathcal{V}) e^{\mu_-^\varepsilon \Delta x/\varepsilon} & \psi_{-0}^\varepsilon(-\mathcal{V}) e^{-E\Delta x/\kappa} \end{pmatrix}. \end{aligned}$$

Moreover, the product $\widetilde{N^\varepsilon}(N^\varepsilon)^{-1}$ is invariant if, in both matrices N^ε and $\widetilde{N^\varepsilon}$, we subtract to the last column $e^{-E\Delta x/\kappa}$ times the Kth column, i.e.

$$\mathcal{S}^\varepsilon = \widetilde{\mathcal{N}^\varepsilon} (\mathcal{N}^\varepsilon)^{-1}, \tag{5.17}$$

with

$$\mathcal{N}^\varepsilon = \begin{pmatrix} \psi_+^\varepsilon(\mathcal{V}) & \psi_0^\varepsilon(\mathcal{V}) & \psi_-^\varepsilon(\mathcal{V})e^{\mu_-^\varepsilon \Delta x/\varepsilon} & (\psi_{-0}^\varepsilon(\mathcal{V}) - \psi_0^\varepsilon(\mathcal{V}))e^{-E\Delta x/\kappa} \\ \psi_+^\varepsilon(-\mathcal{V})e^{-\mu_+^\varepsilon \Delta x/\varepsilon} & \psi_0^\varepsilon(-\mathcal{V}) & \psi_-^\varepsilon(-\mathcal{V}) & \psi_{-0}^\varepsilon(-\mathcal{V}) - \psi_0^\varepsilon(-\mathcal{V})e^{-E\Delta x/\kappa} \end{pmatrix},$$
$$\widetilde{\mathcal{N}}^\varepsilon = \begin{pmatrix} \psi_+^\varepsilon(\mathcal{V})e^{-\mu_+^\varepsilon \Delta x/\varepsilon} & \psi_0^\varepsilon(\mathcal{V}) & \psi_-^\varepsilon(\mathcal{V}) & \psi_{-0}^\varepsilon(\mathcal{V}) - \psi_0^\varepsilon(\mathcal{V})e^{-E\Delta x/\kappa} \\ \psi_+^\varepsilon(-\mathcal{V}) & \psi_0^\varepsilon(-\mathcal{V}) & \psi_-^\varepsilon(-\mathcal{V})e^{\mu_-^\varepsilon \Delta x/\varepsilon} & (\psi_{-0}^\varepsilon(-\mathcal{V}) - \psi_0^\varepsilon(-\mathcal{V}))e^{-E\Delta x/\kappa} \end{pmatrix}.$$

Noticing that when $\varepsilon \to 0$, $\psi_{\pm 0}^\varepsilon(\mathcal{V}) \to \exp(-\frac{\mathcal{V}^2}{2\kappa})$, we may pass to the limit $\varepsilon \to 0$ in the latter matrices and get $\mathcal{S}^\varepsilon \to \mathcal{S}^0 = \mathcal{N}^0(\widetilde{\mathcal{N}}^0)^{-1}$ with

$$\mathcal{N}^0 = \begin{pmatrix} \psi_+^0(\mathcal{V}) \;\; \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) & \mathbf{0}_K \\ \mathbf{0}_{K\times K-1} \;\; \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) & \left(\psi_-^0(-\mathcal{V}) \quad (1-e^{-E\Delta x/\kappa})\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\right) \end{pmatrix}, \tag{5.18}$$

$$\widetilde{\mathcal{N}}^0 = \begin{pmatrix} \mathbf{0}_{K\times K-1} \;\; \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) & \left(\psi_-^0(\mathcal{V}) \quad (1-e^{-E\Delta x/\kappa})\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\right) \\ \psi_+^0(-\mathcal{V}) \;\; \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) & \mathbf{0}_K \end{pmatrix}. \tag{5.19}$$

Lemma 5.2 *Under assumption (5.11) on the set of discrete velocities, the S-matrix (5.17) admits the asymptotic expansion in ε,*

$$\boxed{\mathcal{S}^\varepsilon = \begin{pmatrix} \mathbf{0}_K & \mathbf{I}_K - \zeta_+^0\gamma_+ \\ \mathbf{I}_K - \zeta_+^0\gamma_+ & \mathbf{0}_K \end{pmatrix} + \varepsilon B^\varepsilon, \quad B^\varepsilon = \tfrac{1}{\varepsilon}(\widetilde{\mathcal{N}}^\varepsilon(\mathcal{N}^\varepsilon)^{-1} - \widetilde{\mathcal{N}}^0(\mathcal{N}^0)^{-1}),} \tag{5.20}$$

where the matrices $\gamma_+ \in \mathcal{M}_{K-1\times K}(\mathbb{R})$ and $\zeta_+^0 \in \mathcal{M}_{K\times K-1}(\mathbb{R})$ satisfy,

$$\gamma_+ = \begin{pmatrix} \gamma_1^\top \\ \vdots \\ \gamma_{K-1}^\top \end{pmatrix} \text{ where } \gamma_\ell \in \mathbb{R}^K, \quad \gamma_\ell^\top \psi_k^0(\mathcal{V}) = \delta_{k\ell}, \quad \gamma_\ell^\top \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) = 0; \tag{5.21}$$

$$\zeta_\pm^\varepsilon = \left(\zeta_{\pm 1}^\varepsilon \cdots \zeta_{\pm(K-1)}^\varepsilon\right), \qquad \zeta_{\pm\ell}^\varepsilon = \psi_{\pm\ell}^\varepsilon(\mathcal{V}) - \psi_{\pm\ell}^\varepsilon(-\mathcal{V}) \in \mathbb{R}^K. \tag{5.22}$$

Remark 5.1 Existence of γ_+ is guaranteed by assumption (5.11). Notice that since the limits $\psi_{\pm\ell}^0$ in (5.10) do not depend on E, the first term in the decomposition of the scattering matrix is independent on E, hence on j.

Proof 1. Let vector $\beta \in \mathbb{R}^K$ be such that

$$\beta^\top \psi_\ell^0(\mathcal{V}) = 0; \quad \beta^\top \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) = 1. \tag{5.23}$$

Moreover, since

$$\gamma_+ = \begin{pmatrix} \gamma_1^\top \\ \vdots \\ \gamma_{K-1}^\top \end{pmatrix}, \text{ it comes that } \begin{pmatrix} \gamma_+ \\ \beta^\top \end{pmatrix} = \left(\psi_+^0(\mathcal{V}) \;\; \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\right)^{-1}, \tag{5.24}$$

where the latter matrix is invertible thanks to assumption (5.11). It brings also that,

$$\sum_{\ell=1}^{K-1} \psi_\ell^0(\mathcal{V})\gamma_\ell^\top + \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\beta^\top = I_K. \tag{5.25}$$

2. Similarly, as $\psi_{-\ell}^0(\mathcal{V}) = (-1)^\ell \psi_\ell^0(-\mathcal{V})$, then denoting

$$\gamma_- = \begin{pmatrix} -\gamma_1^\top \\ \gamma_2^\top \\ \vdots \\ (-1)^{K-1}\gamma_{K-1}^\top \end{pmatrix},$$

it comes that,

$$\begin{pmatrix} \gamma_- \\ \frac{1}{1-e^{-E\Delta x/\kappa}}\beta^\top \end{pmatrix} = \left(\psi_-^0(-\mathcal{V}) \;\; (1-e^{-E\Delta x/\kappa})\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\right)^{-1}. \tag{5.26}$$

3. We deduce from both (5.24) and (5.26) that,

$$(\mathcal{N}^0)^{-1} = \begin{pmatrix} \begin{pmatrix} \gamma_+ \\ \beta^\top \end{pmatrix} & \mathbf{0}_K \\ \begin{pmatrix} \mathbf{0}_{K-1\times K} \\ -\frac{1}{1-e^{-E\Delta x/\kappa}}\beta^\top \end{pmatrix} & \begin{pmatrix} \gamma_- \\ \frac{1}{1-e^{-E\Delta x/\kappa}}\beta^\top \end{pmatrix} \end{pmatrix},$$

and so, with (5.18), (5.19),

$$\mathcal{S}^\varepsilon \underset{\varepsilon\to 0}{\longrightarrow} \mathcal{S}^0 := \widetilde{\mathcal{N}}^0(\mathcal{N}^0)^{-1},$$

has the form (5.20), with

$$\widetilde{\mathcal{N}}^0(\mathcal{N}^0)^{-1} = \begin{pmatrix} \mathbf{0}_K & \sum_{\ell=1}^{K-1} \psi_\ell^0(-\mathcal{V})\gamma_\ell^\top + \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\beta^\top \\ \sum_{\ell=1}^{K-1} \psi_\ell^0(-\mathcal{V})\gamma_\ell^\top + \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\beta^\top & \mathbf{0}_K \end{pmatrix}.$$

Using (5.25) allows to complete the proof. □

Lemma 5.3 *For $E > 0$,*

$$B^0 := \lim_{\varepsilon \to 0} B^\varepsilon = \begin{pmatrix} B^{10} & B^{20} \\ B^{30} & B^{40} \end{pmatrix}, \tag{5.27}$$

where

$$\begin{aligned}
B^{10} &= \frac{1}{1 - e^{-\frac{E\Delta x}{\kappa}}} \frac{2E\mathcal{V}}{\kappa} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \beta^\top \\
&\quad - \frac{1}{1 - e^{-\frac{E\Delta x}{\kappa}}} \zeta_+^0 \gamma_+ \left(\frac{E\mathcal{V}}{\kappa} - \frac{E^2}{\kappa}\right) \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \beta^\top; \\
B^{20} &= \left(\frac{d\zeta_-^\varepsilon}{d\varepsilon}_{|\varepsilon=0} + \zeta_+^0 \gamma_+ \frac{d\psi_-^\varepsilon(-\mathcal{V})}{d\varepsilon}_{|\varepsilon=0}\right) \gamma_- - \frac{e^{-\frac{E\Delta x}{\kappa}}}{1 - e^{-\frac{E\Delta x}{\kappa}}} \frac{2E\mathcal{V}}{\kappa} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \beta^\top \\
&\quad - \frac{1}{1 - e^{-\frac{E\Delta x}{\kappa}}} \zeta_+^0 \gamma_+ \left(\frac{E^2}{\kappa} + \frac{2E\mathcal{V}}{\kappa} e^{-\frac{E\Delta x}{\kappa}}\right) \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \beta^\top; \\
B^{30} &= \left(\zeta_+^0 \gamma_+ \frac{d\psi_-^\varepsilon(\mathcal{V})}{d\varepsilon}_{|\varepsilon=0} - \frac{d\zeta_+^\varepsilon}{d\varepsilon}_{|\varepsilon=0}\right) \gamma_+ - \frac{1}{1 - e^{-\frac{E\Delta x}{\kappa}}} \frac{2E\mathcal{V}}{\kappa} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \beta^\top \\
&\quad + \frac{1}{1 - e^{-\frac{E\Delta x}{\kappa}}} \zeta_+^0 \gamma_+ \left(\frac{E\mathcal{V}}{\kappa} + \frac{E^2}{\kappa}\right) \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \beta^\top; \\
B^{40} &= \frac{e^{-\frac{E\Delta x}{\kappa}}}{1 - e^{-\frac{E\Delta x}{\kappa}}} \left(\frac{2E\mathcal{V}}{\kappa} - \zeta_+^0 \gamma_+ \left(\frac{E^2}{\kappa} + \frac{E\mathcal{V}}{\kappa}\right)\right) \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \beta^\top.
\end{aligned}$$

Proof Rewriting $B^\varepsilon = \frac{1}{\varepsilon}(\widetilde{\mathcal{N}}^\varepsilon - \widetilde{\mathcal{N}}^0 (\mathcal{N}^0)^{-1} \mathcal{N}^\varepsilon)(\mathcal{N}^\varepsilon)^{-1}$, it comes,

$$B^\varepsilon \mathcal{N}^\varepsilon = \frac{1}{\varepsilon}(\widetilde{\mathcal{N}}^\varepsilon - \widetilde{\mathcal{N}}^0 (\mathcal{N}^0)^{-1} \mathcal{N}^\varepsilon) = \frac{1}{\varepsilon} \begin{pmatrix} A^{1\varepsilon} & A^{2\varepsilon} \\ A^{3\varepsilon} & A^{4\varepsilon} \end{pmatrix},$$

with

$$\begin{aligned}
A^{1\varepsilon} &= \left((\zeta_+^\varepsilon + \zeta_+^0 \gamma_+ \psi_+^\varepsilon(-\mathcal{V})) e^{-\frac{\mu_+^\varepsilon \Delta x}{\varepsilon}} \quad \zeta_0^\varepsilon + \zeta_+^0 \gamma_+ \psi_0^\varepsilon(-\mathcal{V})\right); \\
A^{2\varepsilon} &= \left(\zeta_-^\varepsilon + \zeta_+^0 \gamma_+ \psi_-^\varepsilon(-\mathcal{V}) \quad \zeta_{-0}^\varepsilon + \zeta_+^0 \gamma_+ \psi_{-0}^\varepsilon(-\mathcal{V}) - (\zeta_0^\varepsilon + \zeta_+^0 \gamma_+ \psi_0^\varepsilon(-\mathcal{V})) e^{-\frac{E\Delta x}{\kappa}}\right); \\
A^{3\varepsilon} &= \left(\zeta_+^0 \gamma_+ \psi_+^\varepsilon(\mathcal{V}) - \zeta_+^\varepsilon \quad \zeta_+^0 \gamma_+ \psi_0^\varepsilon(\mathcal{V}) - \zeta_0^\varepsilon\right); \\
A^{4\varepsilon} &= \left((\zeta_+^0 \gamma_+ \psi_-^\varepsilon(\mathcal{V}) - \zeta_-^\varepsilon) e^{\frac{\mu_-^\varepsilon \Delta x}{\varepsilon}} \quad (\zeta_0^\varepsilon - \zeta_{-0}^\varepsilon + \zeta_+^0 \gamma_+ (\psi_{-0}^\varepsilon(\mathcal{V}) - \psi_0^\varepsilon(\mathcal{V}))) e^{-\frac{E\Delta x}{\kappa}}\right).
\end{aligned}$$

$$\boxed{\text{When } E > 0, \quad \zeta_{-0}^\varepsilon = 0, \ \text{ whereas if } E < 0, \quad \zeta_0^\varepsilon = 0.}$$

Accordingly, for $E > 0$,

$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\psi_0^\varepsilon(\mathcal{V})-\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\right)=\frac{d\psi_0^\varepsilon(\mathcal{V})}{d\varepsilon}_{|\varepsilon=0}=\frac{E\mathcal{V}}{\kappa}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right);$$
$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\left(\psi_{-0}^\varepsilon(\mathcal{V})-\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\right)=-\frac{E^2}{\kappa}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right);$$
$$\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}\zeta_0^\varepsilon=\frac{2E\mathcal{V}}{\kappa}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right),$$

and the expression (5.27) follows by doing $B^0=\left(\lim_{\varepsilon\to 0}\frac{1}{\varepsilon}A^\varepsilon\right)(\mathcal{N}^0)^{-1}$. □

5.6 Uniform accuracy with respect to ε of the final scheme

We deduce the final scheme from (1.7), which reads like (4.13),

$$\begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V})\end{pmatrix}+\frac{\Delta t}{\varepsilon\Delta x}\mathbb{V}\begin{pmatrix} f_j^{n+1}(\mathcal{V})-(\mathbf{I}_K-\zeta_+^0\gamma_+)f_j^{n+1}(-\mathcal{V}) \\ f_{j-1}^{n+1}(-\mathcal{V})-(\mathbf{I}_K-\zeta_+^0\gamma_+)f_{j-1}^{n+1}(\mathcal{V})\end{pmatrix}$$
$$=\begin{pmatrix} f_j^n(\mathcal{V}) \\ f_{j-1}^n(-\mathcal{V})\end{pmatrix}+\frac{\Delta t}{\Delta x}\mathbb{V}B_{j-\frac12}^\varepsilon\begin{pmatrix} f_{j-1}^n(\mathcal{V}) \\ f_j^n(-\mathcal{V})\end{pmatrix}. \tag{5.28}$$

Denoting again $B^\varepsilon=\begin{pmatrix} B^{1\varepsilon} & B^{2\varepsilon} \\ B^{3\varepsilon} & B^{4\varepsilon}\end{pmatrix}$, the scheme (5.28) rewrites as

$$\frac{1}{\varepsilon}\mathcal{R}^\varepsilon\begin{pmatrix} f_j^{n+1}(\mathcal{V}) \\ f_j^{n+1}(-\mathcal{V})\end{pmatrix}=\begin{pmatrix} f_j^n(\mathcal{V}) \\ f_j^n(-\mathcal{V}))\end{pmatrix}+\frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} B_{j-\frac12}^{1\varepsilon}f_{j-1}^n(\mathcal{V})+B_{j-\frac12}^{2\varepsilon}f_j^n(-\mathcal{V}) \\ B_{j+\frac12}^{3\varepsilon}f_j^n(\mathcal{V})+B_{j+\frac12}^{4\varepsilon}f_{j+1}^n(-\mathcal{V})\end{pmatrix}, \tag{5.29}$$

where

$$\mathcal{R}^\varepsilon=\varepsilon\mathbf{I}_{2K}+\frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix}\mathbf{I}_K & \zeta_+^0\gamma_+-\mathbf{I}_K \\ \zeta_+^0\gamma_+-\mathbf{I}_K & \mathbf{I}_K\end{pmatrix}.$$

After inversion of the matrix $\mathcal{R}^\varepsilon$, by construction, the scheme (5.28) satisfies the well-balanced property and is asymptotic preserving. We also define:

$$\sigma_0=\sum_{k=1}^K\omega_k e^{-v_k^2/2\kappa},\qquad \sigma_2=\sum_{k=1}^K\omega_k v_k^2\,e^{-v_k^2/2\kappa}. \tag{5.30}$$

We can now state our main result for the Vlasov–Fokker–Planck equation:

Theorem 5.1 *The scheme (5.29) is a well-balanced approximation for the Vlasov–Fokker–Planck system (5.1). It is asymptotic-preserving (AP) with respect to ε. More precisely, if we assume that (5.11)–(5.13) hold, and that $\sigma_2=\kappa\sigma_0$ in (5.30). Then, as $\varepsilon\to 0$, the macroscopic density $\rho_j^n:=\sum_{k=-K}^K\omega_k f_j^n(v_k)$ satisfies the Sharfetter–Gummel discretization (5.3).*

Remark 5.2 By integration by parts, we notice that, based on (5.30),

$$\int_0^{+\infty} v^2 e^{-v^2/(2\kappa)}\, dv = \kappa \int_0^{+\infty} e^{-v^2/(2\kappa)}\, dv.$$

Therefore, assuming $\sigma_2 = \kappa\sigma_0$ in Theorem 5.1 boils down to assume that the latter equality is also true at the discrete level.

Proof As above, we have $\mathcal{R}^\varepsilon = \mathcal{R}^0 + \varepsilon \mathbf{I}_{2K}$, where

$$\mathcal{R}^0 := \frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} \mathbf{I}_K & \zeta_+^0\gamma_+ - \mathbf{I}_K \\ \zeta_+^0\gamma_+ - \mathbf{I}_K & \mathbf{I}_K \end{pmatrix}.$$

Assuming that f admits a Hilbert expansion $f = f^0 + \varepsilon f^1 + o(\varepsilon)$, we get by identifying the terms in power of ε in (5.29),

$$\mathcal{R}^0 \begin{pmatrix} \{f^0\}_j^{n+1}(\mathcal{V}) \\ \{f^0\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} = 0, \tag{5.31}$$

and

$$\mathcal{R}^0 \begin{pmatrix} \{f^1\}_j^{n+1}(\mathcal{V}) \\ \{f^1\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} = \begin{pmatrix} \{f^0\}_j^{n}(\mathcal{V}) - \{f^0\}_j^{n+1}(\mathcal{V}) \\ \{f^0\}_j^{n}(-\mathcal{V}) - \{f^0\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} + \frac{\Delta t}{\Delta x}\mathbb{V}\begin{pmatrix} B^{10}_{j-\frac12}\{f^0\}_{j-1}^n(\mathcal{V}) + B^{20}_{j-\frac12}\{f^0\}_j^n(-\mathcal{V}) \\ B^{30}_{j+\frac12}\{f^0\}_{j}^n(\mathcal{V}) + B^{40}_{j+\frac12}\{f^0\}_{j+1}^n(-\mathcal{V}) \end{pmatrix}. \tag{5.32}$$

Under assumptions (5.11)–(5.13), we may apply Lemma C.1 in Appendix. Hence

- $\operatorname{Ker}(\mathcal{R}^0) = \operatorname{span}\left(\exp(-\frac{\mathcal{V}^2}{2\kappa})\right) = \operatorname{span}\left(\psi_0^0(\mathcal{V})\right)$,
- $\operatorname{Im}(\mathcal{R}^0) = \left\{Z = (Z_1\ Z_2)^\top,\ Z_i \in \mathbb{R}^K \text{ such that } \sum_{k=1}^K \omega_k(Z_{1k} + Z_{2k}) = 0\right\}$.

Then, Eq. (5.31) implies that f^0 is an element of $\operatorname{Ker}(\mathcal{R}^0)$:

$$\{f^0\}_j^{n+1}(\pm\mathcal{V}) = \frac{\rho_j^{n+1}}{2\sigma_0}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right).$$

Injecting this expression into (5.32), we deduce,

$$\mathcal{R}^0 \begin{pmatrix} \{f^1\}_j^{n+1}(\mathcal{V}) \\ \{f^1\}_j^{n+1}(-\mathcal{V}) \end{pmatrix} = \frac{1}{2\sigma_0}\begin{pmatrix} (\rho_j^n - \rho_j^{n+1})\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \\ (\rho_j^n - \rho_j^{n+1})\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \end{pmatrix} + \frac{\Delta t}{2\sigma_0\Delta x}\mathbb{V}\begin{pmatrix} B^{10}_{j-\frac12}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\rho_{j-1}^n + B^{20}_{j-\frac12}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\rho_j^n \\ B^{30}_{j+\frac12}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\rho_j^n + B^{40}_{j+\frac12}\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\rho_{j+1}^n \end{pmatrix}. \tag{5.33}$$

This equation admits a solution iff the right hand side belongs to $\mathrm{Im}(\mathcal{R}^0)$. Applying again Lemma C.1, we deduce the solvability condition:

$$\rho_j^n - \rho_j^{n+1} + \frac{\Delta t}{2\sigma_0 \Delta x} \sum_{k=1}^{K} \omega_k v_k \left((B^{10}_{j-\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right))_k \rho_{j-1}^n + (B^{20}_{j-\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right))_k \rho_j^n \right.$$
$$\left. + (B^{30}_{j+\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right))_k \rho_j^n + (B^{40}_{j+\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right))_k \rho_{j+1}^n \right) = 0.$$

Using [see (5.21) and (5.23)]

$$\gamma_\pm \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) = \mathbf{0}_{\mathbb{R}^{K-1}}, \qquad \beta^\top \mathbf{1}_{\mathbb{R}^K} = 1,$$

we deduce from the expression (5.27) of B^0,

$$\sum_{k=1}^{K} \omega_k v_k \left(B^{10}_{j-\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \right)_k = \frac{1}{1 - e^{-E_{j-\frac12}\Delta x/\kappa}} \frac{2E_{j-\frac12}}{\kappa} \sum_{k=1}^{K} \omega_k v_k^2 \exp\left(-\frac{v_k^2}{2\kappa}\right);$$
$$\sum_{k=1}^{K} \omega_k v_k \left(B^{20}_{j+\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \right)_k = -\frac{e^{-E_{j-\frac12}\Delta x/\kappa}}{1 - e^{-E_{j-\frac12}\Delta x/\kappa}} \frac{2E_{j-\frac12}}{\kappa} \sum_{k=1}^{K} \omega_k v_k^2 \exp\left(-\frac{v_k^2}{2\kappa}\right);$$
$$\sum_{k=1}^{K} \omega_k v_k \left(B^{30}_{j+\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \right)_k = -\frac{1}{1 - e^{-E_{j+\frac12}\Delta x/\kappa}} \frac{2E_{j+\frac12}}{\kappa} \sum_{k=1}^{K} \omega_k v_k^2 \exp\left(-\frac{v_k^2}{2\kappa}\right);$$
$$\sum_{k=1}^{K} \omega_k v_k \left(B^{40}_{j+\frac12} \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) \right)_k = \frac{e^{-E_{j+\frac12}\Delta x/\kappa}}{1 - e^{-E_{j+\frac12}\Delta x/\kappa}} \frac{2E_{j+\frac12}}{\kappa} \sum_{k=1}^{K} \omega_k v_k^2 \exp\left(-\frac{v_k^2}{2\kappa}\right).$$

Thus, we may rewrite the limiting scheme as

$$0 = \rho_j^n - \rho_j^{n+1}$$
$$+ \frac{\sigma_2 \Delta t}{\sigma_0 \Delta x} \left(\frac{E_{j-\frac12}}{\kappa} \frac{\rho_{j-1}^n - e^{-E_{j-\frac12}\Delta x/\kappa} \rho_j^n}{1 - e^{-E_{j-\frac12}\Delta x/\kappa}} - \frac{E_{j+\frac12}}{\kappa} \frac{\rho_j^n - e^{-E_{j+\frac12}\Delta x/\kappa} \rho_{j+1}^n}{1 - e^{-E_{j+\frac12}\Delta x/\kappa}} \right).$$

By assumption $\sigma_2 = \kappa\sigma_0$, we recognize the Sharfetter–Gummel scheme (5.3). □

6 Conclusion and outlook

In this paper, we proved (at the price of heavy technicalities) that most of the discretizations advocated in [27, Part II], for 1 + 1 kinetic models endowed with a non-trivial diffusive limit, converge toward Il'in/Scharfetter–Gummel's "exponential-fitting" scheme. Such a property implies that IMEX discretizations (4.14) and (5.29), which rely on S-matrices, should be "uniformly accurate" (in the sense of, e.g., [7,23,54]) with respect to the Peclet number,

$$\mathrm{Pe} = |E_{j-\frac{1}{2}}| \text{ for (4.4)}, \qquad \mathrm{Pe} = \left| \frac{E_{j-\frac{1}{2}}}{\kappa} \right| \text{ for (5.3)}.$$

In order to ensure strong stability properties for the overall discretization, the S-matrices should be endowed with left/right-stochastic properties, as recalled in Lemma 1.1: in particular, the requirement (1.15) is important for mass-preservation. This is closely related to "*matrix balancing* techniques" and Sinkhorn's algorithm [37,56]. Especially, results in [37] ensure that one can often adjust a slightly noisy S-matrix to recover a closely related one satisfying both (1.15) and the "right-stochastic" criterion.

Besides, computations in Sect. 5 indicate the importance of having steady solutions $\mathbb{R}_*^+ \ni v \mapsto \Psi_{\pm n}(x, v)$ being a T-system for any $x > 0$ and $n < N \in \mathbb{N}$. Such an issue appears to be specific to kinetic models like Fokker–Planck equations, involving a local differential operator as the collision mechanism. Indeed, the corresponding stationary boundary-value problem is usually solved by means of a modulation of Sturm–Liouville eigenfunctions, for which the so–called "Haar property" (A.1) is not obvious; for instance it may lead to "generalized polynomials", like e.g. exponential ones, for which the equivalent condition (A.2) is not satisfied in general, as recalled in our Appendix D.1

We now emphasize two possible applications of these schemes, one partly studied, the other being essentially an outlook extending the present work:

- Some $1+1$ kinetic models of chemotaxis dynamics exhibit (in sharp contrast with diffusive Keller–Segel approximations) *bi-stability phenomena of traveling waves*, within certain ranges of parameters. Practical computational simulations were achieved in [13] thanks to numerical algorithms based on both S-matrices and $\mathcal{L}$-splines discretizations of diffusive equations [31].
- In [14, Chap. 6] and [15, Chap. 5] Cercignani explains how the formalism of "Case's elementary solutions" can be extended to linearized BGK models of the Boltzmann equation in $1+3$ dimensions (see also the paper [45] and numerical computations in [26]). In [15, pp. 106–108], a (formal) passage from kinetic heat transfer system toward linearized Navier–Stokes–Fourier equations is presented. The discretization of the heat transfer system was presented in e.g. [27, Chap. 14], so that some techniques developed in this paper may shed light onto the corresponding macroscopic behavior.

An important question deals about the possibility of extending these numerical methods toward problems posed in several space dimensions. Indeed, exponential-fit methods in multi-d proceed usually by *dimensional-splitting*, relying on existing one-dimensional numerical fluxes. Exceptions are, e.g., the finite-element method in [10] and the finite-difference scheme in [8]. Defining rigorously a robust notion of well-balanced scheme in several space dimensions isn't straightforward: a tentative was recently proposed in [32].

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A Haar property, Chebyshev T-systems and Markov systems

We first recall basic notions from standard (one-dimensional) approximation theory, following mostly [18, Chapter 3].

Definition A.1 Let $n \in \mathbb{N}$ and $F_n = (f_1, f_2, \ldots, f_n)$ be a family of functions, continuous on an interval $I \subset \mathbb{R}$: it is endowed with the Haar property if, for any strictly increasing family $X = (x_1, x_2, \ldots, x_n) \in I^n$, the family of n vectors $(f_1(X), f_2(X), \ldots, f_n(X))$ is linearly independent. Equivalently, the determinant never vanishes: $\forall\, (x_1, x_2, \ldots, x_n) \in I^n,\ x_1 < x_2 < \cdots < x_n$,

$$\begin{vmatrix} f_1(x_1) & f_2(x_1) & \cdots & f_n(x_1) \\ f_1(x_2) & f_2(x_2) & \cdots & f_n(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ f_1(x_n) & f_2(x_n) & \cdots & f_n(x_n) \end{vmatrix} \neq 0. \tag{A.1}$$

Such a family F_n constitutes a Chebyshev T-system on the interval I.

The simplest example of T-system on $I = \mathbb{R}$ is the monomials family, for which the determinant (A.1) is the well-known *Vandermonde* determinant.

Definition A.2 Let $F = (f_1, f_2, \ldots)$ be an infinite sequence of functions, continuous on an interval $I \subset \mathbb{R}$: it is said to be a Markov system if, for any $n \in \mathbb{N}$, the extracted finite family $F_n \subset F$ is a Chebyshev T-system.

A standard, yet important result is the following:

Proposition A.1 *Let $n \in \mathbb{N}$ and $F_n = (f_1, f_2, \ldots f_n)$ be as in Definition A.1: it is a T-system on I if and only if any (real, and non trivial) linear combination,*

$$\forall (a_1, a_2, \ldots, a_n) \in \mathbb{R}^n, \qquad I \ni x \mapsto \sum_{i=1}^{n} a_i\, f_i(x), \tag{A.2}$$

admits at most $n - 1$ real roots on I.

Remark A.1 Determinants of the type (A.1) are called "alternant determinants", see [57, Chapter 4]. Moreover, the Haar property is closely related to "total positivity" of matrices, see e.g. [24]. Being the "Hadamard product" the component-wise product of two $n \times n$ matrices,

$$(A \circ B)_{1 \le i,j \le n} := A_{i,j}\, B_{i,j},$$

Garloff and Wagner in [24, page 100], explain that the Haar property is not generally preserved by multiplying elements of two T-systems with each other. A first exception is given by two generalized Vandermonde matrices $G_n = (x_i^{\alpha_j})_{1 \le i,j,n}$ sharing either the set of points X or the exponents α_i's. A second one is given by non-negative exponential monomials: see Theorem D.1.

B. Some properties on Case's eigenelements

In this Appendix, we establish some useful properties on the eigenfunctions defined in Proposition 3.1. First we show that the set of Case's eigenfunctions is endowed with the Haar property (see Definition A.1).

Proposition B.1 *Denote $\phi_\lambda(v) = \frac{1}{1-\lambda v}$ for $\lambda \geq 0$, then the following properties hold:*

(i) Let $0 < \lambda_1 < \cdots < \lambda_{K-1}$ and $0 < v_1 < \cdots < v_K$. We denote $\mathcal{V} = (v_1, \dots, v_K)^\top$. Then, the family $\{\mathbf{1}_{\mathbb{R}^K}, \phi_{\lambda_1}(\mathcal{V}), \dots, \phi_{\lambda_{K-1}}(\mathcal{V})\}$ is a basis of $\mathbb{R}^K$.
(ii) The set $(\phi_\lambda)_{\lambda \geq 0}$ is a Markov system on $\mathbb{R}_*^+$ in the sense of Definition A.2.
(iii) There exists $\beta \in \mathbb{R}^K$ and $\gamma \in \mathcal{M}_{K-1\times K}(\mathbb{R})$ such that

$$\begin{pmatrix} \beta^\top \\ \gamma \end{pmatrix} = \begin{pmatrix} \mathbf{1}_{\mathbb{R}^K} & \phi_{\lambda_1}(\mathcal{V}) & \cdots & \phi_{\lambda_{K-1}}(\mathcal{V}) \end{pmatrix}^{-1}.$$

Proof These properties are shown by studying convenient polynomials.

(i) As the family contains K vectors, it suffices to show its linear independence: Assume

$$\exists a_0, a_1, \dots, a_K, \qquad a_0 \mathbf{1}_{\mathbb{R}^K} + \sum_{i=1}^{K-1} a_i \phi_{\lambda_i}(\mathcal{V}) = \mathbf{0}_{\mathbb{R}^K},$$

let us show that $a_0 = a_1 = \cdots = a_{k-1} = 0$. Using the expression of ϕ_λ and multiplying,

$$\forall k \in \{1, \dots, K\}, \qquad \left(a_0 + \sum_{i=1}^{K-1} \frac{a_i}{1 - \lambda_i v_k} \right) \times \prod_{j=1}^{K-1} (1 - \lambda_j v_k) = 0.$$

Thus, for any $k \in \{1, \dots, K\}$, the polynomial

$$v \mapsto P(v) := a_0 \prod_{j=1}^{K-1} (1 - \lambda_j v) + \sum_{i=1}^{K-1} a_i \prod_{j=1, j \neq i}^{K-1} (1 - \lambda_j v)$$

has degree $K - 1$, but K roots $\{v_1, \dots, v_K\}$, so that P is a null polynomial, i.e.

$$\forall v \in \mathbb{R}, \qquad P(v) = 0.$$

Identifying the term of higher degree, we deduce that $a_0 = 0$. Then, taking $v = 1/\lambda_i$, $i \in \{1, \dots, K-1\}$, we obtain $a_i = 0$, for all $i \in \{1, \dots, K-1\}$.

(ii) From (i), since the values of both $K \in \mathbb{N}$ and λ's are arbitrary, the set $(\phi_\lambda(v))_{\lambda \geq 0}$ clearly constitutes a Markov system.

(iii) The point (i) implies that the matrix $\begin{pmatrix} \mathbf{1}_{\mathbb{R}^K} & \phi_{\lambda_1}(\mathcal{V}) & \cdots & \phi_{\lambda_{K-1}}(\mathcal{V}) \end{pmatrix}$ is invertible. □

For our next property, we consider two sets of positive numbers $0 < \lambda_1 < \cdots < \lambda_{K-1}$ and $0 < \mu_1 < \cdots < \mu_{K-1}$ with corresponding Case's eigenfunctions $(\phi_\lambda)_\lambda$ and $(\phi_\mu)_\mu$. We denote γ_1, respectively γ_2, the corresponding matrices defined in Proposition B.1 (iii) for the set $(\lambda_i)_i$, respectively (μ_i). We introduce

$$\zeta_1 = \Big(\phi_{\lambda_1}(\mathcal{V}) - \phi_{\lambda_1}(-\mathcal{V}), \ldots, \phi_{\lambda_{K-1}}(\mathcal{V}) - \phi_{\lambda_{K-1}}(-\mathcal{V})\Big)$$
$$\zeta_2 = \Big(\phi_{\mu_1}(\mathcal{V}) - \phi_{\mu_1}(-\mathcal{V}), \ldots, \phi_{\mu_{K-1}}(\mathcal{V}) - \phi_{\mu_{K-1}}(-\mathcal{V})\Big)$$

Then, let us denote

$$\mathcal{H} = \begin{pmatrix} \mathbf{I}_K & \zeta_2\gamma_2 - \mathbf{I}_K \\ \zeta_1\gamma_1 - \mathbf{I}_K & \mathbf{I}_K \end{pmatrix}.$$

The following Lemma shed light onto the kernel and the range of $\mathcal{H}$:

Lemma B.1 *With the above notations, let us assume moreover that*

$$\forall i, \quad \sum_{k=1}^{K} \omega_k v_k(\phi_{\lambda_i}(v_k) - \phi_{\lambda_i}(-v_k)) = \sum_{k=1}^{K} \omega_k v_k(\phi_{\mu_i}(v_k) - \phi_{\mu_i}(-v_k)) = 0.$$

Then, the matrix $\mathcal{H}$ is such that:

- *$Ker(\mathcal{H}) = Span(\mathbf{1}_{\mathbb{R}^{2K}})$,*
- *$Im(\mathcal{H}) = \Big\{Z = (Z_1\ Z_2)^\top,\ Z_i \in \mathbb{R}^K$ such that $\sum_{k=1}^K \omega_k(Z_{1k} + Z_{2k}) = 0\Big\}$.*

Proof – Pick $Y = (Y_1\ Y_2)^\top \in \mathrm{Ker}(\mathcal{H})$, then

$$Y_1 - Y_2 = \zeta_1\gamma_1 Y_1 = -\zeta_2\gamma_2 Y_2.$$

Since, from Proposition B.1, the families $\{\mathbf{1}_{\mathbb{R}^K}, \phi_{\lambda_1}(\mathcal{V}), \ldots, \phi_{\lambda_{K-1}}(\mathcal{V})\}$ and $\{\mathbf{1}_{\mathbb{R}^K}, \phi_{\mu_1}(\mathcal{V}), \ldots, \phi_{\mu_{K-1}}(\mathcal{V})\}$ are basis of $\mathbb{R}^K$, we may write

$$Y_1 = a_0 + \sum_{\ell=1}^{K-1} a_\ell \phi_{\lambda_\ell}(\mathcal{V}), \qquad Y_2 = b_0 + \sum_{\ell=1}^{K-1} b_\ell \phi_{\mu_\ell}(\mathcal{V}).$$

By definition of ζ_i and γ_i, $i = 1, 2$, we have

$$\zeta_1\gamma_1 Y_1 = \sum_{\ell=1}^{K-1} a_\ell(\phi_{\lambda_\ell}(\mathcal{V}) - \phi_{\lambda_\ell}(-\mathcal{V})), \qquad \zeta_2\gamma_2 Y_2 = \sum_{\ell=1}^{K-1} b_\ell(\phi_{\mu_\ell}(\mathcal{V}) - \phi_{\mu_\ell}(-\mathcal{V})).$$

Thus from the equalities $Y_1 = Y_2 - \zeta_2\gamma_2 Y_2$ and $Y_2 = Y_1 - \zeta_1\gamma_1 Y_1$, we deduce

$$a_0 - b_0 + \sum_{\ell=1}^{K-1} \Big(a_\ell \phi_{\lambda_\ell}(\mathcal{V}) - b_\ell \phi_{\mu_\ell}(-\mathcal{V}) \Big) = 0,$$
$$a_0 - b_0 + \sum_{\ell=1}^{K-1} \Big(a_\ell \phi_{\lambda_\ell}(-\mathcal{V}) - b_\ell \phi_{\mu_\ell}(\mathcal{V}) \Big) = 0.$$

We now proceed as in the proof of Proposition B.1 by introducing the polynomial

$$\begin{aligned} v \mapsto Q(v) := (a_0 - b_0) &\prod_{i=1}^{K-1} (1 - \lambda_i v) \prod_{j=1}^{K-1} (1 + \mu_j v) \\ &+ \sum_{\ell=1}^{K-1} a_\ell \prod_{i=1, i\neq \ell}^{K-1} (1 - \lambda_i v) \prod_{j=1}^{K-1} (1 + \mu_j v) \\ &- \sum_{\ell=1}^{K-1} b_\ell \prod_{i=1}^{K-1} (1 - \lambda_i v) \prod_{j=1, j\neq \ell}^{K-1} (1 + \mu_j v). \end{aligned}$$

This is a polynomial of degree $2(K-1)$ which admits the $2K$ roots, $\pm v_1, \dots, \pm v_K$ (from above equalities). So it is the null polynomial. Picking the values $v = 1/\lambda_\ell$ and $v = -1/\mu_\ell$, $\ell = 1, \dots, K-1$, we deduce that $a_0 = b_0$, $a_\ell = 0$, and $b_\ell = 0$, for $\ell = 1, \dots, K-1$. Therefore, $Y_1 = Y_2 = a_0 \mathbf{1}_{\mathbb{R}^K}$.

– Consider an element in the range of $\mathcal{H}$, $Z = \mathcal{H}Y$, with $Z = (Z_1\ Z_2)^\top$, $Y = (Y_1\ Y_2)^\top$, $Z_i \in \mathbb{R}^K$, $Y_i \in \mathbb{R}^K$, $i = 1, 2$. Then,

$$\sum_{k=1}^{K} \omega_k (Z_{1k} + Z_{2k}) = \sum_{k=1}^{K} \omega_k v_k \sum_{\ell=1}^{K} \big((\zeta_1\gamma_1)_{k\ell} Y_{1\ell} + (\zeta_2\gamma_2)_{k\ell} Y_{2\ell} \big).$$

Applying our assumption, we get

$$\forall \ell, \qquad \sum_{k=1}^{K} \omega_k v_k (\zeta_1\gamma_1)_{k\ell} = 0, \quad \sum_{k=1}^{K} \omega_k v_k (\zeta_2\gamma_2)_{k\ell} = 0,$$

so, for any $Z = (Z_1\ Z_2)^\top \in \mathrm{Im}(\mathcal{H})$, we have $\sum_{k=1}^{K} \omega_k (Z_{1k} + Z_{2k}) = 0$. The dimension of $\mathrm{Ker}(\mathcal{H})$ is 1, so, thanks to the rank-nullity Theorem, equalities are as claimed in Lemma B.1. □

C. Properties of eigenelements of VFP

This appendix is devoted to the proof of an analogue of Lemma B.1 for the VFP case under assumptions on the set of discrete velocities. We first define the useful notations.

Let ψ_ℓ^0, $\ell = 0, \ldots, K-1$, be defined as in (5.10). Let us assume that assumptions (5.11)–(5.13) on the velocity quadrature hold. Therefore, there exists $\beta \in \mathbb{R}^K$ and $\gamma \in \mathcal{M}_{K-1\times K}(\mathbb{R})$ such that

$$\begin{pmatrix} \beta^\top \\ \gamma \end{pmatrix} = \begin{pmatrix} \psi_0^0(\mathcal{V}) & \psi_1^0(\mathcal{V}) & \cdots & \psi_{K-1}^0(\mathcal{V}) \end{pmatrix}^{-1}.$$

We introduce $\zeta_\ell := \psi_\ell^0(\mathcal{V}) - \psi_\ell^0(-\mathcal{V})$, and $\zeta := \begin{pmatrix} \zeta_1 & \ldots & \zeta_{K-1} \end{pmatrix} \in \mathcal{M}_{K\times K-1}(\mathbb{R})$. Then we denote the matrix

$$\mathcal{H} = \begin{pmatrix} \mathbf{I}_K & \zeta\gamma - \mathbf{I}_K \\ \zeta\gamma - \mathbf{I}_K & \mathbf{I}_K \end{pmatrix}.$$

Lemma C.1 *With the above notations, if we assume that* (5.11)–(5.13) *hold. Then,*

- *Ker*$(\mathcal{H})$ = *span* $\left(\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)\right)$ = *span* $\left(\psi_0^0(\mathcal{V})\right)$,
- *Im*$(\mathcal{H}) = \left\{Z = (Z_1\ Z_2)^\top,\ Z_i \in \mathbb{R}^K \text{ such that } \sum_{k=1}^K \omega_k(Z_{1k} + Z_{2k}) = 0\right\}$.

Proof We proceed as in the proof of Lemma B.1.

- Let $Y = (Y_1\ Y_2)^\top \in \mathrm{Ker}(\mathcal{H})$, then

$$Y_1 - Y_2 = \zeta\gamma Y_1 = -\zeta\gamma Y_2.$$

By assumption (5.11), the family $\{\psi_0^0(\mathcal{V}),\ \psi_1^0(\mathcal{V}), \ldots,\ \psi_{K-1}^0(\mathcal{V})\}$ is a basis of $\mathbb{R}^K$, then, we may write

$$Y_1 = \sum_{\ell=0}^{K-1} a_\ell \psi_\ell^0(\mathcal{V}), \qquad Y_2 = \sum_{\ell=0}^{K-1} b_\ell \psi_\ell^0(\mathcal{V}).$$

Simple computations using the definition of ζ and γ and recalling that $\psi_0^0(\mathcal{V}) = \exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right)$, give

$$\zeta\gamma Y_1 = \sum_{\ell=1}^{K-1} a_\ell(\psi_\ell^0(\mathcal{V}) - \psi_\ell^0(-\mathcal{V})), \qquad \zeta\gamma Y_2 = \sum_{\ell=1}^{K-1} b_\ell(\psi_\ell^0(\mathcal{V}) - \psi_\ell^0(-\mathcal{V})).$$

Thus the equalities $Y_1 = Y_2 - \zeta\gamma Y_2$ and $Y_2 = Y_1 - \zeta\gamma Y_1$ imply

$$(a_0 - b_0)\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) + \sum_{\ell=1}^{K-1}\left(a_\ell\psi_\ell^0(\mathcal{V}) - b_\ell\psi_\ell^0(-\mathcal{V})\right) = 0,$$

$$(a_0 - b_0)\exp\left(-\frac{\mathcal{V}^2}{2\kappa}\right) + \sum_{\ell=1}^{K-1}\left(a_\ell\psi_\ell^0(-\mathcal{V}) - b_\ell\psi_\ell^0(\mathcal{V})\right) = 0.$$

From assumption (5.12), we deduce that $a_0 = b_0$, $a_\ell = 0$, $b_\ell = 0$, for $\ell = 1, \dots, K-1$. As a consequence $Y_1 = Y_2 = a_0 \psi_0^0(\mathcal{V})$.

- Consider an element in the range of $\mathcal{H}$, $Z = \mathcal{H}Y$, with $Z = (Z_1\ Z_2)^\top$, $Y = (Y_1\ Y_2)^\top$, $Z_i \in \mathbb{R}^K$, $Y_i \in \mathbb{R}^K$, $i = 1, 2$. Then,

$$\sum_{k=1}^{K} \omega_k (Z_{1k} + Z_{2k}) = \sum_{k=1}^{K} \omega_k v_k \sum_{\ell=1}^{K} (\zeta\gamma)_{k\ell} \big(Y_{1\ell} + Y_{2\ell}\big).$$

  Applying our assumption, we get

$$\forall \ell, \qquad \sum_{k=1}^{K} \omega_k v_k (\zeta\gamma)_{k\ell} = 0,$$

  so, for any $Z = (Z_1\ Z_2)^\top \in \mathrm{Im}(\mathcal{H})$, we have $\sum_{k=1}^{K} \omega_k (Z_{1k} + Z_{2k}) = 0$. The dimension of $\mathrm{Ker}(\mathcal{H})$ is 1, so, thanks to the rank-nullity Theorem, $\mathrm{rank}(\mathcal{H}) = K - 1$, which allows to conclude the proof. □

D. Some properties of exponential polynomials

D.1 Elementary proof of the Pólya–Szegö estimate

Hereafter, following [42, page 10], we establish *by induction* a simple bound on the number of real roots of an exponential polynomial; for various extensions, see [58,59]

$$\forall n \in \mathbb{N}, \qquad f_n(x) = \sum_{i=0}^{n-1} P_i(x) \exp(\mu_i\, x), \qquad \mu_i \in \mathbb{R}, \quad \deg(P_i) = k_i.$$

We intend to show that, for any $n \in \mathbb{N}$, f_n admits *at most* $N_n - 1$ roots, where

$$N_n = \left(\sum_{i=0}^{n-1} (1 + k_i) \right). \tag{D.1}$$

We use an induction on n:

- for $n = 1$, the exponential polynomial reads $f_1(x) = P_0(x) \exp(\mu_0\, x)$ so it admits at most $k_0 = N_1 - 1$ roots.
- Assume the property (D.1) holds for f_n, so that it admits at most $N_n - 1$ real roots. Let M be the number ot real roots of f_{n+1}, and define

$$\forall x \in \mathbb{R}, \qquad f_{n+1}(x)\exp(-\mu_n\, x) = \sum_{i=0}^{n} P_i(x)\exp((\mu_i - \mu_n)\, x)$$
$$= P_n(x) + \sum_{i=0}^{n-1} P_i(x)\exp((\mu_i - \mu_n)\, x).$$

By the classical Rolle's theorem for smooth functions, its $(1+k_n)$th derivative

$$\forall x \in \mathbb{R}, \qquad g_{n+1}(x) = \frac{d^{(1+k_n)}}{dx^{(1+k_n)}}[f_{n+1}(x)\exp(-\mu_n\, x)]$$
$$= \sum_{i=0}^{n-1} \frac{d^{(1+k_n)}}{dx^{(1+k_n)}}[P_i(x)\exp((\mu_i - \mu_n)\, x)],$$

admits at least $M-(1+k_n)$ roots. But since g_{n+1} is an exponential polynomial to which (D.1) applies, it comes that

$$M-(1+k_n) \le N_n - 1, \qquad \text{so that} \quad M \le N_n + (1+k_n) - 1 := N_{n+1} - 1.$$

D.2. Haar property for exponential monomials

Although the former estimate suggests that exponential polynomials do not constitute a Chebyshev T-system, *non-negative exponential monomials* do satisfy the Haar property on $(0,+\infty)$:

Theorem D.1 (Krattenthaller [43]) *Let* $(x_0, x_1, \dots, x_{n-1}) \in \mathbb{R}_+^n$, $(y_0, y_1, \dots, y_{n-1}) \in \mathbb{R}_+^n$ *be non-negative with* $y_0 < y_1 < \cdots < y_{n-1}$. *Moreover, let* $(z_0, z_1, \dots, z_{n-1}) \in \mathbb{N}^n$ *be non-negative integers with* $z_0 < z_1 < \cdots < z_{n-1}$. *The generalized Vandermonde determinant,*

$$\det_{0\le i,j<n}\left(e^{y_j x_i} x_i^{z_j}\right) \tag{D.2}$$

vanishes if and only if two of the x_i*'s are equal to each other.*

The proof of this result relies on an expansion of the exponential and the use of Schur functions [44,46,47].

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