Large time asymptotics for a fully discretized Fokker-Planck type equation

R. Plato *

Institute of Mathematics, Technical University Berlin,

Straße des 17. Juni 135, 10623 Berlin, Germany

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Abstract

An initial-value problem for a Fokker-Planck type equation on an unbounded space domain is discretized in time by an implicit Euler scheme and in space by a Galerkin scheme. It is shown that this scheme conserves mass, positivity and decay of the entropy. The approximation properties are investigated and numerical experiments are provided.

1 Introduction

1.1 Basic notations, motivation

In this paper we consider the following initial-value problem for the real-valued function $\rho(t,x),\ t \geq 0,\ x \in \mathbb{R}^d$:

$$\frac{\partial \rho}{\partial t} = \mathbf{div}\big[D\nabla\rho + \rho(D\nabla A + F)\big] \qquad \text{for } x \in \mathbb{R}^d, \quad t > 0, \tag{1.1}$$

$$\rho(t=0,x) = \rho_0(x) \qquad \text{for } x \in \mathbb{R}^d. \tag{1.2}$$

Here $d \geq 1$ holds, and **div** denotes the divergence operator considered with respect to the space variable x. Moreover, the functions

$$D(x) \in \mathbb{R}^{d\times d} \qquad \text{with } D(x) = D(x)^\top, \quad D(x) \text{ positive definite uniformly } \forall\ x \in \mathbb{R}^d,$$
$$A(x) \in \mathbb{R}, \qquad F(t,x) \in \mathbb{R}^d, \qquad \rho_0(x) \in \mathbb{R} \qquad \text{for } t \geq 0,\ x \in \mathbb{R}^d,$$

are given. More conditions on the diffusion matrix $D(x)$, the potential A, the vector field F and the initial function ρ_0 are given below.

The drift-diffusion equation of the form (1.1) with $F \equiv 0$ is known as Fokker-Planck equation (Risken [12], Soize [13]). It arises, for example, in the mathematical modeling of Brownian motion of particles (see again [12], [13]) or the light-induced orientation process of dye-liquid-crystal systems, see Palffy-Muhoray, Kosa and E [10]. Drift-diffusion equations of the form (1.1) may also arise as part of a Gummel iteration for the numerical solution of van Roosbroecks equation which models the charge carrier transport in semiconductor devices (see e.g. Gajewski and Gärtner [5] and the references there).

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1.2 Properties of solutions

We next recall some well-known results on existence, uniqueness and basic properties of solutions to the Fokker-Planck type equation (1.1)-(1.2). If the coefficients of the considered equation (1.1) are sufficiently smooth and decay sufficiently rapidly for $|x|_2 = (\sum_{k=1}^d x_k^2)^{1/2} \to \infty$ and if $\rho_0 \in L^1(\mathbb{R}^d)$ is satisfied, then there exists a strong solution ρ of (1.1)-(1.2) which satisfies $\rho(t,\cdot) \in L^1(\mathbb{R}^d)$ and $\rho_t(t,\cdot) \in L^1(\mathbb{R}^d)$ for each $t > 0$, and this solution is unique within that class of functions. Additionally, positivity of the initial function ρ_0 implies positivity of that solution ρ (cf. e.g., Friedman [4] for more details) and we have conservation of mass, i.e., $\int_{\mathbb{R}^d} \rho(t,x)dx = \int_{\mathbb{R}^d} \rho_0(x)dx,\ t \geq 0$, holds (which results from an integration of (1.1) with respect to x). We now consider the following function,

$$\rho_\infty(x) := \exp(-A(x)) \qquad \text{for } \ x \in \mathbb{R}^d, \tag{1.3}$$

and assume for a moment that $\mathbf{div}[\rho_\infty F(t,\cdot)] = 0$ holds for each $t \geq 0$ (below we will consider a weak formulation). If the functions ρ_∞ and ρ_0 are integrable on $\mathbb{R}^d$ and $\int_{\mathbb{R}^d} \rho_0(x)dx = \int_{\mathbb{R}^d} \rho_\infty(x)dx$ is satisfied, then the considered solution ρ converges to the steady state ρ_∞ of (1.1) as $t \to \infty$. The corresponding speed of convergence to the steady state can be measured in terms of certain convex functionals and decays exponentially, respectively. For more details see e.g., Arnold et. al. [1] or Section 4 of this paper.

For the numerical solution of problems of the form (1.1), certain time-discrete schemes and its properties like conservation of positivity and mass as well as speed of convergence of the approximate states towards equilibrium are investigated recently, see e.g. Arnold and Unterreiter [2] or Jordan, Kinderlehrer and Otto ([6], [7]). In the present paper we consider a standard numerical scheme for (1.1)–(1.2) which is discrete both with respect to time and space and has similar conservation properties.

1.3 Formulation of assumptions

For the numerical solution of the Fokker-Planck type equation (1.1)-(1.2), the unknown function ρ in (1.1)-(1.2) is scaled as follows,

$$u(t,x) = \rho(t,x)/\rho_\infty(x) \qquad \text{for } \ x \in \mathbb{R}^d, \quad t > 0,$$

which leads to the following initial value problem for the function u,

$$\rho_\infty \frac{\partial u}{\partial t} \ = \ \mathbf{div}(\rho_\infty D \nabla u) \ + \ \mathbf{div}(\rho_\infty u F) \qquad \text{for } \ x \in \mathbb{R}^d, \quad t > 0, \tag{1.4}$$

$$u(t=0,x) \ = \ \rho_0(x)/\rho_\infty(x) \qquad \text{for } \ x \in \mathbb{R}^d. \tag{1.5}$$

As a further preparation we introduce weighted L^2- and weighted Sobolev spaces of real-valued functions:

$$L^2_{\rho_\infty}(\mathbb{R}^d) \ = \ \Big\{ u : \mathbb{R}^d \to \mathbb{R} : \int_{\mathbb{R}^d} |u|^2 \rho_\infty dx < \infty \Big\},$$

$$H^1_{\rho_\infty, D}(\mathbb{R}^d) \ = \ \Big\{ u \in L^2_{\rho_\infty}(\mathbb{R}^d) : \int_{\mathbb{R}^d} \nabla^\top u \cdot D \cdot \nabla u \rho_\infty dx < \infty \Big\},$$

which are equipped with the following inner products,

$$\begin{aligned}\langle u,v\rangle_{L^2_{\rho_\infty}} &= \int_{\mathbb{R}^d} uv\rho_\infty dx \qquad \text{for } u,v\in L^2_{\rho_\infty}(\mathbb{R}^d),\\ \langle u,v\rangle_{H^1_{\rho_\infty,D}} &= \int_{\mathbb{R}^d} uv\rho_\infty dx \;+\; \int_{\mathbb{R}^d} \nabla^\top u\cdot D\cdot\nabla v\rho_\infty dx \qquad \text{for } u,v\in H^1_{\rho_\infty,D}(\mathbb{R}^d),\end{aligned}$$

respectively. Here, all derivatives are understood in a weak sense, and in addition the following assumptions are imposed:

A.1 $D^{1/2}(\cdot)\in[L^\infty(\mathbb{R}^d)]^{d\times d}$;

A.2 $D^{-1/2}(\cdot)F(t,\cdot)\in[L^\infty(\mathbb{R}^d)]^d$ uniformly for $t\geq 0$;

A.3 $\rho_\infty\in L^1(\mathbb{R}^d)$, $\qquad \rho_0\in L^1(\mathbb{R}^d)$, $\qquad \int_{\mathbb{R}^d}\rho_0(x)dx=\int_{\mathbb{R}^d}\rho_\infty(x)dx$.

Conditions A.1 and A.2 are needed below for a weak formulation of an iterative scheme to solve the scaled Fokker-Planck type equation (1.4)-(1.5). The first assumption in A.3 implies that constant functions belong to $L^2_{\rho_\infty}(\mathbb{R}^d)$, and on the other hand it excludes the case $A\equiv 0$, i.e., the consideration of the classical diffusion equation. We finally note that for nonnegative functions ρ_0, the mass identity in A.3 can always be obtained by replacing the potential A with $A+c$ for an appropriate real number c.

We additionally suppose that $\mathbf{div}[\rho_\infty F(t,\cdot)]=0$ holds for each $t\geq 0$ in the following weak sense,

A.4 $$\int_{\mathbb{R}^d} v\nabla^\top v\cdot F(t,\cdot)\rho_\infty dx \;=\; 0 \qquad \forall v\in H^1_{\rho_\infty,D}(\mathbb{R}^d), \qquad t\geq 0.$$

This weak formulation is obtained by multiplying $\mathbf{div}[\rho_\infty F(t,\cdot)]$ with the function v^2 and employing a partial integration then. Note that it follows from assumption A.2 that the integral in A.4 in fact exists.

1.4 A numerical scheme

In the sequel we consider a discretized version of the initial-value problem for the scaled Fokker-Planck type equation (1.4)-(1.5). We suppose that the three assumptions A.1 – A.3 are satisfied, and then the time derivative $\frac{\partial u}{\partial t}$ on the left-hand side of the scaled Fokker-Planck type equation (1.4) is replaced by backward differences. For the resulting method we consider a weak formulation, and for this purpose let

$$\mathcal{S}\subset H^1_{\rho_\infty,D}(\mathbb{R}^d), \qquad u^0\in\mathcal{S}, \tag{1.6}$$

with $u^0\approx\rho_0/\rho_\infty$, and $\mathcal{S}$ is supposed to be a linear subspace. The resulting scheme is of the following form: determine functions u^m for $m=1,2,\ldots$ with

$$\begin{aligned}u^m\in\mathcal{S}, \qquad \int_{\mathbb{R}^d} u^m v\rho_\infty dx \;&=\; \int_{\mathbb{R}^d} u^{m-1}v\rho_\infty dx \;-\; \Delta t\int_{\mathbb{R}^d}\nabla^\top u^m\cdot D\cdot\nabla v\rho_\infty dx\\ &\quad -\;\Delta t\int_{\mathbb{R}^d} u^m\nabla^\top v\cdot F(m\Delta t,\cdot)\rho_\infty dx \qquad \forall v\in\mathcal{S},\\ &\qquad\qquad m=1,2,\ldots,\end{aligned} \tag{1.7}$$

with the intention

$$\rho^m := u^m \rho_\infty \approx \rho(m\Delta t, \cdot) \qquad \text{for } \; m = 0, 1, \dots \; . \tag{1.8}$$

The special situation $\mathcal{S} = H^1_{\rho_\infty, D}(\mathbb{R}^d)$ and $u^0 = \rho_0/\rho_\infty \in H^1_{\rho_\infty, D}(\mathbb{R}^d)$ with $u^0 \geq 0$ on $\mathbb{R}^d$ is considered in Arnold and Unterreiter [2]. There, with similar assumptions as in A.1-A.4 existence, uniqueness, nonnegativity and convergence towards the steady state is shown for the approximations $\rho^m = u^m \rho_\infty$ with $u^m \in H^1_{\rho_\infty, D}(\mathbb{R}^d)$ for $m = 1, 2, \dots$. In the present paper we derive similar results for a finite-dimensional setting which is obtained by considering linear subspaces $\mathcal{S} \subset H^1_{\rho_\infty, D}(\mathbb{R}^d)$ with $\dim \mathcal{S} < \infty$. In addition we will consider the approximation properties of the scheme (1.7) at fixed times $t > 0$, respectively.

2 Matrix version of the numerical scheme, mass conservation

In the sequel we suppose that the four assumptions A.1 – A.4 are satisfied and consider the scheme (1.7) with a finite-dimensional subspace $\mathcal{S} \subset H^1_{\rho_\infty, D}(\mathbb{R}^d)$. Using the notation $N := \dim \mathcal{S}$, we assume that

$$s_1, s_2, \dots, s_N \in \mathcal{S} \quad \text{is a basis} \tag{2.1}$$

of the subspace $\mathcal{S}$. With the notations

$$u^m \;=\; \sum_{\ell=1}^{N} \alpha_\ell^m s_\ell, \qquad \alpha^m \;=\; (\alpha_\ell^m)_{\ell=1..N} \in \mathbb{R}^N \qquad \text{for } \; m = 0, 1, \dots, \tag{2.2}$$

the scheme (1.7) can be written in the following form,

$$(G \;+\; \Delta t(B \;+\; C_m))\alpha^m \;=\; G\alpha^{m-1} \qquad \text{for } \; m = 1, 2, \dots \; . \tag{2.3}$$

Here, the matrices $G \in \mathbb{R}^{N\times N}$ and $B \in \mathbb{R}^{N\times N}$ are defined as follows,

$$G \;=\; \begin{pmatrix} g_{11} \cdots & g_{1N} \\ \vdots \;\; \ddots & \vdots \\ g_{N1} \cdots & g_{NN} \end{pmatrix} \qquad \text{with} \quad g_{k\ell} \;=\; \int_{\mathbb{R}^d} s_\ell s_k \rho_\infty dx,$$

and

$$B \;=\; \begin{pmatrix} b_{11} \cdots & b_{1N} \\ \vdots \;\; \ddots & \vdots \\ b_{N1} \cdots & b_{NN} \end{pmatrix} \qquad \text{with} \quad b_{k\ell} \;=\; \int_{\mathbb{R}^d} \nabla^\top s_\ell \cdot D \cdot \nabla s_k \rho_\infty dx. \tag{2.4}$$

Moreover, the matrix C_m is defined as follows,

$$C_m \;=\; \begin{pmatrix} c_{11}^m \cdots & c_{1N}^m \\ \vdots \;\; \ddots & \vdots \\ c_{N1}^m \cdots & c_{NN}^m \end{pmatrix} \qquad \text{with} \quad c_{k\ell}^m \;=\; \int_{\mathbb{R}^d} s_\ell \nabla^\top s_k \cdot F(m\Delta t, \cdot)\rho_\infty dx.$$

Obviously, the matrix $G \in \mathbb{R}^{N\times N}$ is symmetric and positive definite, and the matrix $B \in \mathbb{R}^{N\times N}$ is symmetric and positive semidefinite. In addition, for each m the matrix $C_m \in \mathbb{R}^{N\times N}$ defines an alternating quadratic form, i.e., we have $\alpha^\top C_m \alpha \geq 0$ for each $\alpha \in \mathbb{R}^N$ which in fact follows from assumption A.4. This implies that the matrix $G + \Delta t(B + C_m) \in \mathbb{R}^{N\times N}$ in the implicit iteration scheme (2.3) is nonsingular.

We now consider mass conservation of the iterates $\rho^m = u^m \rho_\infty$ with u^m determined by the scheme (1.7). For this purpose we suppose that $\mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}$ holds, where $\mathbf{1}_{\mathbb{R}^d} : \mathbb{R}^d \to \mathbb{R}$ denotes the characteristic function on $\mathbb{R}^d$, i.e.,

$$\mathbf{1}_{\mathbb{R}^d}(x) = 1 \qquad \text{for } \; x \in \mathbb{R}^d.$$

An application of the identity (1.7) with the constant function $v \equiv \mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}$ then yields $\int_{\mathbb{R}^d} u^m \rho_\infty dx = \int_{\mathbb{R}^d} u^{m-1} \rho_\infty dx$ for $m = 1, 2, \dots$. We summarize these results in the following proposition.

Proposition 2.1 *Let A.1 – A.4 and (1.6) be satisfied, and let the linear subspace $\mathcal{S} \subset H^1_{\rho_\infty,D}(\mathbb{R}^d)$ be finite-dimensional. Then the iterates u^m considered in (1.7) exist and are uniquely determined for $m = 1, 2, \dots$. If additionally $\mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}$ holds, then for the approximations $\rho^m = u^m \rho_\infty$ there holds*

$$\int_{\mathbb{R}^d} \rho^m dx \;=\; \int_{\mathbb{R}^d} \rho^0 dx \qquad \textit{for } \; m = 0, 1, \dots \; .$$

The starting vector $\alpha^0 \in \mathbb{R}^N$ for the matrix-vector-version (2.3) of the scheme (1.7) can be determined, e.g., by solving the following linear system of equations,

$$G\alpha^0 \;=\; b \qquad \text{with} \quad b = (\langle \rho_0/\rho_\infty, s_k \rangle_{L^2_{\rho_\infty}})_{k=1..N} \in \mathbb{R}^N. \tag{2.5}$$

Then u^0 is the $L^2_{\rho_\infty}$-orthogonal projection of the function ρ_0/ρ_∞ onto the considered finite element space $\mathcal{S}$. We then have $\int_{\mathbb{R}^d} u^0 \rho_\infty dx = \int_{\mathbb{R}^d} \rho_0 dx$ provided that $\mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}$ holds. On the other hand, $\rho_0 \geq 0$ does not necessarily implies $\alpha^0 \geq 0$ in (2.5) even under canonical assumptions on the basis functions. At the end of Section 3, another strategy for choosing the starting function will be considered which guarantee nonnegativity.

3 Non-negativity of the approximations

In the sequel we suppose that the conditions (1.6) and (2.1) are satisfied, and additionally we assume that there exists some parameter $h = h(\mathcal{S})$ representing the grid size such that the following conditions are satisfied:

$$0 \;\leq\; s_\ell \;\leq\; 1 \quad \text{for } \; \ell = 1, 2, \dots, N, \qquad \sum_{\ell=1}^{N} s_\ell = \mathbf{1}_{\mathbb{R}^d}, \tag{3.1}$$

$$b_{k\ell} \;\leq\; -\frac{c_1}{h^2} \int_{\mathcal{T}_k \cap \mathcal{T}_\ell} \rho_\infty dx \qquad \text{for } \; k \neq \ell \qquad \text{with} \quad \mathcal{T}_\ell := \operatorname{supp}(s_\ell), \tag{3.2}$$

where $b_{k\ell}$ is as in (2.4), and $c_1 > 0$ denotes some constant which is independent of the finite element space $\mathcal{S}$. Additionally, $\mathrm{supp}(s_\ell)$ in (3.2) denotes the support of the function s_ℓ. We need two more natural assumptions:

$$|\nabla s_k|_1 \leq \frac{c_2}{h} \quad \text{on } \mathcal{T}_k \qquad \text{for } k = 1, 2, \ldots, N, \tag{3.3}$$

$$\int_{\mathbb{R}^d} s_k \rho_\infty dx \geq c_3 \int_{\mathcal{T}_k} \rho_\infty dx \qquad \text{for } k = 1, 2, \ldots, N, \tag{3.4}$$

with some positive constants c_2 and c_3 which are independent of $\mathcal{S}$. In (3.3), the notation $|z|_1 = \sum_{k=1}^d |z_k|$ for $z = (z_k) \in \mathbb{R}^d$ is used. If the Fokker-Planck type equation (1.1) is considered with $F \equiv 0$ then the two assumptions (3.3) and (3.4) in fact can be discarded.

We next present an example where the conditions (3.1)–(3.3) are satisfied.

Remark 3.1 In the two-dimensional case $d = 2$ and if D is the identity matrix, then the conditions (3.1)–(3.3) are satisfied, for example, if the subspace $\mathcal{S} \subset H^1_{\rho_\infty, D}(\mathbb{R}^2)$ is a space of continuous functions on $\mathbb{R}^2$ with the following properties:

(i) There exists a convex bounded domain Ω of $\mathbb{R}^2$ with a polygonal boundary as well as a quasiuniform triangulation of this set Ω. All inner angles of triangles belonging to that triangulation are obtuse, i.e., they are smaller than 90 degrees.

(ii) On each triangle of the considered triangulation, the elements of $\mathcal{S}$ are linear functions, respectively.

(iii) The considered basis functions $s_1, s_2, \ldots, s_N$ are standard hat functions on Ω, respectively.

(iv) Outside the considered domain Ω, each element of $\mathcal{S}$ is a constant function.

For more details about triangulations and linear splines on two-dimensional bounded domains, see e.g., Knabner and Angermann [9]. The one-dimensional case $d = 1$ is considered in the numerical tests, cf. Section 6.

We consider some elementary consequences of the assumptions in (3.1):

$$\mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}, \tag{3.5}$$

$$\sum_{\ell=1}^N b_{k\ell} = 0, \qquad \sum_{\ell=1}^N g_{k\ell} = \int_{\mathcal{T}_k} s_k \rho_\infty dx \qquad \text{for } k = 1, 2, \ldots, N, \tag{3.6}$$

$$\sum_{\ell=1}^N c^m_{k\ell} = \int_{\mathcal{T}_k} \nabla^\top s_k F(m\Delta t, \cdot) \rho_\infty dx \qquad \text{for } k = 1, 2, \ldots, N, \tag{3.7}$$

$$0 \leq g_{k\ell} \leq \int_{\mathcal{T}_k \cap \mathcal{T}_\ell} \rho_\infty dx \qquad \text{for } k, \ell = 1, 2, \ldots, N. \tag{3.8}$$

We next show that the iteration matrix $G + \Delta t(B + C_m)$ is an M-Matrix for appropriate choices of the time stepsize Δt. Recall (see, e.g., [11]) that a matrix $A = (a_{k\ell}) \in \mathbb{R}^{N \times N}$ is by definition an M-Matrix if the following holds:

(a) The matrix A is regular, with an inverse that has nonnegative entries, $A^{-1} \geq 0$.

(b) All entries of the matrix A, except for those on the diagonal, are nonpositive, i.e., $a_{k\ell} \leq 0$ for all indices k, ℓ with $k \neq \ell$.

In the sequel we use the notation $|z|_\infty = \max_{k=1,\dots,d} |z_k|$ for $z = (z_k) \in \mathbb{R}^d$.

Theorem 3.2 *Let the assumptions A.1 – A.4 be fulfilled and the conditions (1.6), (2.1) and (3.1)-(3.4) be satisfied. Moreover we suppose that there exists a constant $0 < L < \infty$ such that for each $t \geq 0$ there holds $|F(t,x)|_\infty \leq L$ for a.e. $x \in \mathbb{R}^d$. Then for each time stepsize Δt satisfying*

$$c_5 h^2 \ \leq \ \Delta t \ < \ \frac{c_4}{L} h, \tag{3.9}$$

with the constants $c_4 = c_3/c_2$ and $c_5 = (1+c_3)/c_1$, the matrix $G + \Delta t(B + C_m)$ considered in the implicit iteration scheme (2.3) is an M-Matrix.

Proof. It is sufficient (see [11]) to show that the following holds for the considered matrix $G + \Delta t(B + C_m)$ with time stepsizes Δt satisfying (3.9): the matrix is strictly diagonal dominant, all off-diagonal entries are nonpositive, and all diagonal entries are positive. In fact, for a fixed index k, each off-diagonal element in the kth row of the matrix $G + \Delta t(B + C_m)$ is nonpositive:

$$\begin{aligned} g_{k\ell} \ + \ \Delta t(b_{k\ell} + c_{k\ell}^m) \ &\overset{(*)}{\leq} \ \Big\{1 \ - \ c_1 \frac{\Delta t}{h^2} \ + \ c_2 L \frac{\Delta t}{h}\Big\} \int_{\mathcal{T}_k \cap \mathcal{T}_\ell} \rho_\infty dx \\ &\overset{(**)}{\leq} \ 0 \qquad \text{for} \ \ k \neq \ell. \end{aligned}$$

Here, estimate $(*)$ follows from (3.2), (3.3) and (3.8), and estimate $(**)$ is a consequence of the time stepsize condition (3.9). Additionally, for the considered values of h and Δt, the sum of the modulus of all off-diagonal elements in the kth row of the matrix $G + \Delta t(B + C_m)$ is smaller than the diagonal element in the kth row:

$$\begin{aligned} \sum_{\substack{\ell=1,\dots,N \\ \ell \neq k}} |g_{k\ell} \ + \ \Delta t(b_{k\ell} + c_{k\ell}^m)| \ \ &= \ \ \sum_{\substack{\ell=1,\dots,N \\ \ell \neq k}} \big\{ - g_{k\ell} \ - \ \Delta t(b_{k\ell} \ + \ c_{k\ell}^m)\big\} \\ &\overset{(*)}{=} \ g_{kk} \ + \ \Delta t(b_{kk} \ + \ c_{kk}^m) \ - \ \int_{\mathbb{R}^d} s_k \rho_\infty dx \ - \ \Delta t \int_{\mathbb{R}^d} \nabla^\top s_k F(m\Delta t, \cdot) \rho_\infty dx \\ &\overset{(**)}{<} \ g_{kk} \ + \ \Delta t(b_{kk} \ + \ c_{kk}^m). \end{aligned}$$

Here, the identity $(*)$ follows easily from (3.6) and (3.7), and the estimate $(**)$ follows from the conditions (3.3) and (3.4). These statements hold for each k so that $G + \Delta t(B + C_m)$ is in fact an M-Matrix. ∎

As an immediate consequence of Theorem 3.2 we obtain the following result.

Corollary 3.3 *In addition to the assumptions in Theorem 3.2 (including time stepsize condition (3.9)), let the initial function $u^0 \in \mathcal{S}$ be nonnegative. Then the approximations $\rho^m = u^m \rho_\infty$, $m = 1, 2, \dots$ obtained by the scheme (2.2)-(2.3) are nonnegative, respectively.*

We conclude this section with some remarks.

Remark 3.4 1. A starting function $u^0 \in \mathcal{S}$ such that the states $\rho^m = u^m \rho_\infty$ for $m = 1, 2, \ldots$ preserve nonnegativity and mass, respectively, can be obtained as follows.

(i) For a given initial function ρ_0 which satisfies $\rho_0 \geq 0$, at a first step determine a nonnegative approximation $\tilde{u}^0 \in \mathcal{S}$ to the scaled function $\rho_0/\rho_\infty \geq 0$. For spaces $\mathcal{S}$ consisting of linear splines this can be obtained, e.g., by interpolation.

(ii) At a second step, compute the function $u^0 = c\tilde{u}^0 \in \mathcal{S}$ where $c = \int_{\mathbb{R}^d} \rho_0 dx / \int_{\mathbb{R}^d} \tilde{u}^0 \rho_\infty dx$. The property $\rho_0 \geq 0$ then necessarily implies $u^0 \geq 0$, and in addition there holds $\int_{\mathbb{R}^d} u^0 \rho_\infty dx = \int_{\mathbb{R}^d} \rho_0 dx$.

2. In the situation $F \equiv 0$, the statements in Theorem 3.2 and Corollary 3.3 remain valid without the conditions (3.3) and (3.4), respectively, and the condition (3.9) on the stepsize reduces to

$$\tfrac{1}{c_1} h^2 \;\leq\; \Delta t, \tag{3.10}$$

with c_1 as in (3.2).

4 Large time asymptotics

For a fixed function ρ_∞ of the form (1.3) with $\rho_\infty \in L^1(\mathbb{R}^d)$, we now consider the following convex functional,

$$e(\rho|\rho_\infty) \;=\; \int_{\mathbb{R}^d} \psi\Big(\frac{\rho}{\rho_\infty}\Big)\rho_\infty dx \qquad \text{for} \quad \rho/\rho_\infty \in L^2_{\rho_\infty}(\mathbb{R}^d), \qquad \rho \geq 0, \tag{4.1}$$

with the generating function

$$\psi(\sigma) \;=\; \sigma \ln \sigma - (\sigma - 1) \qquad \text{for} \;\; \sigma > 0, \qquad \psi(0) = 1, \tag{4.2}$$

c.f. Arnold et. al. [1]. From the elementary inequality $0 \leq \psi(\sigma) \leq (\sigma - 1)^2$ for $\sigma \geq 0$ it follows that the functional $e(\rho|\rho_\infty)$ is well-defined and satisfies

$$0 \;\leq\; e(\rho|\rho_\infty) \;\leq\; \int_{\mathbb{R}^d} (\rho - \rho_\infty)^2 \rho_\infty^{-1} dx \qquad (\rho/\rho_\infty \in L^2_{\rho_\infty}(\mathbb{R}^d), \quad \rho \geq 0). \tag{4.3}$$

Remark 4.1 There exist different terminologies. For example, in Arnold et. al. [1], Arnold and Unterreiter [2] or Dolbeault and Illner [3] the number $e(\rho|\rho_\infty)$ is denoted as relative logarithmic entropy of the state ρ. If in addition $\int_{\mathbb{R}^d} \rho dx = \int_{\mathbb{R}^d} \rho_\infty dx$ holds then $e(\rho|\rho_\infty)$ also can be written as follows,

$$e(\rho|\rho_\infty) \;=\; \int_{\mathbb{R}^d} \rho \ln \rho dx \;+\; \int_{\mathbb{R}^d} \rho A dx. \tag{4.4}$$

In the case $F \equiv 0$ and $D = I$, the number $e(\rho|\rho_\infty)$ in (4.4) is known as the free energy of the state ρ. The first integral on the right-hand side of the identity in (4.4) is known as an energy of the state ρ, and the second integral is the negative of the Gibbs-Boltzmann entropy (cf. Jordan, Kinderlehrer and Otto [6]). In the sequel the number $e(\rho|\rho_\infty)$ in (4.4) will be simple denoted as the free energy of the state ρ.

Under certain conditions on the involved functions there exists a solution ρ of the Fokker-Planck type equation (1.1) such that the free energies (4.1) of its states decay exponentially as $t \to \infty$, i.e.,

$$0 \;\le\; e(\rho(t,\cdot)|\rho_\infty) \;\le\; e(\rho_0|\rho_\infty)e^{-\lambda t} \qquad \text{for } \; t \ge 0 \tag{4.5}$$

for some parameter $\lambda > 0$, see e.g., Arnold et. al. [1] for the details. A semidiscrete version of (4.5) can be found in Arnold and Unterreiter [2] where in fact the scheme (1.7) is considered with $\mathcal{S} = H^1_{\rho_\infty,D}(\mathbb{R}^d)$. In this section a discrete version of (4.5) is considered for the approximations $\rho^m = u^m\rho_\infty$ which is obtained by the scheme (1.7) with a finite-dimensional subspace $\mathcal{S} \subset H^1_{\rho_\infty,D}(\mathbb{R}^d)$. As a preparation we suppose that the following Poincaré inequality is satisfied:

A.5 There exists a real constant $\lambda > 0$ with

$$\|v\|^2_{L^2_{\rho\infty}} \;\le\; \frac{2}{\lambda}\int_{\mathbb{R}^d} \nabla^\top v \cdot D \cdot \nabla v \rho_\infty dx \quad \forall v \in H^1_{\rho_\infty,D}(\mathbb{R}^d) \quad \text{with} \quad \int_{\mathbb{R}^d} v\rho_\infty dx \;=\; 0. \tag{4.6}$$

For example, in the case $D = I$ the Poincaré inequality (4.6) is satisfied if the potential A is uniformly convex on $\mathbb{R}^d$.

We now present a first result on the exponential time decay of the approximations.

Proposition 4.2 *Let assumptions A.1-A.5 and (1.6) hold, and additionally let* $\mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}$ *and* $\int_{\mathbb{R}^d} u^0\rho_\infty dx = \int_{\mathbb{R}^d} \rho_\infty dx$ *be satisfied. Then for the approximations* $\rho^m = u^m\rho_\infty$ *with the iterates* u^m *obtained by the scheme (1.7), the following estimate holds,*

$$\int_{\mathbb{R}^d} (\rho^m - \rho_\infty)^2 \rho_\infty^{-1} dx \;\le\; (1+\lambda\Delta t)^{-m} \int_{\mathbb{R}^d} (\rho^0 - \rho_\infty)^2 \rho_\infty^{-1} dx \qquad \textit{for } \; m = 0, 1, \dots \; . \tag{4.7}$$

Proof. We begin with the following calculations:

$$\begin{aligned}
\|u^{m-1} - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho\infty}} \;&=\; \int_{\mathbb{R}^d} (u^m - \mathbf{1}_{\mathbb{R}^d} - (u^m - u^{m-1}))^2 \rho_\infty dx \\
&\ge\; \|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho\infty}} \;-\; 2\int_{\mathbb{R}^d} (u^m - \mathbf{1}_{\mathbb{R}^d})(u^m - u^{m-1})\rho_\infty dx \\
&\overset{(*)}{=}\; \|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho\infty}} \;+\; 2\Delta t \int_{\mathbb{R}^d} \nabla^\top u^m \cdot D \cdot \nabla u^m \rho_\infty dx \\
&\qquad +\; 2\Delta t \int_{\mathbb{R}^d} u^m \nabla^\top u^m \cdot F(m\Delta t, \cdot)\rho_\infty dx \qquad \text{for } \; m = 1, 2, \dots \; .
\end{aligned}$$

Here, $(*)$ follows from the identity (1.7) applied with the function $v = u^m - \mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}$, c.f. (3.5). From assumption A.4 applied with the function $v = u^m$ we conclude that the last integral in the previous calculations vanishes:

$$\int_{\mathbb{R}^d} u^m \nabla^\top u^m \cdot F(m\Delta t, \cdot)\rho_\infty dx \;=\; 0 \qquad \text{for } \; m = 1, 2, \dots \; . \tag{4.8}$$

We now consider the Poincaré inequality (4.6) applied with the function $v = u^m - \mathbf{1}_{\mathbb{R}^d} \in \mathcal{S}$, which is possible due to Proposition 2.1 on the mass conservation. From this and the estimate (4.8) we finally obtain

$$\begin{aligned} \|u^{m-1} - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho_\infty}} &\geq \|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho_\infty}} + 2\Delta t \int_{\mathbb{R}^d} \nabla^\top u^m \cdot D \cdot \nabla u^m \rho_\infty dx \\ &\geq (1 + \lambda\Delta t)\|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho_\infty}} \qquad \text{for } m = 1, 2, \dots . \end{aligned}$$

This statement is equivalent to

$$\int_{\mathbb{R}^d} (\rho^m - \rho_\infty)^2 \rho_\infty^{-1} dx \leq (1 + \lambda\Delta t)^{-1} \int_{\mathbb{R}^d} (\rho^{m-1} - \rho_\infty)^2 \rho_\infty^{-1} dx \qquad \text{for } m = 1, 2, \dots,$$

and the statement of the theorem now follows by mathematical induction. □

Remark 4.3 In the situation $F = 0$, the factor $(1+\lambda\Delta t)^{-m/2}$ in (4.7) can be replaced by the factor $(1 + \lambda\Delta t/2)^{-m}$. This follows by using a different technique, details are omitted here.

We continue to consider the large time behavior of the approximations $\rho^m = u^m\rho_\infty \approx \rho(m\Delta t, \cdot)$. In fact, as an immediate consequence of Proposition 4.2 and inequality (4.3) we obtain the following estimate:

Corollary 4.4 *In addition to the assumptions in Proposition 4.2 we suppose that the conditions (3.1)-(3.4) are satisfied and that the initial function u^0 for the iteration scheme (1.7) is nonnegative. Let the time stepsize Δt be chosen according to (3.9) (or according to (3.10), if $F = 0$ holds). Then there holds*

$$0 \leq e(\rho^m|\rho_\infty) \leq c(1 + \lambda\Delta t)^{-m} \qquad \textit{for } m = 0, 1, \dots \tag{4.9}$$

with the constant $c = \int_{\mathbb{R}^d} (\rho^0 - \rho_\infty)^2 \rho_\infty^{-1} dx$.

Remark 4.5 (a) If the function ρ^0/ρ_∞ is bounded then the constant c in (4.9) can be estimated as follows,

$$c \leq 2\Big\{ \sup_{x\in\mathbb{R}^d} |\rho^0/\rho_\infty| \Big\} e(\rho^0|\rho_\infty). \tag{4.10}$$

This follows from the fact that the generating function ψ considered in (4.2) satisfies the elementary inequality $\psi(\sigma) \geq \frac{1}{2\sigma_0}(\sigma - 1)^2$ for $0 \leq \sigma \leq \sigma_0$ with $\sigma_0 > 0$. Estimate (4.10) implies that the free energy decay of the approximations $\rho^m = u^m\rho_\infty$, $m = 1, 2, \dots$ can be estimated in terms of the free energy of the initial state $\rho^0 = u^0\rho_\infty$.

(b) Convex functionals $e(\cdot|\rho_\infty)$ of the form (4.1) with generating functions of the form $\psi(\sigma) = \sigma^p - 1 - p(\sigma - 1)$ for $\sigma \geq 0$ $(1 < p < 2)$ admit estimates which are similar to (4.3) (c.f. Arnold et. al. [1]) as well as (4.9). The verification is also similar and details are therefore omitted here.

5 Approximation properties at fixed times

5.1 Preparations

For the sake of completeness, in this section the approximation properties of the scheme (1.7), (1.6) are considered. We continue to suppose that the assumptions A.1-A.5 are satisfied, and for technical reasons we restrict the considerations to time-independent vector fields F, i.e.,

$$F(x) = F(t,x) \qquad \text{for} \quad x \in \mathbb{R}^d, \quad t \geq 0. \tag{5.11}$$

The condition (5.11) in fact guarantees that differentiation and the Ritz projector R considered below commute.

5.2 A Ritz projection

Under the conditions stated in Section 5.1 we consider the bilinear form $a : H^1_{\rho_\infty,D}(\mathbb{R}^d) \times H^1_{\rho_\infty,D}(\mathbb{R}^d) \to \mathbb{R}$ given by

$$\begin{aligned} a(u,v) \;&=\; \int_{\mathbb{R}^d} \nabla^\top u \cdot D \cdot \nabla v \rho_\infty dx \;+\; \int_{\mathbb{R}^d} u \nabla^\top v \cdot F \rho_\infty dx, \\ &\qquad\qquad u, v \in H^1_{\rho_\infty,D}(\mathbb{R}^d). \end{aligned} \tag{5.12}$$

The bilinear form $a(\cdot,\cdot)$ given by (5.12) is elliptic with respect to all those functions $v \in H^1_{\rho_\infty,D}(\mathbb{R}^d)$ which have a weighted mean zero, cf. (4.6) and assumption A.4. The conditions A.1-A.2 imply continuity of the bilinear form a with respect to the space $H^1_{\rho_\infty,D}(\mathbb{R}^d)$.

For a given finite-dimensional subspace $\mathcal{S} \subset H^1_{\rho_\infty,D}(\mathbb{R}^d)$ and for $u \in H^1_{\rho_\infty,D}(\mathbb{R}^d)$ we consider the Ritz projection $Ru \in \mathcal{S}$ determined by the following two conditions:

$$a(Ru,v) \;=\; a(u,v) \qquad \forall v \in \mathcal{S} \quad \text{with} \quad \int_{\mathbb{R}^d} v \rho_\infty dx \;=\; 0, \tag{5.13}$$

$$\int_{\mathbb{R}^d} (Ru) \rho_\infty dx \;=\; \int_{\mathbb{R}^d} u \rho_\infty dx. \tag{5.14}$$

For each element $u \in H^1_{\rho_\infty,D}(\mathbb{R}^d)$, the Ritz projection $Ru \in \mathcal{S}$ determined by the two conditions (5.13) and (5.14) in fact exists and is unique.

5.3 Error estimate

For solutions of the scaled Fokker-Planck type equation (1.4)-(1.5) which are sufficiently smooth, e.g., for a twice continuously differentiable function $u : [0,\infty) \to H^1_{\rho_\infty,D}(\mathbb{R}^d)$ (with the notation $u(t) = u(t,\cdot)$) the following error estimate can be obtained by standard techniques, see, e.g., Knabner and Angermann [9], Theorem 6.13:

$$\begin{aligned} \|u^m - u(m\Delta t)\|_{L^2_{\rho_\infty}} \;\leq\; &\int_0^{m\Delta t} \|(I-R)u'(s)\|_{L^2_{\rho_\infty}} ds \;+\; \Delta t \int_0^{m\Delta t} \|u''(s)\|_{L^2_{\rho_\infty}} ds \\ &+ \|u^0 - Ru(0)\|_{L^2_{\rho_\infty}} \;+\; \|(I-R)u(m\Delta t)\|_{L^2_{\rho_\infty}} \end{aligned} \tag{5.15}$$

for $m = 0, 1, \ldots$. We now consider convergence w.r.to x, and for this purpose let $\mathcal{S}_0, \mathcal{S}_1, \ldots$ be a sequence of finite-dimensional subspaces of the Sobolev space $H^1_{\rho_\infty, D}(\mathbb{R}^d)$ with $\cup_{N=0,1,\ldots} \mathcal{S}_N$ being dense in $H^1_{\rho_\infty, D}(\mathbb{R}^d)$, and the corresponding approximations in (1.7) are denoted by u^m_N instead of u^m. As a consequence of the error estimate (5.15) we obtain convergence in the following sense:

$$\begin{aligned} \|u^m_N - u(m\Delta t)\|_{L^2_{\rho_\infty}} \;&\le\; C(\inf_{v \in \mathcal{S}_N} \|v - u(m\Delta t)\|_{H^1_{\rho_\infty, D}} + \Delta t) \\ &\text{for} \quad m, N = 0, 1, \ldots, \qquad m\Delta t \le T, \end{aligned} \tag{5.16}$$

where $T > 0$ is fixed, and C denotes some real positive constant which is independent of N, m and Δt, and $\inf_{v \in \mathcal{S}_N} \|v - u(m\Delta t)\|_{H^1_{\rho_\infty, D}} \to 0$ holds as $N \to \infty$. As initial function u^0_N, the Ritz projection or the $L^2_{\rho_\infty}$-orthogonal projection of the original initial function ρ_0/ρ_∞ may be considered.

6 Numerical Experiments

Numerical tests are employed for the one-dimensional setting $d = 1$, the potential $A(x) = x^2/2$, the constant diffusion coefficient $D = 1$, and the function F vanishes, $F = 0$. The Poincaré inequality is satisfied then with $\lambda = 2$.

For the Galerkin scheme (1.7) we use spaces of linear splines with respect to grid points $-\infty < x_1 < x_2 < \ldots < x_N < \infty$,

$$\begin{aligned} \mathcal{S} \;=\; \big\{ u : \mathbb{R} \to \mathbb{R} : \quad & u \;\text{ continuous on } \mathbb{R}, \quad u \;\text{ is linear on } \; [x_{k-1}, x_k] \;\text{ for} \\ & k = 2, 3, \ldots, N, \quad u \;\text{ const. on } (-\infty, x_1] \;\text{ and on } \; [x_N, \infty), \;\; \text{resp..} \big\}. \end{aligned}$$

As basis functions we use hat functions $s_\ell \in \mathcal{S}$ with $s_\ell(x_\ell) = 1$ and $s_\ell(x_k) = 0$ for $k \ne \ell$ $(k, \ell = 1, 2, \ldots, N)$. Moreover, the functions s_ℓ vanish outside the interval $[x_1, x_N]$, with the two exceptions $s_1(x) \equiv 1$ for $x \in (-\infty, x_1]$, and $s_N(x) \equiv 1$ for $x \in [x_N, \infty)$. In the numerical experiments we use a uniform space grid

$$x_k \;=\; a + (k-1)h \qquad \text{for} \;\; k = 1, 2, \ldots, N, \qquad\qquad h \;=\; (b-a)/(N-1),$$

with $a = -4, b = 6$ and $N = 41$. The conditions (3.1)-(3.2) then are satisfied with $c_1 = 1$. We consider the time step size $\Delta t = 0.07$ so that the condition (3.10) is satisfied then. The entries of the considered matrices B and G are computed by using sufficiently accurate quadrature formulas. Experiments are employed using the interactive program system Octave (see the URL http://www.octave.org). We consider two different initial functions.

Example 6.1 We first consider $\rho_0(x) = c \exp(-x^2/2 + 2x)$ as initial function, with the constant c chosen such that $\int_{-\infty}^{\infty} \rho_0 dx = \int_{-\infty}^{\infty} \rho_\infty dx$ holds, i.e., $c \approx 7.3941$. As initial function u^0 the $L^2_{\rho_\infty}$–orthogonal projection of the original initial function ρ_0/ρ_∞ onto the finite element space $\mathcal{S}$ is considered. It turns out in the numerical experiments that the initial function u^0 for the iteration scheme (1.7) is nonnegative, and then all functions u^m for $m \ge 1$ are nonnegative (see Corollary 3.3). Graphical illustrations are given in Figures

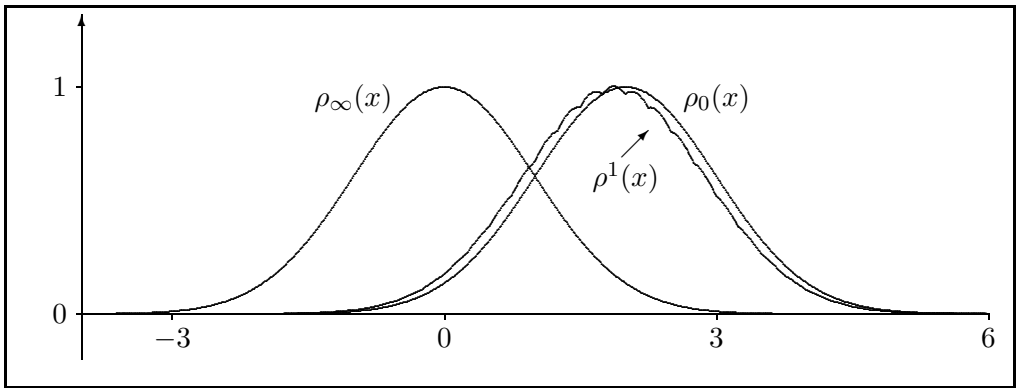

Figure 1: Plots of the initial function ρ_0, the approximation $\rho_1 = u_1\rho_\infty$ at the first time level $t = 0.07$, and the equilibrium ρ_∞, Example 6.1.

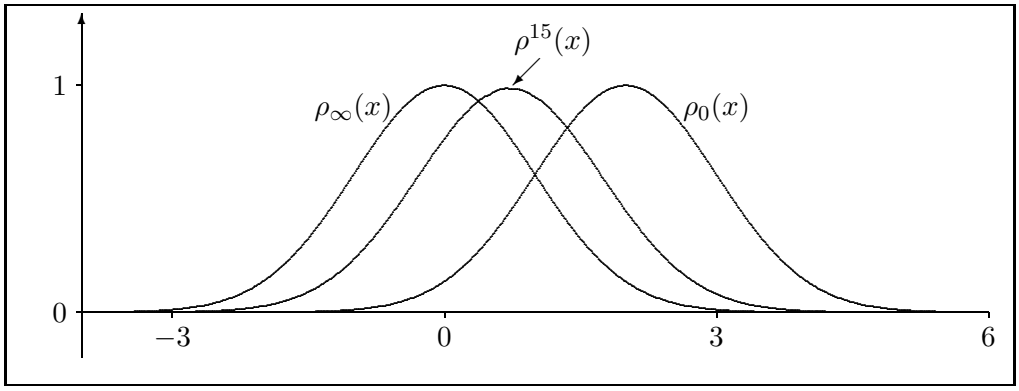

Figure 2: Plots of the initial function ρ_0, the approximation $\rho^{15} = u^{15}\rho_\infty$ at time level $t = 15\Delta t = 1.05$, and the equilibrium ρ_∞, Example 6.1.

1, 2 and 3, respectively. In Figure 4, the free energies of the states of Example 6.1 are shown for the first 60 time steps. Additionally we illustrate the statement of Corollary 4.4 and present in Table 1 the free energies $e(\rho^m|\rho_\infty)$ for some values of m.

Example 6.2 In a second numerical experiment we consider $\rho_0(x) = (1+x)\exp(-x^2/2)$ as initial function. This function has also negative values and therefore no free energies are considered here. As initial function u^0 again the $L^2_{\rho_\infty}$–orthogonal projection of ρ_0/ρ_∞ onto the space $\mathcal{S}$ is considered. The numerical results for the large time asymptotics w.r.t. the L^2-norm are shown in Table 2.

7 Conclusions

For an initial-value problem for a Fokker-Planck type equation on an unbounded space domain we considered a discretization in time by an implicit Euler scheme, and as space discretization a Galerkin scheme is considered. It is shown that, without restrictive assumptions on the geometry of the triangulation, we have conservation of mass, positivity and exponential decay of the free energy. The approximation properties at fixed times are investigated and numerical experiments are provided.

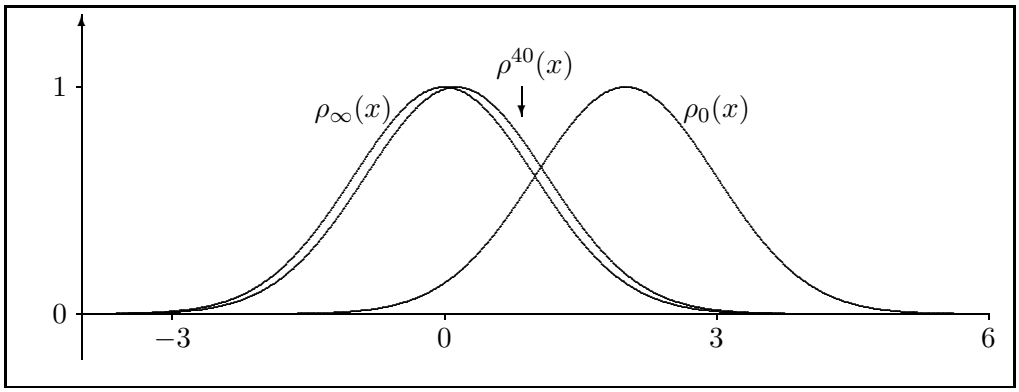

Figure 3: Plots of the initial function ρ_0, the approximation $\rho^{40} = u^{40}\rho_\infty$ at time level $t = 40\Delta t = 2.80$, and the equilibrium ρ_∞, Example 6.1.

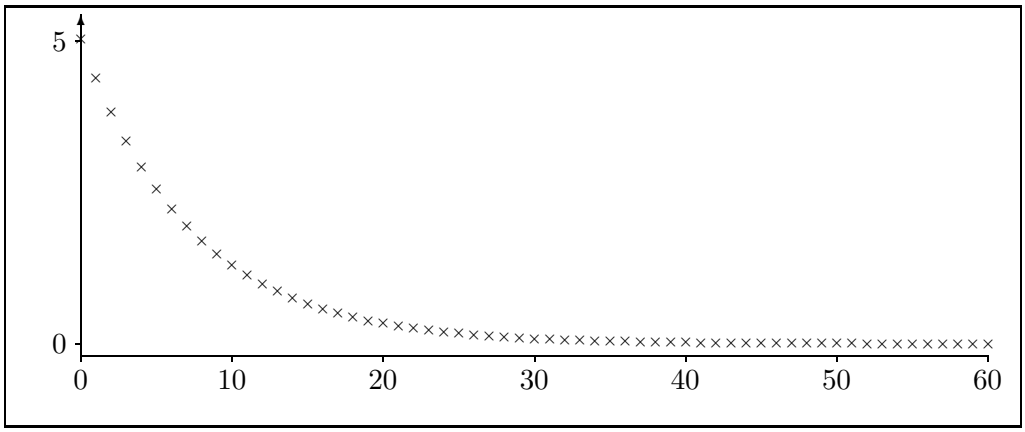

Figure 4: The free energy $e(\rho^m|\rho_\infty)$ with $\rho^m = u^m\rho_\infty$ for $m = 0, 1, \ldots, 60$, Example 6.1.

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m	t	$e(\rho^m\|\rho_\infty)$	$e(\rho^m\|\rho_\infty)/q^m$	$\|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho_\infty}}$	$\|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho_\infty}}/q^m$
0	0.0	5.0410	5.0	931.5306	931.5
10	0.7	1.3009	4.8	4.9270	18.3
20	1.4	0.3362	4.6	0.7909	10.9
30	2.1	0.0868	4.4	0.1815	9.2
40	2.8	0.0224	4.2	0.0454	8.6
50	3.5	0.0058	4.1	0.0116	8.1
60	4.2	0.0015	3.9	0.0030	7.8
70	4.9	0.0004	3.7	0.0008	7.4

Table 1: Some numerical results for Example 6.1, with $q = 1/(1 + \lambda\Delta t)$.

m	t	$\|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho_\infty}}$	$\|u^m - \mathbf{1}_{\mathbb{R}^d}\|^2_{L^2_{\rho_\infty}}/(1 + \lambda\Delta t)^{-m}$
0	0.0	2.7863	2.78633
10	0.7	0.6582	2.44000
20	1.4	0.1700	2.33689
30	2.1	0.0439	2.23832
40	2.8	0.0113	2.14375
50	3.5	0.0029	2.05488
60	4.2	0.0008	1.98044
70	4.9	0.0002	1.95655

Table 2: Some numerical results for Example 6.2.

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