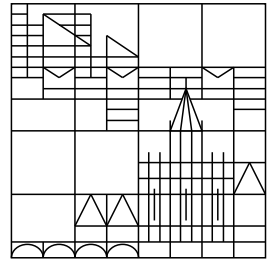


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# Positive Entropic Schemes for a Nonlinear Fourth-order Parabolic Equation

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## Abstract

A finite-difference scheme with positivity-preserving and entropy-decreasing properties for a nonlinear fourth-order parabolic equation arising in quantum systems and interface fluctuations is derived. Initial-boundary value problems, the Cauchy problem and a rescaled equation are discussed. Based on this scheme we elucidate properties of the long-time asymptotics for this equation.

## 1 Introduction

We analyse the evolution of a function  $u(t, x)$  that satisfies the fourth-order parabolic equation

$$u_t = -(u(\log u)_{xx})_{xx}, \quad x \in (-L, L), \quad t \geq 0, \quad (1.1)$$

with initial data

$$u(0, x) = u_0(x) > 0. \quad (1.2)$$

Three different types of boundary conditions will be considered:

1. Periodic boundary conditions:

$$u(t, x + 2L) = u(t, x). \quad (1.3)$$

2. Reflecting boundary conditions:

$$u_x(t, -L) = u_x(t, L) = u_{xxx}(t, -L) = u_{xxx}(t, x) = 0. \quad (1.4)$$

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### 3. Fixed boundary conditions:

$$u(t, -L) = u(t, L) = 1, \quad u_x(t, -L) = u_x(t, L) = 0. \quad (1.5)$$

Equation (1.1) arises as a scaling limit in the study of interface fluctuations in a certain spin system [13]. It also models the electron concentration in a quantum semiconductor device with zero temperature and negligible electric field [16].

Local in time positive classical solutions of (1.1) with strictly positive initial data and with periodic boundary conditions (1.3) have been obtained in [9]. In this paper also the existence of *global* (in time) solutions for “small” initial data has been proved. Global non-negative weak solutions have been proven to exist in [16] using the fixed boundary conditions (1.5). The existence of global non-negative solutions for equation (1.1) using non-negative initial data with either periodic or reflecting boundary conditions as well as the Cauchy problem remains open.

Concerning the long-time asymptotics of this equation, it has been proved in [18] that a weak solution of (1.1) with fixed boundary conditions (1.5) converges exponentially fast to the constant steady state  $u = 1$ . The long-time asymptotics for the Cauchy problem or for the initial-boundary-value problem with either periodic or reflecting boundary conditions is yet not understood.

However, we can state some conjectures about the asymptotic behavior based on similar situations for the thin film equation [12] and for diffusion equations [11, 10, 14]. We conjecture that the self-similar solution

$$u_s(t, x) = (1 + t)^{-1/4} \exp\left(-\frac{x^2}{4\sqrt{1+t}}\right) \quad (1.6)$$

is the intermediate asymptotics for the Cauchy problem of equation (1.1), for initial data with the same initial mass. More precisely, it is conjectured that the solutions will converge as  $t \rightarrow \infty$  towards the self-similar equation (1.6) (multiplied by a constant factor due to mass conservation) algebraically fast in the  $L^1$  norm. For the initial boundary value problem with either periodic or reflecting boundary conditions, one expects exponential convergence towards a constant steady state determined by the initial mass.

In this paper we focus on two objectives. We first derive a numerical scheme that preserves important properties of this equation, namely: positivity, mass conservation (in some cases) and monotonicity of the (negative) physical entropy

$$\mathcal{S}(u) = \int u(\log u - 1) dx. \quad (1.7)$$

The decrease of the entropy for the numerical scheme is of paramount importance to achieve meaningful results for the long-time asymptotics. In fact, the above-mentioned conjectures on the long-time asymptotics are based on a careful study of the evolution of this entropy. The second aim of this paper is to use this numerical scheme to verify the above conjectures numerically.

In recent years, the question of positivity preservation for the dynamics of nonlinear fourth-order equations was thoroughly investigated in the context of lubrication-type equations [2, 3, 4, 5, 7, 21]. They arise in the study of thin liquid films and spreading droplets (for an overview see [6] and the references therein). Numerically, several discretization methods have been presented. In [8] a positivity-preserving numerical scheme with finite differences has been developed. Finite element techniques have been used in [1] imposing the non-negativity property as a constraint such that at each time level a variational inequality has to be solved. Entropy consistent schemes are derived in [15].

For related numerical results we refer to [19] where relaxation schemes for degenerate diffusion equations have been designed and to [17] where a positivity-preserving semi-implicit scheme for the quantum drift-diffusion model has been derived.

This paper is organized as follows. In Section 2 we review some of the properties of equation (1.1). Section 3 is devoted to the derivation of the numerical scheme possessing the properties of positivity, mass conservation (in some cases) and monotonicity of the entropy. Finally, in Section 4 some numerical results are shown.

## 2 Basic properties

In this section we recall some basic properties of the solutions to (1.1)-(1.2). In particular, we review the long-time behavior of the solutions in the case of the fixed boundary conditions (1.5). In the sequel we will not make explicit the kind of boundary condition we use except necessary and thus, any asserted property of the solutions holds for any boundary condition.

The following proposition shows the existence of some Lyapunov functionals in the case of classical solutions.

**Proposition 2.1** *For any positive classical solution  $u(t, x)$  of (1.1)-(1.2) the following properties hold:*

1. *The entropy functional*

$$\mathcal{S}(u(t)) = \int_{-L}^L u(t)(\log u(t) - 1) \, dx$$

*is non-increasing for  $t \geq 0$ .*

2. *Stationary states are constant solutions.*
3. *For boundary conditions (1.3) or (1.4), the total mass*

$$\int_{-L}^L u(t) \, dx$$

*is preserved. For boundary conditions (1.5), the total mass is bounded if  $\int_{-L}^L (u_0 - \log u_0) \, dx < \infty$ .*

4. For boundary conditions (1.3) or (1.4), the Fisher information functional

$$I(u(t)) = \int_{-L}^L \frac{u(t)_x^2}{2u(t)} dx$$

is non-increasing for  $t \geq 0$ .

*Proof.* Properties 1 and 3 can be obtained through a direct calculation. For the second property, the case of fixed boundary conditions was studied in [18], and in fact, the solution converges exponentially towards the unique stationary state  $u_\infty = 1$ . Now we consider the other two kinds of boundary conditions. A stationary solution  $u_\infty(x)$  satisfies

$$(u_\infty(\log u_\infty)_{xx})_{xx} = 0, \quad x \in [-L, L].$$

This means that for certain constants  $C_0$  and  $C_1$ ,

$$(u_\infty(\log u_\infty)_{xx})_x = C_1,$$

$$u_\infty(\log u_\infty)_{xx} = C_1x + C_0. \quad (2.1)$$

By a calculation at the boundaries, we have  $C_1 = 0$  for the reflecting boundary conditions (1.4). Moreover, the vanishing of  $(\log u_\infty)_x$  at  $x = \pm L$  implies that there exists a point in  $[-L, L]$  where  $(\log u_\infty)_{xx} = 0$ . Because  $u_\infty$  is positive,  $C_0$  has to be 0. On the other hand, a non-constant periodic function  $\log u_\infty$  has infinitely many inflection points over  $\mathbb{R}$ , and the only possible case is again  $C_1 = C_0 = 0$ .

By virtue of the positivity of  $u_\infty$ , (2.1) gives

$$u_\infty = \exp(C_3x + C_2).$$

It is then straight forward to show that only a constant solution meets the boundary conditions (1.3) or (1.4).

The last property is a consequence of the computation of the derivative of the Fisher information functional:

$$\frac{d}{dt}I(u) = - \int_{-L}^L \frac{1}{u} \left( u_{xx} - \frac{u_x^2}{u} \right)_x dx. \quad (2.2)$$

Let us verify the last formula. Taking the derivative in time, integrating by parts and taking into account boundary conditions, we deduce

$$\begin{aligned} \frac{d}{dt}I(u) &= - \int_{-L}^L u_t \left( \left( \frac{u_x}{u} \right)_x + \frac{u_x^2}{2u^2} \right) dx \\ &= - \int_{-L}^L u_t \left( \frac{u_{xx}}{u} - \frac{u_x^2}{2u^2} \right) dx. \end{aligned}$$

Since  $u$  satisfies (1.1), we have equivalently

$$u_t = - \left( u_{xx} - \frac{u_x^2}{u} \right)_{xx}$$

and thus, by substituting  $u_t$  and integrating by parts, one finds (2.2).  $\square$

Let us point out that, by the conservation of mass, the unique stationary solution possibly giving the asymptotic behavior for the initial data  $u_0(x)$  is

$$u_\infty = \frac{1}{2L} \int_{-L}^L u_0(x) dx. \quad (2.3)$$

We explain now the long-time behavior of the solutions to (1.1)-(1.2). Consider first the initial-value problem with the fixed boundary conditions (1.5). If the initial datum satisfies  $u_0 \geq 0$  in  $(-L, L)$  and  $u_0 - \log u_0 \in L^1(-L, L)$ , it is shown in [16] that there exists a weak solution  $u$  to (1.1)-(1.2), (1.5) satisfying

$$u \geq 0 \text{ in } (-L, L), \quad u \in L_{\text{loc}}^2(0, \infty; H^2(-L, L)) \cap W_{\text{loc}}^{1,1}(0, \infty; H^{-2}(-L, L)).$$

Moreover, the transient weak solution converges exponentially to the unique steady state  $u_\infty = 1$  as  $t \rightarrow \infty$  (see [18]).

The main idea of the convergence result can be sketched as follows. Assume that there is a classical solution to this initial-boundary-value problem. (The following results can be justified for weak solutions by an approximation argument; see [18] for details.) A direct calculation shows that the entropy  $\eta(u) = \int (u(\log u - 1) + 1) dx$  is non-increasing and moreover, it holds

$$\frac{d}{dt} \eta(u) = - \int_{-L}^L u(\log u)_{xx}^2 dx = -D(u),$$

where  $D(u)$  is the entropy dissipation. By logarithmic Sobolev-type inequalities one can show that the entropy dissipation can be related to the entropy itself by  $\eta(u) \leq (N+2)/8 \cdot D(u)$ , where  $N = \int u(t) dx \leq \text{const}$ . Therefore,

$$\frac{d}{dt} \eta(u) \leq -\frac{8}{N+2} \eta(u),$$

and we conclude the exponential decay in the entropy ‘norm’:

$$\eta(u(t)) \leq \eta(u_0) e^{-8t/(N+2)}.$$

By a Csiszar-Kullback inequality, we infer that

$$\|u(t) - 1\|_{L^1(-L, L)} \leq \sqrt{\eta(u_0)} (1 + \sqrt{N}) e^{-4t/(N+2)}.$$

Thus, the convergence rate in the  $L^1$  norm is half of the rate in the entropy ‘norm’.

Let us now turn to the Cauchy problem. First, we want to remark that several properties related to entropies and self-similar solutions of the Cauchy problem for the equation

$$u_t = -(u(\log u)_{xx})_{xx}, \quad x \in \mathbb{R}, \quad (2.4)$$

are related to similar entropies for second-order diffusion equations. In fact, we consider the time-space rescaling (see [10, 11, 14, 20])

$$w(t, x) = \alpha(t)u(\beta(t), \alpha(t)x), \quad (2.5)$$

with  $\alpha(t) = e^t$  and  $\beta(t) = (e^{4t} - 1)/4$ . Then  $w$  verifies

$$w_t = -(w(\log w)_{xx})_{xx} + (xw)_x, \quad x \in \mathbb{R}. \quad (2.6)$$

Moreover, it can be easily checked that the self-similar solution (1.6) of equation (2.4) translates into a stationary solution for equation (2.6), i.e. the Gaussian distribution

$$w_s(x) = \exp\left(-\frac{x^2}{2}\right). \quad (2.7)$$

Furthermore, equation (2.6) can be written as

$$w_t = -\left[w\left(\log\frac{w}{w_s}\right)_{xx}\right]_{xx} + \left[w\left(\log\frac{w}{w_s}\right)_x\right]_x, \quad x \in \mathbb{R}. \quad (2.8)$$

It is then obvious to check that

$$\mathcal{S}_r(w(t)) = \int_{\mathbb{R}} w(t) \log\left(\frac{w(t)}{w_s}\right) dx \quad (2.9)$$

is an entropy or Lyapunov functional, assuming that the solutions are positive and classical. We remark that this entropy coincides with the natural entropy used in the linear second-order diffusion Fokker-Planck equation

$$\xi_t = \left[\xi\left(\log\frac{\xi}{w_s}\right)_x\right]_x = (x\xi + \xi_x)_x, \quad x \in \mathbb{R}. \quad (2.10)$$

Let us assume that we deal with global in time positive classical solutions of this problem and let us explain the grounds on which the conjecture about the asymptotic behavior is based. In fact, we can compute the evolution of this entropy exactly using (2.8) finding that

$$\frac{d}{dt}\mathcal{S}_r(w) = -\int_{\mathbb{R}} w\left(\log\frac{w}{w_s}\right)_{xx}^2 dx - \int_{\mathbb{R}} w\left(\log\frac{w}{w_s}\right)_x^2 dx.$$

From here, it is easy to deduce that

$$\frac{d}{dt}\mathcal{S}_r(w) \leq - \int_{\mathbb{R}} w \left( \log \frac{w}{w_s} \right)_x^2 dx = -D(w),$$

where  $D(w)$  is nothing else than the standard dissipation of the physical entropy (2.9) for the linear Fokker-Planck equation (2.10) (see [10, 11]). Now, we use the well-known logarithmic Sobolev inequality that gives  $2\mathcal{S}_r(w) \leq D(w)$  to conclude with

$$\frac{d}{dt}\mathcal{S}_r(w) \leq -2\mathcal{S}_r(w),$$

and thus, the exponential decay of the entropy  $\mathcal{S}_r(w)$  follows. Finally, the Csiszar-Kullback inequality implies that

$$\|w(t) - w_s\|_{L^1(\mathbb{R})}^2 \leq 2\mathcal{S}_r(w)$$

and therefore, we deduce the exponential decay of the  $L^1$  deviation to  $w_s$  with a rate which is half of the rate for the entropy  $\mathcal{S}_r(w)$ . By means of the change of variables (2.5), we obtain an algebraic decay towards the self-similar profile (1.6), i.e.

$$\|u(t) - u_s(t)\|_{L^1(\mathbb{R})} \leq C(1+t)^{-1/4}.$$

Let us finally mention that the Fisher information  $I(u)$  is also a Lyapunov functional for the Cauchy problem for (2.4). This functional translates into the Lyapunov functional

$$I_r(w) = \int_{\mathbb{R}} \frac{x^2}{2} u dx + \int_{\mathbb{R}} \frac{u_x^2}{2u} dx$$

for the rescaled equation (2.6).

### 3 Numerical Scheme

In this section we shall design a numerical scheme that preserves the positivity of the solutions to (1.1) and for which the discrete entropy is non-increasing, for both the boundary value problems and the Cauchy problem.

#### 3.1 The boundary value problems

The construction of the scheme will be performed in two steps. First, we derive a semi-discrete scheme and then a fully discrete scheme.

The space domain  $[-L, L]$  is discretized by a uniform mesh with  $2N + 1$  subintervals of length  $\Delta x = 2L/(2N + 1)$ , centered at  $x_i = i\Delta x$  for  $i = -N, \dots, N$ . For a function  $f(x)$ , a standard three-stencil centered difference is

$$f_{i,xx} = \frac{f_{i-1} + f_{i+1} - 2f_i}{(\Delta x)^2}, \tag{3.1}$$

with  $f_i = f(x_i)$ . If we introduce the abbreviations  $F = (f_{-N}, \dots, f_N)^T$  and

$$D = \frac{1}{(\Delta x)^2} \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix} \in \mathbb{R}^{(2N+1) \times (2N+1)},$$

then (3.1) can be written as

$$F_{,xx} = DF + \left( \frac{1}{(\Delta x)^2} f_{-N-1}, 0, \dots, 0, \frac{1}{(\Delta x)^2} f_{N+1} \right)^T,$$

where  $f_{-N-1}$  and  $f_{N+1}$  are approximations of  $f(x_{-N-1})$  and  $f(x_{N+1})$ , respectively, at the ghost points  $x_{-N-1}$  and  $x_{N+1}$  (see below).

The idea of the discretization of (1.1) is to introduce an augmented variable  $v = \log u$  and to discretize the coupled system

$$\begin{aligned} u_t &= -(uv_{xx})_{xx}, \\ v_t &= -\frac{(uv_{xx})_{xx}}{u}. \end{aligned}$$

Using centered differences for the discretization of the  $x$ -variable, we obtain a system of ordinary differential equations for the semi-discrete functions  $(u_i(t), v_i(t))$  approximating  $(u(t, x_i), v(t, x_i))$ :

$$\frac{du_i}{dt} = -(u_i v_{i,xx})_{,xx}, \quad (3.2)$$

$$\frac{dv_i}{dt} = -\frac{(u_i v_{i,xx})_{,xx}}{u_i}, \quad (3.3)$$

with initial data

$$u_i(0) = u_0(x_i), \quad v_i(0) = \log(u_i(0)).$$

For the *periodic boundary conditions*, the index  $i$  in (3.2)-(3.3) varies from  $-N$  to  $N$ . There are four ghost points involved, namely  $x_{\pm(N+1)}$  and  $x_{\pm(N+2)}$ . The  $2L$ -periodicity can be stated as

$$\begin{aligned} u_{\pm(N+1)}(t) &= u_{\mp N}(t), & u_{\pm(N+2)}(t) &= u_{\mp(N-1)}(t), \\ v_{\pm(N+1)}(t) &= v_{\mp N}(t), & v_{\pm(N+2)}(t) &= v_{\mp(N-1)}(t), \end{aligned}$$

This implies

$$u_{\pm(N+1)}(v_{\pm(N+1)})_{,xx} = u_{\mp N}(v_{\mp N})_{,xx}.$$

Therefore, the centered differences for  $u$  and  $uv_{xx}$  may be rewritten into a homogeneous form, namely

$$F_{,xx} = D_P F,$$

with

$$D_P = \frac{1}{(\Delta x)^2} \begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 0 & 1 \\ 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 1 & 0 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix}.$$

With the abbreviations  $U = (u_{-N}, \dots, u_N)^T$ ,  $V = (v_{-N}, \dots, v_N)^T$ , and  $\Lambda_U = \text{diag}(u_{-N}, \dots, u_N)$ , the semi-discrete scheme then reads

$$\begin{aligned} \frac{dU}{dt} &= -D_P \Lambda_U D_P V, \\ \frac{dV}{dt} &= -\Lambda_U^{-1} D_P \Lambda_U D_P V. \end{aligned}$$

Similarly, for the *reflecting boundary conditions* in semi-discrete form

$$\begin{aligned} u_{\pm(N+1)}(t) &= u_{\pm N}(t), & u_{\pm(N+2)}(t) &= u_{\pm(N-1)}(t), \\ v_{\pm(N+1)}(t) &= v_{\pm N}(t), & v_{\pm(N+2)}(t) &= v_{\pm(N-1)}(t), \end{aligned}$$

it is easy to show that

$$u_{\pm(N+1)}(v_{\pm(N+1)})_{,xx} = u_{\pm N}(v_{\pm N})_{,xx}$$

and thus, the semi-discrete scheme reads

$$\begin{aligned} \frac{dU}{dt} &= -D_R \Lambda_U D_R V, \\ \frac{dV}{dt} &= -\Lambda_U^{-1} D_R \Lambda_U D_R V, \end{aligned}$$

with the matrix

$$D_R = \frac{1}{(\Delta x)^2} \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 1 & -1 \end{bmatrix}.$$

Finally, for the *fixed boundary conditions*, the index  $i$  varies from  $-N + 1$  to  $N - 1$ , since the value of  $u$  at the boundary is fixed. Only two additional points  $x_{\pm(N+1)}$  are used. The boundary conditions are

$$u_{\pm(N+1)}(t) = u_{\pm N}(t) = 1, \quad v_{\pm(N+1)}(t) = v_{\pm N}(t) = 0.$$

An elementary computation shows that in this case the scheme can be written as

$$\begin{aligned} \frac{dU}{dt} &= -D_F^T \Lambda_U D_F V, \\ \frac{dV}{dt} &= -\Lambda_U^{-1} D_F^T \Lambda_U D_F V, \end{aligned}$$

with

$$D_F = \frac{1}{(\Delta x)^2} \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & -2 & 1 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -2 & 1 & 0 \\ 0 & 0 & 0 & \cdots & 1 & -2 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \end{bmatrix}.$$

Noticing the symmetry in  $D_P$  and  $D_R$ , all three cases can be unified as

$$\frac{dU}{dt} = -D_B^T \Lambda_U D_B V, \quad (3.4)$$

$$\frac{dV}{dt} = -\Lambda_U^{-1} D_B^T \Lambda_U D_B V. \quad (3.5)$$

where  $D_B$  is taken as  $D_P$ ,  $D_R$ , or  $D_F$ , respectively.

We now discretize the semi-discrete system (3.2)-(3.3) (or (3.4)-(3.5)) in time. At the time level  $t = t_n$ , let  $(u_i^n, v_i^n)$  be an approximation of  $(u_i(t_n), v_i(t_n))$ . We describe an evolution from  $(u_i^n, v_i^n)$  to  $(u_i^{n+1}, v_i^{n+1})$  in two steps. The consistency is assumed at  $t_n$ , namely  $v_i^n = \log u_i^n$ .

First, we perform a semi-implicit integration

$$u_i^* - u_i^n = -\Delta t (u_i^n v_{i,xx}^*)_{,xx}, \quad (3.6)$$

$$v_i^* - v_i^n = -\frac{\Delta t}{u_i^n} (u_i^n v_{i,xx}^*)_{,xx}. \quad (3.7)$$

This is a decoupled linear system. First,  $v_i^*$  is computed from (3.7) and then,  $u_i^*$  is obtained from (3.6). With the notation  $U^n = (u_{-N}^n \dots, u_N^n)^T$ ,  $U^* = (u_{-N}^* \dots, u_N^*)^T$ ,  $V^n = (v_{-N}^n \dots, v_N^n)^T$ , and  $V^* = (v_{-N}^* \dots, v_N^*)^T$ , the equations (3.6)-(3.7) can be recasted as

$$U^* = U^n - \Delta t \Lambda_{U^n} A V^*, \quad (3.8)$$

$$V^* = (I + \Delta t A)^{-1} V^n, \quad (3.9)$$

where  $A = \Lambda_{U^n}^{-1} D_B^T \Lambda_{U^n} D_B$ . The linear algebraic system (3.9) may be solved by a standard method such as LU decomposition.

By a routinary calculation, the local truncation error can be found to be of the order  $O(\Delta t, (\Delta x)^2)$ . The total mass of  $u$  is preserved for the periodic or the reflecting boundary conditions. Indeed, by virtue of the zero-sum for each row in  $D_B$  in these two cases, we have

$$\begin{aligned} \sum_{i=-N}^N u_i^* &= (1, \dots, 1) U^* \\ &= (1, \dots, 1) U^n - \Delta t (1, \dots, 1) D_B^T \Lambda_{U^n} D_B V^* \\ &= \sum_{i=-N}^N u_i^n. \end{aligned}$$

Moreover, the monotonicity of the discrete entropy

$$\mathcal{S}_D^n \equiv \sum_{i=-N}^N u_i^n (v_i^n - 1)$$

is maintained. In order to see this we multiply (3.7) by  $u_i^n$  and take the difference of the resulting equation and (3.6) to get

$$u_i^* = u_i^n (1 + v_i^* - v_i^n). \quad (3.10)$$

Using this identity, (3.8) and (3.9) we infer

$$\begin{aligned} \mathcal{S}_D^* - \mathcal{S}_D^n &= \sum_{i=-N}^N [u_i^* (v_i^* - 1) - u_i^n (v_i^n - 1)] \\ &= \sum_{i=-N}^N (u_i^* - u_i^n) v_i^* \\ &= (\Lambda_{U^n} (V^* - V^n))^T V^* \\ &= -\Delta t (\Lambda_{U^n} A V^*)^T V^* \\ &= -\Delta t V^{*T} D_B^T \Lambda_{U^n} D_B V^* \\ &= -\Delta t (D_B V^*)^T \Lambda_{U^n} D_B V^* \\ &\leq 0. \end{aligned}$$

The consistency between  $u$  and  $v$  is forced in the second step of the discretization of the the semi-discrete system. Observe that, due to (3.10),

$$u_i^* = u_i^n (1 + v_i^* - v_i^n) \leq u_i^n \exp(v_i^* - v_i^n) = \exp v_i^*. \quad (3.11)$$

We define, with a threshold  $V_L \leq 1$ ,

$$(u_i^{n+1}, v_i^{n+1}) = \begin{cases} (u_i^*, \log u_i^*), & \text{if } v_i^* > V_L, \\ (\exp v_i^*, v_i^*), & \text{if } v_i^* \leq V_L. \end{cases}$$

Generally speaking, the conservation in  $u$  is lost. However, the deviation is only of the order  $(v^* - v^n)^2 \sim (\Delta t)^2$  due to (3.11). Moreover, positivity is likely gained at this step. As a matter of fact,  $u_i^*$  becomes negative when the increment  $-\Delta t(u_i^n v_{i,xx}^*)_{,xx}$  is negative with a too big absolute value. As  $v_i^*$  takes an increment proportionally, this typically occurs when  $v_i^* \leq V_L$  if we choose  $V_L$  not too small. The substitution by  $\exp v_i^*$  for  $u_i^{n+1}$  then ensures the positivity.

We can show that positivity of the discrete solution  $u_i^{n+1}$  holds if one of the following conditions are satisfied.

(S1) At time  $t_n$ , it holds  $v_i^n \leq V_L + 1$  for all  $i$ .

(S2) The time step size is small enough such that

$$1 - \Delta t e_i (I + \Delta t A)^{-1} A V^n > 0,$$

where  $I$  is the identity matrix, and  $e_i$  is the  $i$ -th unit row-vector.

The justification of (S1) is straight forward. Indeed, by (3.10), we have

$$u_i^* = u_i^n (1 + v_i^* - v_i^n) \geq u_i^n (v_i^* - V_L).$$

Therefore, the positivity would be lost only if  $v_i^* \leq V_L$ , but in this case it is forced in the second step.

Concerning (S2), direct calculations show

$$u_i^* = u_i^n (1 - \Delta t e_i (I + \Delta t A)^{-1} A V^n). \quad (3.12)$$

When  $\Delta t$  is small enough,  $u_i^*$  stays positive, since  $u_i^n$  is so. Therefore,  $u_i^{n+1}$  is positive.

Now we make a few remarks. First, it turns out in the numerical simulations that (S1) is satisfied and positivity is guaranteed. In fact, if we take  $V_L = 1$ , (S1) means  $u \leq \exp 2 = 7.389$ . Second, noticing the invariance of the equation under a multiplication of a constant, we may indeed select the threshold  $V_L$  as big as suitable for the specific problem (where the initial data may be large). However, then the entropy function should be modified to

$$\mathcal{S} = \int_{-L}^L u (\log u - V_L) dx,$$

and  $\mathcal{S}_D^n$  is changed accordingly. We notice that  $u(v - V_L)$  is non-increasing if either  $u$  increases for  $v \leq V_L$ , or  $v$  decreases for  $u \geq 0$ . Thus in the second step, each local term satisfies  $u_i^{n+1}(v_i^{n+1} - V_L) \leq u_i^*(v_i^* - V_L)$ , by (3.11). Thus the total entropy is non-increasing.

We conclude this subsection by the following theorem.

**Theorem 3.1** *The fully discrete scheme (3.6)-(3.7) yields a positive solution as long as (S1) or (S2) holds. Moreover, the discrete entropy is non-increasing, i.e.*

$$\mathcal{S}_D^{n+1} \leq \mathcal{S}_D^n.$$

*Proof.* The first assertion follows from the above considerations. To prove the second assertion, it suffices to show that  $\mathcal{S}_D^{n+1} \leq \mathcal{S}_D^*$ . Now, if  $v_i^* \leq V_L \leq 1$ , we get for any  $i$

$$u_i^{n+1}(v_i^{n+1} - 1) = \exp v_i^*(v_i^* - 1) \leq u_i^*(v_i^* - 1),$$

using the inequality (3.11). If  $v_i^* > V_L$ , we have

$$u_i^{n+1}(v_i^{n+1} - 1) = u_i^*(\log u_i^* - 1) \leq u_i^*(v_i^* - 1).$$

This shows  $\mathcal{S}_D^{n+1} \leq \mathcal{S}_D^* \leq \mathcal{S}_D^n$ .  $\square$

### 3.2 Cauchy problem

A Cauchy problem is usually approximated by solving the equation in a finite interval  $[-L, L]$ . Numerical boundary conditions are then needed at the cut-off points  $x = \pm L$ . We take the reflecting boundary conditions (1.4) here. This implies that the conservation of  $u$  does not hold in the finite interval  $[-L, L]$ . For the exact solution

$$u_s(t, x) = (1+t)^{-1/4} \exp\left(-\frac{x^2}{4\sqrt{1+t}}\right), \quad (3.13)$$

the deviation at time  $t$  is only

$$\int_{-L}^L |u_s(t, x) - u_s(0, x)| dx = 4 \int_{L/2\sqrt[4]{1+t}}^{L/2} e^{-\xi^2} d\xi.$$

This means that the conservation is basically correct at time  $t = o(L^4)$ . Our numerical results justify this set of boundary conditions.

We shall also need to investigate the rescaled equation (2.6). Therefore, we need to devise the numerical treatment for the Cauchy problem of equation (2.6) or (2.8). Taking a similar strategy as before, we introduce an augmented variable

$$v = \log \frac{w}{w_s},$$

and specify proper boundary conditions at the cut-off points  $x = \pm L$  to approximate the Cauchy problem. By requiring both the conservation of  $w$  and the monotonicity of the entropy function  $\mathcal{S}_w$  over this finite interval, the following boundary conditions seem to be natural:

$$v_x(t, \pm L) = 0, \quad (wv_{xx})_x(t, \pm L) = 0. \quad (3.14)$$

Introducing as in Section 3.1  $W = (w_{-N}, \dots, w_N)^T$ ,  $V = (v_{-N}, \dots, v_N)^T$ , and  $\Lambda_W = \text{diag}(w_{-N}, \dots, w_N)$ , we define the semi-discrete scheme

$$\begin{aligned}\frac{dW}{dt} &= -(D_B^T \Lambda_W D_B + D_1^T \Lambda_W D_1)V, \\ \frac{dV}{dt} &= -\Lambda_W^{-1}(D_B^T \Lambda_W D_B + D_1^T \Lambda_W D_1)V.\end{aligned}$$

Here, the term  $D_B^T \Lambda_W D_B V$  is an approximation of  $(wv_{xx})_{xx}$ , and  $-D_1^T \Lambda_W D_1 V$  approximates  $(wv_x)_x$ . To get the expressions of  $D_B$  and  $D_1$ , we recast the boundary conditions into the semi-discrete form

$$\begin{aligned}v_{\pm(N+1)} &= v_{\pm N}, \\ w_{\pm(N+1)}(v_{\pm(N+2)} + v_{\pm N} - 2v_{\pm(N+1)}) &= w_{\pm N}(v_{\pm(N+1)} + v_{\pm(N-1)} - 2v_{\pm N}).\end{aligned}$$

It is then readily shown that

$$w_{\pm(N+1)}(v_{\pm(N+2)} - v_{\pm N}) = -w_{\pm N}(v_{\pm(N+1)} - v_{\pm(N-1)}). \quad (3.15)$$

Taking the centered difference for the first order derivatives by

$$f_{i,x} = \frac{f_{i+1} - f_{i-1}}{2\Delta x}, \quad (3.16)$$

the discrete derivative of a vector  $F$  becomes

$$F_{,x} = D^1 F + \left( -\frac{f_{-N-1}}{2\Delta x}, 0, \dots, 0, \frac{f_{N+1}}{2\Delta x} \right)^T, \quad (3.17)$$

with

$$D^1 = \frac{1}{2\Delta x} \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 0 \end{bmatrix},$$

Coming back to the boundary terms, we see that (3.15) implies

$$(wv_x)_{\pm(N+1)} = -(wv_x)_{\pm N}.$$

Therefore, the vector approximating the term  $(wv_x)_x$  is (with a slight abuse of notation)

$$\begin{bmatrix} (wv_x)_{x,-N} \\ (wv_x)_{x,-N+1} \\ (wv_x)_{x,-N+2} \\ \vdots \\ (wv_x)_{x,N-2} \\ (wv_x)_{x,N-1} \\ (wv_x)_{x,N} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & -1 \end{bmatrix} \begin{bmatrix} (wv_x)_{-N} \\ (wv_x)_{-N+1} \\ (wv_x)_{-N+2} \\ \vdots \\ (wv_x)_{N-2} \\ (wv_x)_{N-1} \\ (wv_x)_N \end{bmatrix}.$$

Moreover,

$$\begin{bmatrix} (wv_x)_{-N} \\ (wv_x)_{-N+1} \\ (wv_x)_{-N+2} \\ \vdots \\ (wv_x)_{N-2} \\ (wv_x)_{N-1} \\ (wv_x)_N \end{bmatrix} = \Lambda_W \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix} V.$$

As a conclusion, we obtain

$$D_1 = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 & 0 \\ -1 & 0 & 1 & \cdots & 0 & 0 & 0 \\ 0 & -1 & 0 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 1 & 0 \\ 0 & 0 & 0 & \cdots & -1 & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & -1 & 1 \end{bmatrix}. \quad (3.18)$$

On the other hand, by a similar argument as above, we may show that  $D_B = D_R$ .

We now describe the fully discrete scheme. At a time level  $t = t_n$ ,  $(W^n, V^n)$  denotes an approximation of  $(W(t_n), V(t_n))$ . The time discretization is

$$W^* - W^n = -\Delta t (D_B^T \Lambda_{W^n} D_B + D_1^T \Lambda_{W^n} D_1) V^*, \quad (3.19)$$

$$V^* - V^n = -\Delta t \Lambda_{W^n}^{-1} (D_B^T \Lambda_{W^n} D_B + D_1^T \Lambda_{W^n} D_1) V^*. \quad (3.20)$$

We first solve the linear problem on  $V^*$  from (3.20) and then obtain  $W^*$  from (3.19). By exactly the same argument as before, this step maintains the conservation of  $w$  and the monotonicity of the entropy

$$\mathcal{S}_{Dr}^n = \sum_{i=-N}^N w_i^n v_i^n.$$

The property corresponding to (3.11) is now

$$w_i^* = w_i^n (1 + v_i^* - v_i^n) \leq w_i^n \exp(v_i^* - v_i^n) = w_s(x_i) \exp(v_i^*). \quad (3.21)$$

This allows us to make a second step to relate  $w$  and  $v$ . With a threshold  $V_L \leq 1$ , we define

$$(w_i^{n+1}, v_i^{n+1}) = \begin{cases} (w_i^*, \log(w_i^*/w_s(x_i))), & \text{if } v_i^* > V_L, \\ (w_s(x_i) \exp v_i^*, v_i^*), & \text{if } v_i^* \leq V_L. \end{cases}$$

With the same arguments as in the previous section, we can show the following properties of the derived fully discrete scheme.

**Theorem 3.2** *The fully discrete scheme (3.19)-(3.20) yields a positive solution as long as either one of the following conditions holds.*

(S1') *At time  $t_n$ , it holds  $v_i^n \leq V_L + 1$  for all  $i$ .*

(S2') *The time step size is small enough such that*

$$1 - \Delta t e_i (I + \Delta t A_w)^{-1} A_w V^n > 0,$$

$$\text{where } A_w = D_B^T \Lambda_{W^n} D_B + D_1^T \Lambda_{W^n} D_1.$$

*Moreover, the discrete entropy is non-increasing, i.e.*

$$\mathcal{S}_{Dr}^{n+1} \leq \mathcal{S}_{Dr}^n. \quad (3.22)$$

## 4 Numerical simulations

In this section we present our numerical results for the original equation (1.1) and the rescaled equation (2.6).

### 4.1 Original equation

We consider the evolution with the initial data

$$u(0, x) = 0.01 + 0.99 \sin^2 \pi x, \quad x \in [-0.5, 0.5]. \quad (4.1)$$

The computations are performed with 201 gridpoints ( $N = 100$ ) and  $\Delta t = 10^{-4}$ . The scheme is stable with this time-step size due to the semi-implicitness. For an explicit scheme, one expects  $\Delta t \sim (\Delta x)^4$  for such a fourth-order problem. The threshold for  $v$  is taken as  $V_L = 1$ .

The evolution of the solution with periodic boundary conditions is displayed in Figure 1(a). The solution converges quickly to the constant steady state  $u = u_\infty$ . The plots in Figure 2 illustrate the conservation of  $u$  (solid line) and the monotonicity of the entropy as well as the Fisher information functional. Note that the conservation in  $u$  is not exact numerically. The local increment is of the order  $(\Delta t)^2$ . Therefore, we may reduce it by taking smaller  $\Delta t$ . In Figure 2(a) (dotted line), we observe the difference with  $\Delta t = 5 \times 10^{-5}$ . The convergence towards equilibrium  $u_\infty(x)$  is exponential, as clearly seen from subplot (d). The modified entropy  $\int_{-L}^L (u - u_\infty)(\log u - \log u_\infty) dx$ , which diminishes at equilibrium, decays exponentially as well, twice faster than the  $L^1$  deviation. See subplots (e) and (f).

The solution with reflecting boundary conditions (1.4) is shown in Figure 1(b). As the initial data is symmetric, so is the solution itself. In this case, the reflecting boundary

conditions are equivalent to the periodic boundary conditions and give the same solutions. However, if there is no symmetry, the solutions corresponding to both boundary conditions are different. For instance, in Figure 3, we use the initial data

$$u(0, x) = 0.01 + 0.99 \sin^2 \pi(0.5 - (x - 0.5)(x + 0.5)(x - 1.5)).$$

We observe that the solution is ‘skew’ for reflecting boundary conditions. The convergence towards a constant state is slower, as it is not a constant at  $t = 0.01$ . In the periodic case, on the other hand, the evolution is as fast as in the symmetric case.

With the fixed boundary conditions (1.5), the solution approaches to a uniform profile  $u_\infty(x) = 1$ , as shown in [18] (see Figure 4 for initial data (4.1)). The conservation of  $u$  clearly does not hold in this case, and the evolution of  $\int_{-L}^L u(t, x) dx$  is shown in Figure 5(a). The entropy  $\mathcal{S}_D$  decreases, as depicted in subplot (b). The monotonicity of two other functionals

$$\eta(u(t)) = \int_{-L}^L (u(t, x)(\log u(t, x) - 1) + 1) dx,$$

and

$$\theta(u(t)) = \int_{-L}^L |u(t, x) - 1| dx$$

are shown in the subplots (c) and (d), respectively. As predicted in [18], they decrease exponentially, with the rates shown in subplots (e) and (f). Though the numerical decay rates are bigger than the theoretical results, we see that the rate for  $\eta$  is about twice than the rate for  $\theta$  which confirms the theoretical results (see Section 2).

Now we approximate the Cauchy problem with a scheme similar as described in Section 3.2. For the initial data we choose the exact solution (3.13) at  $t = 0$ . In Figure 6, we display the numerical solution for  $(t, x) \in [0, 10] \times [-10, 10]$ . The simulation is taken with 201 grid points and  $\Delta t = 0.01$ . We show in Figure 7 the amplitude  $u(t, 0)$  and the snapshot  $u(10, x)$ . The difference between the numerical solution and the exact solution is indiscernable.

If we perturb the Cauchy data by

$$u(0, x) = \begin{cases} e^{-(x+1)^2}, & \text{for } x < -1, \\ 1, & \text{for } |x| \leq 1, \\ e^{-(x-1)^2}, & \text{for } x > 1, \end{cases} \quad (4.2)$$

then the solution will converge to the unperturbed solution  $u_s(t, x)$  up to a scaling asymptotically. This is illustrated in Figure 8, and quantitatively in the subplots of Figure 9. We observe that the convergence is polynomial rather than exponential here.

## 4.2 Rescaled problem

For the rescaled problem, a naive scheme that treats  $(xw)_x$  in (2.6) as a source term may not give the correct solution. In most cases, taking the Gaussian as initial data, the

numerical solution grows. Even if we employ boundary conditions satisfied by the exact solution such as

$$w_x + wx = 0, \quad w(t, \pm L) = w(0, \pm L), \quad (4.3)$$

we still observe the growth (Figure 10). Consequently, the entropy also increases.

Taking the scheme described in the previous section, we can reproduce the Gaussian solution (2.7) (Figure 11). We have taken 201 grid points and  $\Delta t = 0.001$ . Moreover, if we disturb the Gaussian, e.g. by the double-bell profile

$$u(0, x) = \exp\left(-\frac{x^2}{2} + \sin^2 x\right), \quad (4.4)$$

the solution still converges to the Gaussian-shaped solution (Figure 12). The numerical result indicates that the convergence towards the Gaussian  $w_\infty$  with corresponding mass occurs with an exponential rate, as seen in Figure 13(a). The decay exponent of  $\|w(t, \cdot) - w_\infty(\cdot)\|_{L^1}$  for this initial data is about 0.9. The modified entropy corresponding to this solution

$$\int_{-L}^L w \log \frac{w}{w_\infty} dx$$

decreases, as shown in Figure 13(b). For time from around 7, the entropy reaches regime of round-off error, and becomes oscillatory. The decay exponent is about 1.8. This result confirms the formal computations made in Section 2 for the Cauchy problem. We note that for other initial data which decreases fast enough at infinity, e.g. a smoothed step-function, we obtain essentially the same asymptotic Gaussian up to a translation and scaling.

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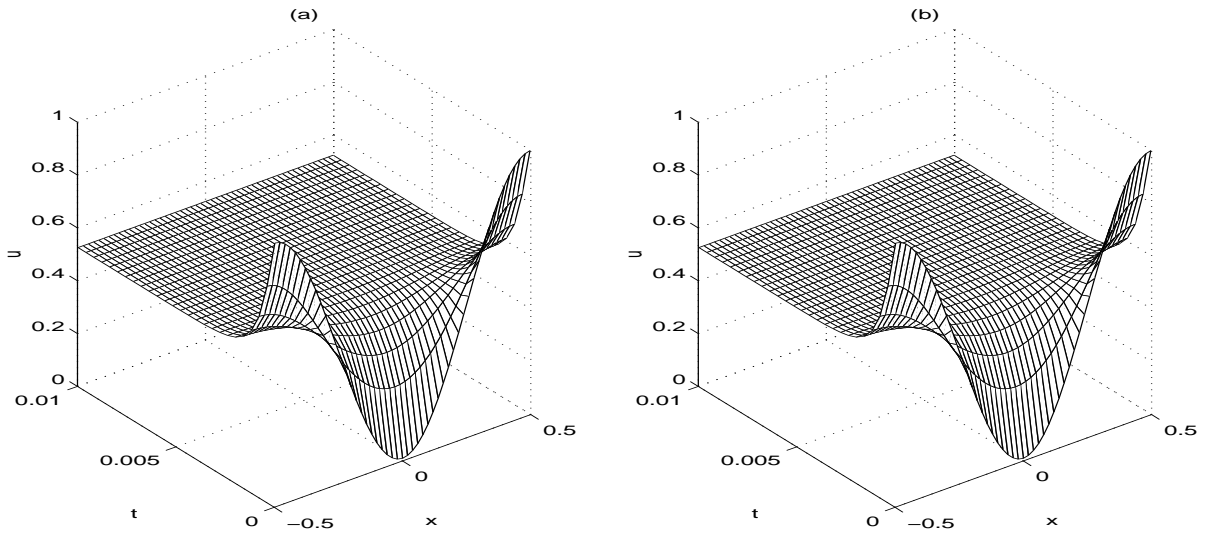


Figure 1: Numerical solution  $u(t, x)$  of (1.1) with (a) periodic boundary conditions; (b) reflecting boundary conditions.

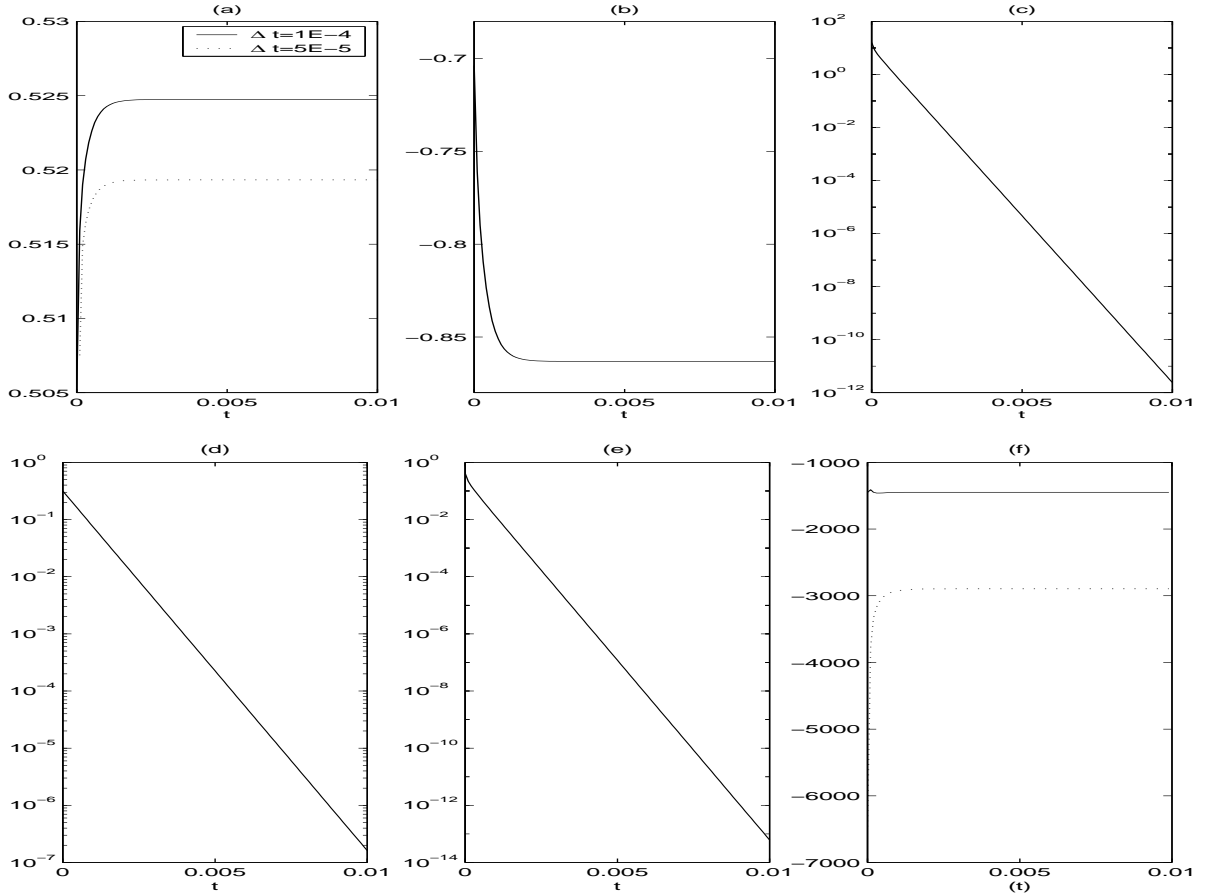


Figure 2: Quantitative properties of the solution with periodic boundary conditions: (a) total mass  $\int_{-L}^L u(t, x) dx$  for  $\Delta t = 10^{-4}$  (solid line) and  $\Delta t = 5 \times 10^{-5}$  (dotted line); (b) entropy  $\mathcal{S}_D$  for  $\Delta t = 10^{-4}$ ; (c) Fisher information functional  $I(u(t))$ ; (d)  $L^1$  deviation from equilibrium  $\|u - u_\infty\|_{L^1}$ ; (e) modified entropy  $\int_{-L}^L (u - u_\infty)(\log u - \log u_\infty) dx$ ; (f) rate of decay, solid for  $L^1$  deviation, dotted for modified entropy.

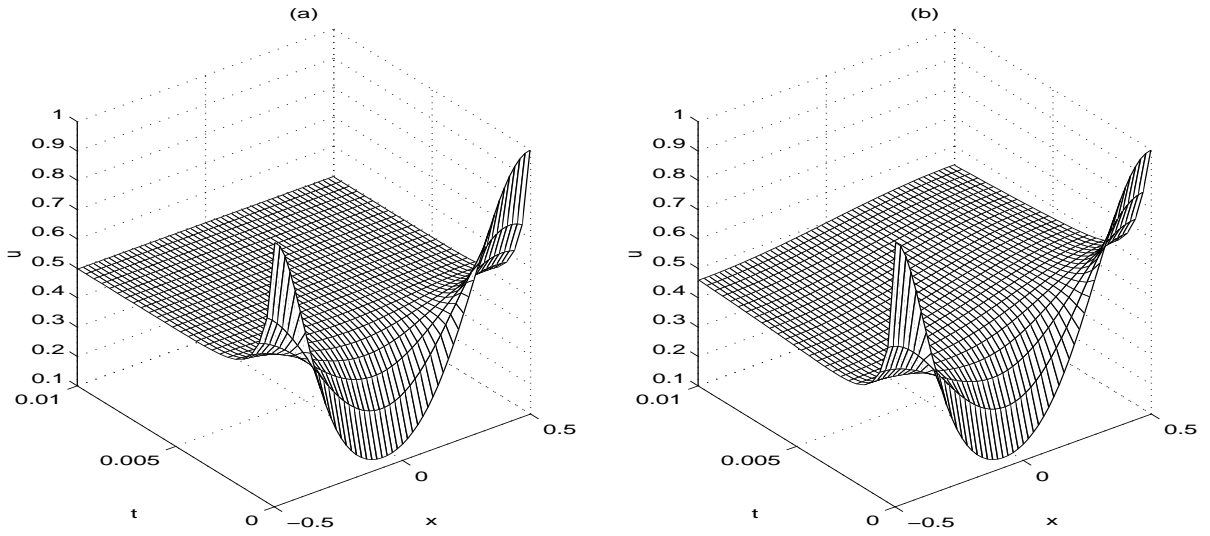


Figure 3: Numerical solution  $u(t, x)$  of (1.1) for nonsymmetric initial data with (a) periodic boundary conditions; (b) reflecting boundary conditions.

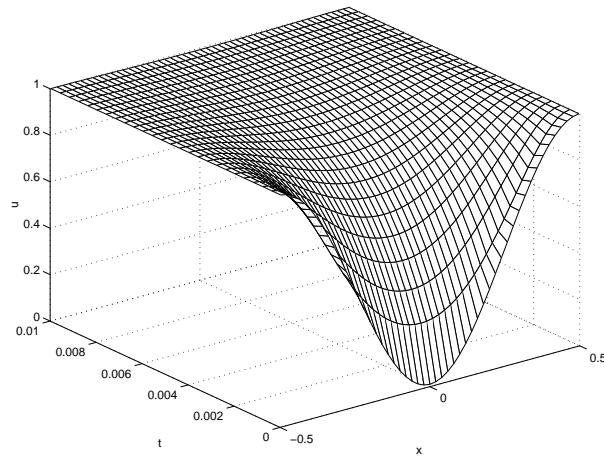


Figure 4: Numerical solution  $u(t, x)$  of (1.1) with fixed boundary conditions.

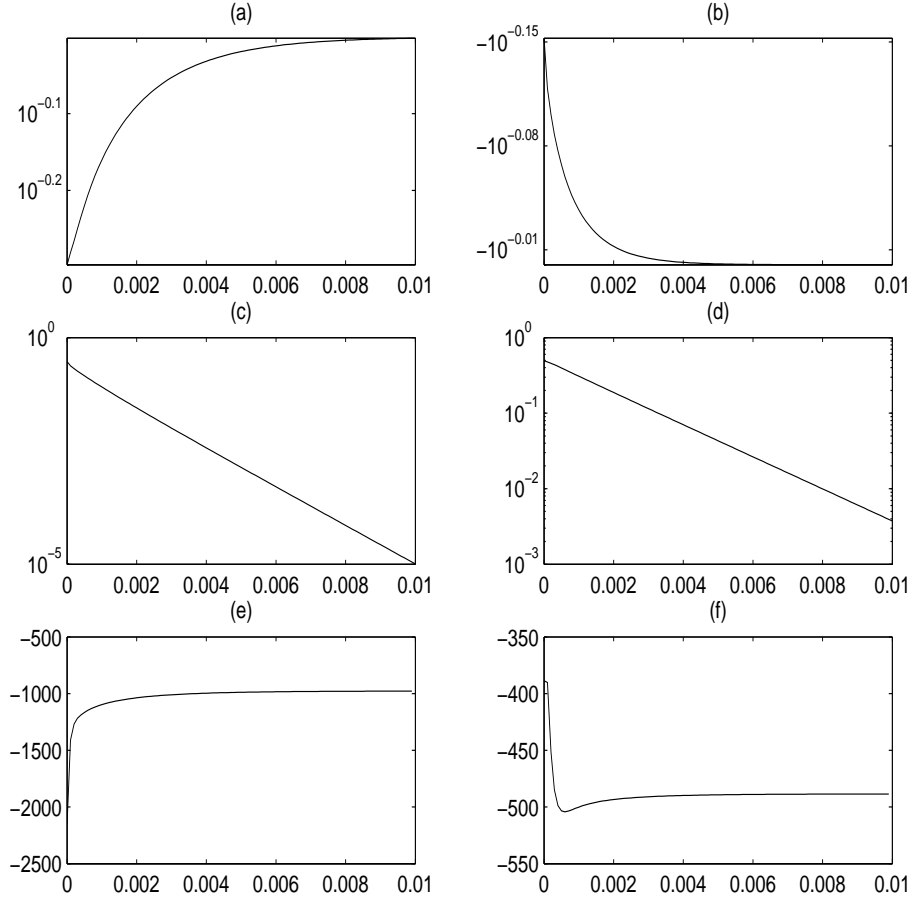


Figure 5: Quantitative properties of the solution with fixed boundary conditions: (a) total mass  $\int_{-L}^L u(t, x) dx$ ; (b) entropy  $\mathcal{S}_D$ ; (c) functional  $\eta(u(t))$ ; (d)  $L^1$  deviation  $\theta(u(t))$ ; (e) convergence rate for  $\eta(u(t))$ ; (f) convergence rate for  $\theta(u(t))$ .

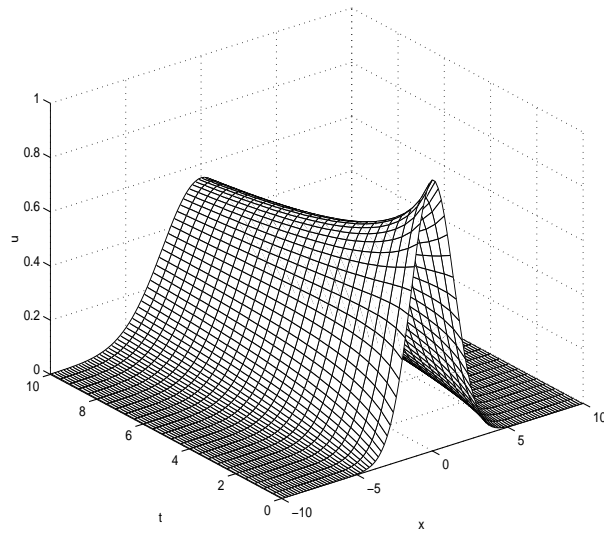


Figure 6: Numerical solution  $u(t, x)$  for the Cauchy problem.

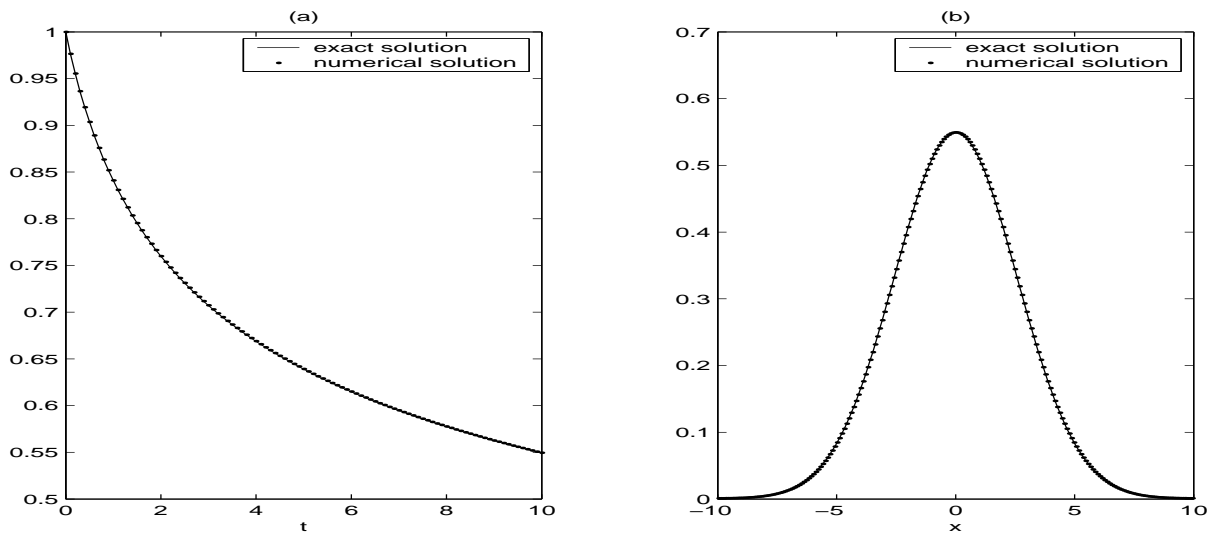


Figure 7: Comparison between the numerical solution and the exact solution: (a)  $u(t, 0)$ ; (b)  $u(10, x)$ .

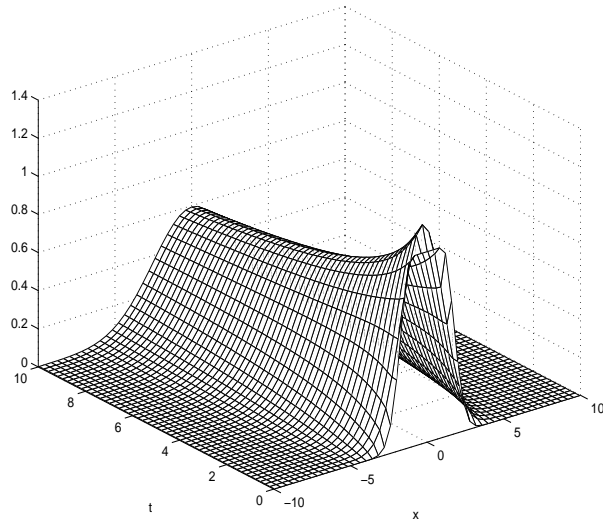


Figure 8: Perturbed Cauchy problem.

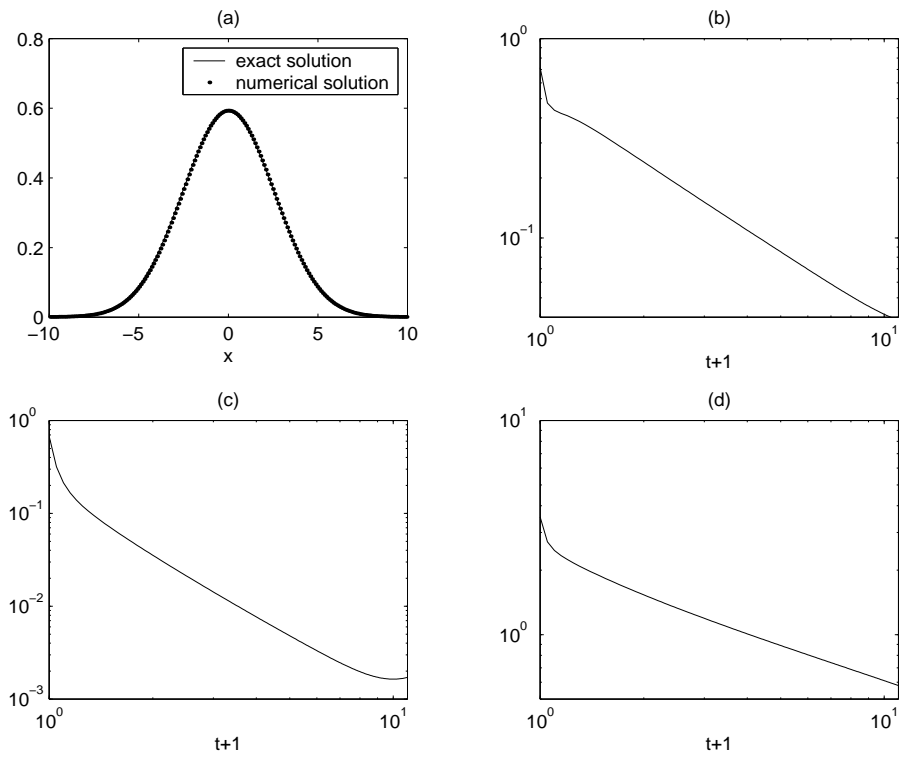


Figure 9: Quantitative properties of the perturbed Cauchy problem: (a) comparison between  $u(10, x)$  and  $u_s(10, x)$ ; (b)  $L^1$  deviation; (c) modified entropy; (d) Fisher information functional  $I(u(t))$ .

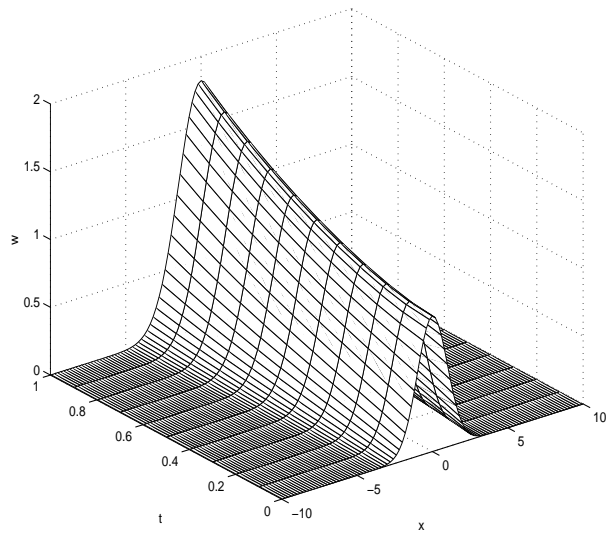


Figure 10: Growth of the numerical solution  $u(t, x)$  for the Cauchy problem with boundary conditions (4.3).

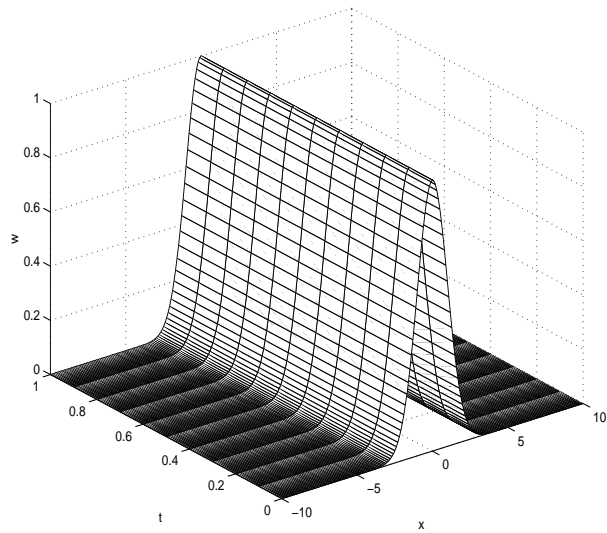


Figure 11: Gaussian solution for the Cauchy problem.

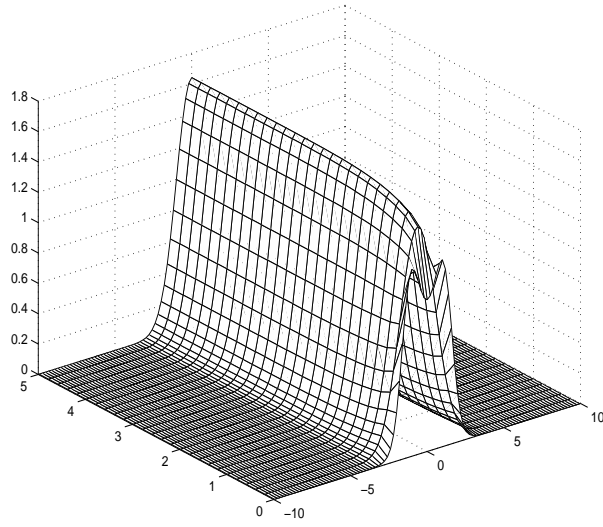


Figure 12: Perturbed solution for the Cauchy problem.

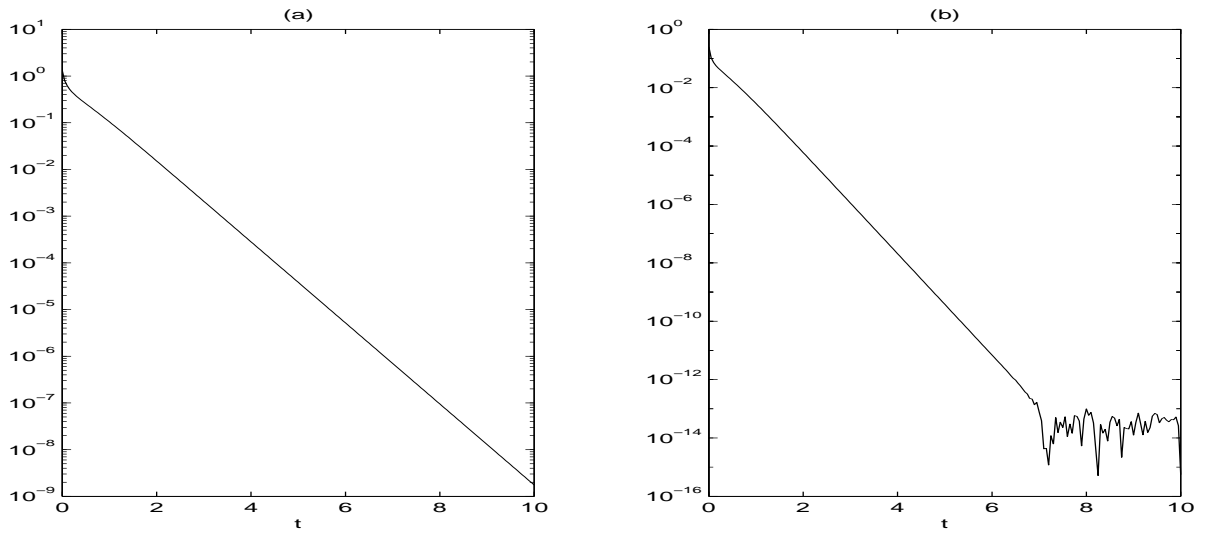


Figure 13: Qualitative behavior of the perturbed solution: (a)  $L^1$ -norm of the deviation from the corresponding Gaussian  $w_\infty$ ; (b) modified entropy.