

A Finite Difference Scheme to the System of Self-interacting Particles

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自己相互作用粒子系への差分法

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1 Introduction

Let $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$) be a bounded domain with the smooth boundary $\partial\Omega$. We consider a parabolic-elliptic system for unknowns $u = u(x, t)$ and $v = v(x, t)$ of $(x, t) \in \bar{\Omega} \times [0, T]$;

$$(1.1) \quad \begin{cases} \frac{\partial u}{\partial t} = \nabla \cdot (\nabla u - u \nabla v) & \text{in } \Omega \times (0, T), \\ 0 = \Delta v - av + u & \text{in } \Omega \times (0, T), \\ \frac{\partial u}{\partial \nu} - u \frac{\partial v}{\partial \nu} = 0, \frac{\partial v}{\partial \nu} = 0 & \text{on } \partial\Omega \times (0, T), \end{cases}$$

where ν denotes the outer unit normal vector to $\partial\Omega$; $\partial/\partial \nu$ the differentiation along ν on $\partial\Omega$; and a a positive constant. We treat (1.1) with the initial condition

$$(1.2) \quad u|_{t=0} = u_0(x) \quad \text{on } \Omega,$$

and assume that $u_0(x)$ is smooth, non-negative, and not identically zero on $\bar{\Omega}$.

In the context of statistical mechanics, the system (1.1) is interpreted as the adiabatic limit of the Fokker-Plank equation, which is associated with the mean field of self-interacting particles subject to a frictional, velocity-dependent force with a random fluctuation. There u denotes the distribution of mass and v the potential. See, for example, Wolansky [11], [12].

Other model leading to (1.1) comes from mathematical biology as a simplified Keller-Segel system of chemotaxis which was introduced by Nagai [6]. That is, the system (1.1) describes the aggregation of slime molds caused by their chemotactic features, where $u(x, t)$ denotes the density of the cellular slime molds and $v(x, t)$ the concentration of the chemical substance. If taking

$$a_0 \frac{\partial v}{\partial t} = \Delta v - av + u \quad \text{in } \Omega \times (0, T) \quad a_0 > 0 : \text{const}$$

instead of the second equation of (1.1), we obtain the original system proposed by Keller and Segel [5].

As was studied by Yagi [10] and Biler [2], the unique classical solution (u, v) of (1.1) exists locally in time if $\partial\Omega$ is smooth enough. The supremum of the existence time of the solution is denoted by $T_{\max}$ and in what follows we shall take $T \in (0, T_{\max})$ otherwise stated. Moreover we have

$$(I) \quad u(x, t) > 0 \quad (x, t) \in \bar{\Omega} \times (0, T] \quad (\text{conservation of the positivity}),$$

$$(II) \quad \int_{\Omega} u(x, t) dx = \int_{\Omega} u_0(x) dx \quad t \in [0, T] \quad (\text{conservation of the total mass}).$$

In fact, (I) is a consequence of the maximum principle and (II) immediately follows from

$$\frac{d}{dt} \int_{\Omega} u(x, t) dx = \int_{\partial\Omega} \left(\frac{\partial u}{\partial \nu} - u \frac{\partial v}{\partial \nu} \right) dS = 0.$$

Another important feature of (1.1) is

$$(III) \quad \frac{d}{dt} W(u(\cdot, t), v(\cdot, t)) \leq 0 \quad t \in [0, T] \quad (\text{existence of the Lyapunov functional})$$

where

$$W(u, v) = \int_{\Omega} (u \log u - u) dx - \frac{1}{2} \int_{\Omega} uv dx.$$

In the one dimensional case ($d = 1$), the dynamics of (1.1) is completely determined by (III). On the other hand, in the two or three dimensional cases ($d = 2, 3$), (III) brings us various information on the behaviour of a solution to (1.1). See, for more detail, the monograph by one of the author ([9]).

From the view point of numerical analysis, it is quite natural to try to make a discrete scheme to (1.1) which inherits analytical properties of the original equation, in particular the discrete analogues of (I), (II) and (III).

We already know several schemes which satisfy some of (I), (II) and (III). For linear convection-diffusion equations

$$(1.3) \quad \frac{\partial u}{\partial t} = \Delta u - \nabla \cdot (\mathbf{b}u), \quad \left(\frac{\partial u}{\partial \nu} - (\mathbf{b} \cdot \nu)u \right) \Big|_{\partial\Omega} = 0, \quad (\mathbf{b} : \text{given flow}),$$

R. Gorenflo ([3]) considered the case $d = 1$ and gave a finite difference scheme satisfying (I) and (II) by a carefully treatment of the flux at the boundary. K. Baba and M. Tabata

([1]) made a finite element scheme to (1.3) which satisfies (I) and (II). The latter work applied an upwind technique, and therefore (I) was guaranteed without any restriction on h , the spatial discretization parameter. It is an important difference between these two works; (I) was guaranteed for a sufficiently small h in [3].

On the other hand, several authors proposed energy conservative or energy dissipative schemes. Here we only refer to D. Furihata's work. He (and his co-workers) derived finite difference schemes which inherited energy conservation or dissipation property of the original equation. They derived discrete equations directly from the variational principle and their method is called the discrete variational method (See, for example, [4]). However, our problem seems to be out of scope from their theory.

The purpose of the present note is to give some considerations to make a finite difference scheme satisfying the discrete analogues of (I), (II) and (III). Roughly speaking, our strategy is as follows. In order to treat (I) and (II), we combine the idea of Gorenflo with that of Baba-Tabata. Then we take a certain time discretization which preserves the discrete analogue of (III). Specifically, we shall propose

$$(1.4) \quad \frac{u^n - u^{n-1}}{\tau_n} = \nabla \cdot (\nabla u^n - u^n \nabla v^{n-1}) \text{ in } \Omega$$

with a suitable boundary condition, where u^n and v^n denote approximations of u and v at the n th time step and $\tau_n > 0$ the n th time mesh size. Equality (1.4) is a linear elliptic equation for u^n so that its numerical implementation is rather easy. Furthermore, as will be verified below, it holds

$$(1.5) \quad \frac{1}{\tau_n} [\mathcal{W}(u^n, v^n) - \mathcal{W}(u^{n-1}, v^{n-1})] \leq 0.$$

Time discretization (1.4) is often applied in actual computations, however, to our knowledge, no emphasis on (1.5) is made.

The organisation of this paper is as follows: In §2, we consider time discrete scheme (1.4) and verify (1.5). §3 is devoted to a finite difference scheme where the time discretization is based on (1.4) and the spatial one is on a combination of [3] with [1]. Because of the limitation of the page number, concerning the spatial discretization, we shall restrict our consideration to the one dimensional case. Finite difference scheme in the two dimensional case and some numerical examples will be reported in a forthcoming paper ([7]).

2 Time discretization

Before preceding to a time discretization, we recall the derivation of (III). We firstly introduce

$$(Gu)(x, t) = \int_{\Omega} \hat{G}(x, y) u(y, t) dy,$$

where $\hat{G}(x, y)$ denotes the Green function associated with $-\Delta + a$ under the homogeneous Neumann boundary condition. Then (1.1) is written as

$$(2.1) \quad \begin{cases} \frac{\partial u}{\partial t} = \nabla \cdot (\nabla u - u \nabla(Gu)) & \text{in } \Omega \times (0, T), \\ (\nabla u - u \nabla(Gu)) \cdot \nu = 0 & \text{on } \partial\Omega \times (0, T), \end{cases}$$

and (III) is equivalent to

$$(III)' \quad \frac{d}{dt} J(u(\cdot, t)) \leq 0 \quad t \in [0, T],$$

where

$$J(u) = \mathcal{W}(u, Gu) = \int_{\Omega} (u \log u - u) dx - \frac{1}{2} \int_{\Omega} (Gu)u dx.$$

We introduce

$$X = \{w \in L^2(\Omega) \mid w(x) > 0 \text{ (} x \in \overline{\Omega})\},$$

and deal with J as a functional over X . We decompose J into $J = I - K$, where

$$I(w) = \int_{\Omega} (w \log w - w) dx, \quad K(w) = \frac{1}{2} \int_{\Omega} (Gw)w dx \quad (w \in X).$$

Fréchet derivatives $DI(w)$ and $DK(w)$ of I and K at $w \in X$ are given as

$$\begin{aligned} (DI(w), \varphi) &= \lim_{s \rightarrow 0} s^{-1} [I(w + s\varphi) - I(w)] = (\log w, \varphi) & (\forall \varphi \in X), \\ (DK(w), \varphi) &= (Gw, \varphi) & (\forall \varphi \in X), \end{aligned}$$

where

$$(v, w) = \int_{\Omega} v(x)w(x) dx \quad (v, w \in L^2(\Omega)).$$

Based on these identities, we shall employ identification

$$DI(w) \sim \log w \quad \text{and} \quad DK(w) \sim Gw$$

in the way of the L^2 inner product.

As a result, noting $\nabla \cdot (\nabla u - u \nabla(Gu)) = \nabla \cdot u \nabla(\log u - Gu)$, we can rewrite (2.1) as

$$(2.2) \quad \begin{cases} \frac{\partial u}{\partial t} = \nabla \cdot u \nabla(DI(u) - DK(u)) & \text{in } \Omega \times (0, T), \\ u \nabla(DI(u) - DK(u)) \cdot \nu = 0 & \text{on } \partial\Omega \times (0, T). \end{cases}$$

Hence, by the chain rule,

$$\begin{aligned} (2.3) \quad \frac{d}{dt} J(u(\cdot, t)) &= \int_{\Omega} u_t (DI(u) - DK(u)) dx \\ &= \int_{\Omega} \nabla \cdot [u \nabla(DI(u) - DK(u))] \cdot [(DI(u) - DK(u))] dx \\ &= - \int_{\Omega} u |\nabla(DI(u) - DK(u))|^2 dx \leq 0. \end{aligned}$$

Now we proceed to a time discretization scheme. The following lemma plays a crucial

Lemma 2.1. *We have*

$$(2.4) \quad J(w) - J(\hat{w}) \leq (DI(w) - DK(\hat{w}), w - \hat{w}), \quad (w, \hat{w} \in X).$$

Proof. Let $w \in X$ and $\hat{w} \in X$. Since $s(>0) \mapsto s \log s - s$ is convex, we have

$$(2.5) \quad I(w) - I(\hat{w}) \leq (DI(w), w - \hat{w}).$$

By Taylor's formula (for example Theorem 4.A of Zeidler [14]), we obtain

$$K(\hat{w} + \varphi) = K(\hat{w}) + (DK(\hat{w}), \varphi) + \frac{1}{2} \int_0^1 (1 - \sigma) D^2 K(\hat{w} + \sigma \varphi) [\varphi, \varphi] d\sigma$$

for any $\varphi \in X$, where $D^2 F(\tilde{w})$ denotes the second Fréchet derivative of F at $\tilde{w} \in X$;

$$D^2 K(\tilde{w})[\varphi, \varphi] = \lim_{s \rightarrow 0} \left(\frac{d}{ds} \right)^2 K[u + s\varphi] = (G\varphi, \varphi), \quad (\varphi \in X).$$

The function $G\varphi$ is a solution of $-\Delta v + av = \varphi$ in Ω with $\partial v / \partial \nu = 0$ on $\partial\Omega$ so that $(G\varphi, \varphi) = \|\nabla(G\varphi)\|_{L^2}^2 + a\|G\varphi\|_{L^2}^2 > 0$. Therefore, by choosing $\varphi = w - \hat{w}$, we have

$$K(w) - K(\hat{w}) \geq (DK(\hat{w}), w - \hat{w}).$$

This, together with (2.5), implies (2.4). $\square$

Based on the observation above, we propose a time discretization to (1.1). Let $\{\tau_n\}_{n=1}^m$ be a set of positive numbers and suppose that the n th time step t_n is determined by

$$(2.6) \quad t_0 = 0, \quad t_n = t_{n-1} + \tau_n = \sum_{k=1}^n \tau_k \quad (n = 1, \dots, m), \quad t_m \leq T.$$

Let $u^n \in C^2(\overline{\Omega})$ be an approximation of $u(\cdot, t_n)$ at the n th time step t_n ($n = 0, 1, 2, \dots$). We set

$$(2.7) \quad u^0 = u_0(x) \quad \text{on } \Omega$$

and obtain $\{u^n\}_{n=1}^m$ by successively solving

$$(2.8) \quad \begin{cases} \frac{u^n - u^{n-1}}{\tau_n} = \nabla \cdot u^n \nabla (DI(u^n) - DK(u^{n-1})) & \text{in } \Omega, \\ u^n \nabla (DI(u^n) - DK(u^{n-1})) \cdot \nu = 0 & \text{on } \partial\Omega \end{cases}$$

or equivalently

$$(2.9) \quad \begin{cases} \frac{u^n - u^{n-1}}{\tau_n} = \nabla \cdot (\nabla u^n - u^n \nabla (Gu^{n-1})) & \text{in } \Omega, \\ (\nabla u^n - u^n \nabla (Gu^{n-1})) \cdot \nu = 0 & \text{on } \partial\Omega. \end{cases}$$

Theorem 2.1. Let $n \in \{1, 2, \dots, m\}$. Assume that $u^n, u^{n-1} \in C^2(\overline{\Omega}) \cap X$ satisfy (2.8). Then we have

$$(III^\tau) \quad \frac{1}{\tau_n} [J(u^n) - J(u^{n-1})] \leq 0.$$

Proof. By Lemma 2.1,

$$\begin{aligned} & J(u^n) - J(u^{n-1}) \\ & \leq \tau_n \int_{\Omega} (DI(u^n) - DK(u^{n-1})) [\nabla \cdot u^n \nabla (DI(u^n) - DK(u^{n-1}))] dx \\ & = -\tau_n \int_{\Omega} u^n |\nabla (DI(u^n) - DK(u^{n-1}))|^2 dx \leq 0, \end{aligned}$$

which implies (III^τ) . $\square$

Remark 2.1. The first equation of (2.9) is written as

$$\left(\frac{1}{\tau_n} + aGu^{n-1} - u^{n-1} \right) u^n - \Delta u^n + (\nabla(Gu^{n-1})) \cdot (\nabla u^n) = \frac{1}{\tau_n} u^{n-1},$$

where the relation $-\Delta(Gu^{n-1}) + aGu^{n-1} = u^{n-1}$ is used. Hence, if τ_n is sufficiently small, there is a unique solution $u^n \in C^2(\overline{\Omega})$ and it satisfies

$$(I^\tau) \quad u^n > 0 \text{ in } \overline{\Omega} \quad (n = 1, \dots, m).$$

On the other hand, integrating both sides of (2.7) over Ω , we have

$$\frac{1}{\tau_n} \left(\int_{\Omega} u^n dx - \int_{\Omega} u^{n-1} dx \right) = \int_{\partial\Omega} (\nabla u^n - u^n \nabla (Gu^{n-1})) \cdot dS = 0,$$

which yields

$$(II^\tau) \quad \int_{\Omega} u^n(x) dx = \int_{\Omega} u_0(x) dx \quad (n = 1, \dots, m).$$

3 Finite difference scheme

In this section, we treat

$$(3.1) \quad \begin{cases} u_t = (u_x - uv_x)_x & (0 < x < 1, 0 < t < T), \\ u_x(0, t) = u_x(1, t) = 0, \\ 0 = v_{xx} - av + u & (0 < x < 1, 0 < t < T), \\ v_x(0, t) = v_x(1, t) = 0, \\ u(x, t) = u_0(x). \end{cases}$$

Take a positive integer N and let $h = 1/N$. We introduce two kinds of mesh points over Ω as

$$x_j = \left(j - \frac{1}{2} \right) h, \quad \hat{x}_j = jh \quad (j = 1, \dots, N).$$

Moreover, for the sake of convenience, virtual mesh points $x_0 = -h/2$, $x_{N+1} = (N + 1/2)h$, $\hat{x}_{-1} = -h$, and $\hat{x}_{N+1} = (N + 1)h$ are often treated. Time discretization makes use of (2.8). We find approximations of $u(\cdot, t_n)$ and $v_x(\cdot, t_n)$ over the *main mesh points* $\{x_j\}_{j=1}^N$:

$$u_j^n \approx u(x_j, t_n) \quad \text{and} \quad b_j^n \approx v_x(x_j, t_n).$$

On the other hand, we compute approximations of $v(\cdot, t_n)$ and $(u_x - uv_x)(\cdot, t_n)$ over the *dual mesh points* $\{\hat{x}_j\}_{j=0}^N$:

$$v_j^n \approx v(\hat{x}_j, t_n) \quad \text{and} \quad F_j^n \approx (u_x - uv_x)(\hat{x}_j, t_n).$$

Firstly, we suppose that $\{u_j^{n-1}\}_{j=1}^N$ and $\{v_j^{n-1}\}_{j=0}^N$ have been obtained. Then we approximate $v_x(\cdot, t_{n-1})$ by

$$b_j^{n-1} = \frac{v_j^{n-1} - v_{j-1}^{n-1}}{h} \quad (j = 1, 2, \dots, N),$$

and set

$$b_j^{n-1,+} = \max\{0, b_j^{n-1}\}, \quad b_j^{n-1,-} = \max\{0, -b_j^{n-1}\}.$$

Following a technique of upwind approximation, we may suppose that u_j^n and u_{j+1}^n are carried into a point $\hat{x}_j$ on flows $b_j^{n-1,+}$ and $-b_{j+1}^{n-1,-}$, respectively. That is, the approximation F_j^n of the flux $u_x - uv_x$ at $(\hat{x}_j, t_n)$ is calculated by

$$F_j^n = \frac{u_{j+1}^n - u_j^n}{h} - b_j^{n-1,+} u_j^n + b_{j+1}^{n-1,-} u_{j+1}^n \quad (j = 1, 2, \dots, N)$$

Based on the observation above, our present scheme is as follows

$$(3.2) \quad \frac{u_j^n - u_j^{n-1}}{\tau_n} = \frac{F_j^n - F_{j-1}^n}{h},$$

or equivalently

$$(3.3) \quad \frac{u_j^n - u_j^{n-1}}{\tau_n} = \Delta_h u_j^n - D_h (b_j^{n-1,+} u_j^n) + D_h^* (b_j^{n-1,-} u_j^n),$$

where

$$D_h w_j = \frac{w_j - w_{j-1}}{h} \quad (\text{backward difference quotient}),$$

$$D_h^* w_j = \frac{w_{j+1} - w_j}{h} \quad (\text{forward difference quotient}),$$

$$\Delta_h w_j = D_h D_h^* w_j = D_h^* D_h w_j.$$

The boundary condition is approximated by

$$(3.4) \quad \begin{cases} F_0^n = \frac{u_1^n - u_0^n}{h} - b_0^{n-1,+} u_0^n + b_1^{n-1,-} u_1^n = 0, \\ F_N^n = \frac{u_{N+1}^n - u_N^n}{h} - b_N^{n-1,+} u_N^n + b_{N+1}^{n-1,-} u_{N+1}^n = 0 \end{cases}$$

and the initial condition by

$$(3.5) \quad u_j^0 = u_0(x_j) \quad (j = 1, \dots, N).$$

Now we describe two ways to determine $\{v_j^n\}_{j=0}^N$ from $\{u_j^n\}_{j=1}^N$. The one is the finite difference method as

$$(3.6) \quad -\Delta_h v_j^n + a v_j^n = \tilde{u}_j^n \quad (j = 0, 1, \dots, N)$$

with $v_{-1}^n = v_1^n$ and $v_{N+1}^n = v_{N-1}^n$, where

$$\tilde{u}_j^n = \begin{cases} u_1^n & (j = 0) \\ (u_{j+1}^n + u_j^n)/2 & (j = 1, 2, \dots, N-1) \\ u_1^N & (j = N). \end{cases}$$

The other is described in terms of the explicit formula of the Green function and we compute as

$$(3.7) \quad v_j^n = \sum_{i=1}^N \hat{G}(\hat{x}_j, x_i) u_i^n \quad (j = 0, 1, \dots, N).$$

Theorem 3.1. *Let $n \in \{1, 2, \dots, m\}$. Suppose that $\{u_j^{n-1}\}_{j=1}^N$ and $\{u_j^n\}_{j=1}^N$ satisfy (3.2) with (3.4). Then*

$$(II)_h^\tau \sum_{j=1}^N u_j^n h = \sum_{j=1}^N u_j^{n-1} h. \quad (\text{conservation of the discrete total mass}).$$

Proof. Taking the summation of both sides of (3.2) from 1 to N , we obtain by (3.4)

$$\frac{1}{\tau} \left(\sum_{j=1}^N u_j^n - \sum_{j=1}^N u_j^{n-1} \right) = \sum_{j=1}^N D_h F_j^n = \frac{F_0^n - F_N^n}{h} = 0.$$

□

Theorem 3.2. *Let $n \in \{1, \dots, m\}$. Suppose that $\{u_j^{n-1}\}_{j=1}^N$ are given and assume*

$$(I)_h^\tau u_j^{n-1} > 0 \quad (j=1, \dots, N).$$

If τ_n is small such that

$$(3.8) \quad 2\tau_n b_{\max}^{n-1} < h \quad \left(b_{\max}^{n-1} = \max_{1 \leq j \leq N} |b_j^{n-1}| \right),$$

then (3.2) with (3.4) admits a unique solution $\{u_j^n\}_{j=1}^N$ and $(I)_h^\tau$ is valid for $\{u_j^n\}_{j=1}^N$.

Proof. Introducing the $N \times N$ matrix $H^n = [H_{kl}]$ by

$$H_{kl} = \begin{cases} -1 - hb_1^{n,+} & (k=l=1) \\ 1 + hb_2^{n,-} & (k=1, l=2) \\ 1 + hb_{k-1}^{n,+} & (2 \leq k \leq N-1, l=k-1) \\ -2 - h(b_k^{n,+} + b_k^{n,-}) & (2 \leq k \leq N-1, l=k+1) \\ 1 + hb_{N-1}^{n,-} & (k=N, l=N-1) \\ -1 - hb_N^{n,+} & (k=l=N). \end{cases}$$

Then we can write (3.2) with (3.4) as

$$(3.9) \quad (I - \lambda_n H^{n-1}) \mathbf{u}^n = \mathbf{u}^{n-1} \quad (n = 1, 2, \dots, m),$$

where $\lambda_n = \tau_n/h^2$ and $\mathbf{u}^n = {}^T(u_1^n, u_2^n, \dots, u_N^n)$. Set $A = [A_{kl}] = I - \lambda H^{n-1}$. Then $A_{kk} > 0$, and $A_{kl} \leq 0$ for $k \neq l$. Moreover under (3.8) we have

$$\sum_{l=1}^N A_{kl} > 0.$$

These imply that A is of M-type (c.f. Varga [13]). Hence A^{-1} exists and $A^{-1} > 0$ (each element is positive). $\square$

Now we are able to state our numerical algorithm as follows:

- Step 0. Take $N \in \mathbb{N}$ and $\varepsilon \in (0, 1)$. Set $\mathbf{u}^0 = {}^T(u_0(x_1), \dots, u_0(x_N))$, $h = 1/N$ and $n = 1$.
- Step 1. Compute $\{v_j^{n-1}\}$ in accordance with (3.6) or (3.7). Then compute $\{b_j^{n-1,-}\}$, $\{b_j^{n-1,+}\}$ and $\{b_j^{n-1,-}\}$. Set $\tau_n = \varepsilon h / (2b_{\max}^n)$.
- Step 2. Solve (3.9) to obtain $\mathbf{u}^n$.
- Step 3. If $n = m$, then finish the computation. If $n < m$, then go to the next step.
- Step 4. Renew n by $n + 1$ and return to Step 1.

Before concluding this paper, we describe a few remarks.

Remark 3.1. By virtue of (I) $_h^\tau$ and (II) $_h^\tau$, we have a priori estimate

$$0 < \min_{1 \leq j \leq N} u_j^n \leq \max_{1 \leq j \leq N} u_j^n \leq \sum_{j=1}^N u_j^0 \leq \frac{1}{h} \max_{0 \leq x \leq 1} u_0(x),$$

which means that $\mathbf{u}^n$ never blows up in finite time. Hence $(0 <) \tau_n < \infty$ is guaranteed for any n and our algorithm always works.

Remark 3.2. The discrete analogue of J is, for example,

$$J_h(\mathbf{u}^n) = \sum_{j=1}^N (u_j^n \log u_j^n - u_j^n) h - \frac{1}{2} \sum_{j=1}^N \frac{v_{j-1}^n + v_j^n}{2} u_j^n,$$

and it is natural to expect that

$$(3.10) \quad \frac{1}{\tau_n} [J_h(\mathbf{u}^n) - J_h(\mathbf{u}^{n-1})] \leq 0.$$

However, the argument of §2 fails in this case. Furthermore numerical results indicate that (3.10) is valid for a small h . See, for more detail, Saito and Suzuki [7].

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March 27, 2003
(2003 年 3 月 27 日)