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by

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Higher order approximations in the heat equation and the truncated moment problem ⋆

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Abstract

In this paper we employ a linear combination of n heat kernels to approximate an L^1 solution to the heat equation. We show that our approximation is of order $O(t^{(\frac{1}{2p}-\frac{2n+1}{2})})$ in L^p-norm, $1 \le p \le \infty$, as $t \to \infty$. For instance, for positive solutions of the heat equation such an approximation is achieved using the theory of truncated moment problems. For a general sign-changing solution, this type of approximation is obtained by simply adding an auxiliary heat kernel. An interesting feature of this approximation is that it converges with a geometric order for a fixed $t > 0$ as $n \to \infty$. The theoretical asymptotic convergence orders for $t > 0$ large and for $n > 0$ large are tested and observed numerically.

1 Introduction

It is well known that

$$u(x,t) = \frac{1}{\sqrt{4\pi t}} \int e^{-(x-y)^2/(4t)} u_0(y)dy \Big(= \int \frac{u_0(c)}{\sqrt{4\pi t}} e^{-(x-c)^2/(4t)} dc \Big) \qquad (1.1)$$

is the bounded solution of the heat equation,

$$u_t = u_{xx}, \quad u(x,0) = u_0(x), \qquad x, u \in \boldsymbol{R}, \quad t > 0, \qquad (1.2)$$

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where, for simplicity, $u_0(x)$ is assumed to be continuous and decay exponentially for $|x|$ large, i.e.,

$$|u_0(x)| = O(e^{-x^2}) \quad \text{as} \quad |x| \to \infty. \tag{1.3}$$

(In this paper we shall refer to (1.1) as the solution of the heat equation (1.2) for the sake of brevity.) It is also well known that any asymptotic convergence order in L^1-norm is not expected for a general solution to a diffusion equation. Hence the asymptotic convergence is usually studied under the assumption that the initial value decays for $|x|$ large with the order that the fundamental solution has (see [2,24]). The decay order in (1.3) is the one that the Gaussian has and makes the moment of $u_0(x)$ be well defined up to any order. We set the first $2n$ moments as

$$\gamma_k \equiv \int x^k u_0(x)dx < \infty, \qquad k = 0, 1, \cdots, 2n-1. \tag{1.4}$$

Even though the explicit formula (1.1) gives the exact value of the solution at any given point $(x,t) \in \boldsymbol{R} \times \boldsymbol{R}^+$, one can only do the integration approximately. In numerical computations finding an efficient way to compute such an integration formula has been an important issue. From this point of view, it is reasonable to consider its approximation in a simpler form. In this article we construct a linear combination of 'n' heat kernels,

$$\phi_n(x,t) \equiv \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{\frac{-(x-c_i)^2}{4t}}. \tag{1.5}$$

There are $2n$ degrees of freedom in choosing ρ_i's and c_i's for $i = 1, \cdots, n$ and it is natural to ask what is the best choice for them. In this paper they are uniquely decided by the following $2n$ equations

$$\lim_{t \to 0} \int x^k \phi_n(x,t)dx = \gamma_k, \qquad k = 0, 1, \cdots, 2n-1. \tag{1.6}$$

(We employ the theory of truncated moment problems [3] to obtained the solvability of the problem.) Then ϕ_n and u share the same first $2n$ moments, and we may show that

$$\|u(t) - \phi_n(t)\|_p = O(t^{(\frac{1}{2p} - \frac{2n+1}{2})}) \quad \text{as} \quad t \to \infty, \quad 1 \le p \le \infty. \tag{1.7}$$

This convergence order indicates that ϕ_n is an excellent approximation of the solution for $t > 0$ large. However, the convergence for n large for a fixed

$t > 0$ is more important if one want to consider $\phi_n(x,t)$ as an approximation of $u(x,t)$. Indeed our approximation has a convergence property with an geometric convergence order such as

$$\frac{\|u(t)-\phi_n(t)\|_\infty}{\|u(t)-\phi_{n+1}(t)\|_\infty} \to 1+4\frac{t}{v} \quad \text{as} \quad n\to\infty, \tag{1.8}$$

where $v > 0$ may depend on the initial value $u_0(x)$. Numerical examples in Section 7.2 show this geometric convergence and the mechanism of such convergence is discussed in Section 6. Note that the geometric convergence order in (1.8) is faster than any other algebraic convergence order for any given $t > 0$. One can find an alternative approximation with a high asymptotic convergence order from [8]. However, obtaining a convergence for $n > 0$ large is limited as tested in Section 7.3.

Our approach is as followings. In Section 2 we show the convergence order (1.7) assuming (1.6). In Section 3, we employ the $2n$ freedom of choices in (1.5) and assign the zero value to the first $2n$ moments of the difference (or the initial approximation error) $u_0(x) - \phi(x,0)$. We remark that the existence and the uniqueness of ρ_i's and c_i's that satisfy the zero moments conditions are given by the theory of the truncated moment problems if the initial value $u_0(x)$ is nonnegative (see [1,3] and Section 3).

For a general sign changing solution the existence and the uniqueness of such ρ_i's and c_i's do not hold. In Section 4 we discuss the issue in detail for three cases with $n = 1,2$ and 3. In Section 5 we construct an approximation for a general sign-changing case by adding an auxiliary heat kernel. The convergence property for $n > 0$ large is discussed in Section 6. The asymptotic convergence orders in (1.7) and (1.8) have been tested numerically in Sections 7.1 and 7.2, respectively.

In a study of a time evolutionary system a special solution which converges to the Dirac-measure as $t \to 0$ serves as the asymptotic structure of the problem(see [26]). In the study of nonlinear diffusion equations, the Barenblatt solution is used as its asymptotic profile and the convergence order of general solutions to this special one has been studied in various cases (see [2,5] and references therein). The diffusion wave and the Gaussian are the asymptotics of convection-diffusion equations for diffusion dominant cases (see [9–11,17]). For convection dominant cases (see [13]) and inviscid convection problems (see [4,7,12,21]) or hyperbolic systems (see [6,18,19]), N-waves represent the asymptotic behavior, where N-waves also converges to the Dirac-measure as $t \to 0$.

In the study of nonlinear diffusion the initial value is usually assumed to have finite first two moments and a higher convergence order is obtained by comparing the solution with the Barenblatt solution of the correct size (mass) placed at the correct place (center of mass) (see [2,12,16]). Therefore the result of this paper can be viewed as an ideal case. The approach in this paper can be directly employed to approximate the solutions to the Burgers equation via the Cole–Hopf transformation. To obtain the rigorous convergence order for the Burgers case it is required to check the well definedness of the transformed solutions as is done in Lemmas 3.1-3.2 and Theorem 3.3 in [16] for the special case with $n = 1$. Considering that the Burgers equation has been used as a tool to study the asymptotic structure of the viscous systems of conservations laws (see e.g. [20]), we hope the approach in this article may be used for more general models.

2 Asymptotic convergence order

2.1 Decay rates of derivatives

Consider an initial value $E_m(x)$ which is continuous and

$$|E_m(x)| = O(e^{-x^2}) \quad \text{as} \quad |x| \to \infty. \tag{2.1}$$

Do not feel strange due to the subindex 'm' of the initial value. We are going to replace $E_m(x)$ with an m-th order antiderivative of an initial approximation error as in Lemma 2.3 and then eventually substitute $2n$ in the place of m. Let $E(x,t)$ be the solution of the heat equation with this initial value, i.e.,

$$E(x,t) = \frac{1}{\sqrt{4\pi t}} \int e^{-(x-y)^2/(4t)} E_m(y)dy.$$

Then $E(x,t)$ also has the same exponential decay order for $|x|$ large with a fixed $t > 0$. The dissipation of the solution can be easily shown by introducing similarity variables:

$$\xi = \frac{x}{\sqrt{t}}, \quad \zeta = \frac{y}{\sqrt{t}}, \quad \tilde{E}(\xi,t) = E(x,t). \tag{2.2}$$

Then $E(x,t)$ is transformed to

$$\tilde{E}(\xi,t) = \frac{1}{\sqrt{4\pi}} \int e^{-(\xi-\zeta)^2/4} E_m(\sqrt{t}\zeta)d\zeta,$$

and its m-th order derivative is given by

$$\partial_\xi^m \tilde{E}(\xi,t) = \partial_x^m E(x,t)(\partial_\xi x)^m = \partial_x^m E(x,t)(\sqrt{t})^m.$$

Now consider the decay order of the m-th order derivative of the solution $E(x,t)$ in L^p-norm, $1 \le p \le \infty$. First, let $p = \infty$. Then, the maximum of the m-th order derivative satisfies

$$(\sqrt{t})^{m+1}|\partial_x^m E(x,t)| = \sqrt{t}|\partial_\xi^m \tilde{E}(\xi,t)| = \frac{\bar{\gamma}_m}{\sqrt{4\pi}}|\int f(\zeta)g_t(\xi-\zeta)d\zeta|, \tag{2.3}$$

where

$$\bar{\gamma}_m \equiv \int E_m(y)dy \neq 0,\ g_t(\xi) = \sqrt{t}E_m(\sqrt{t}\xi)/\bar{\gamma}_m,\ f(\xi) = \partial_\xi^m(e^{-\xi^2/4}). \tag{2.4}$$

After taking the supremum of both sides of (2.3), one obtains for all $t > 0$ that

$$(\sqrt{t})^{m+1}\|\partial_x^m E(t)\|_\infty \le \frac{\bar{\gamma}_m}{\sqrt{4\pi}}\|\partial_\zeta^m(e^{-\zeta^2/4})\|_\infty.$$

If one takes $t \to \infty$ limit to the equation (2.3), then

$$\lim_{t\to\infty}(\sqrt{t})^{m+1}|\partial_x^m E(x,t)| = \frac{\bar{\gamma}_m}{\sqrt{4\pi}}|f(\xi)|.$$

Therefore, after taking the supremum of the both sides again, we obtain

$$\lim_{t\to\infty}(\sqrt{t})^{m+1}\|\partial_x^m E(t)\|_\infty = \frac{|\bar{\gamma}_m|}{\sqrt{4\pi}}\|\partial_\xi^m(e^{-\xi^2/4})\|_\infty\ .$$

On the other hand, if $1 \le p < \infty$, then,

$$\begin{aligned}
t^{(\frac{m+1}{2}-\frac{1}{2p})}&\|\partial_x^m E(t)\|_p \\
&= (\sqrt{t})^{m+1}(1/\sqrt{t})^{1/p}(\textstyle\int |\partial_x^m E(x,t)|^p dx)^{1/p} \\
&= (\textstyle\int |(\sqrt{t})^{m+1}\partial_x^m E(x,t)|^p d(\frac{x}{\sqrt{t}}))^{1/p} \\
&= (\textstyle\int |\sqrt{t}\partial_\xi^m \tilde{E}(\xi,t)|^p d\xi)^{1/p} \\
&= \tfrac{\bar{\gamma}_m}{\sqrt{4\pi}}(\textstyle\int |\int f(\zeta)g_t(\xi-\zeta)d\zeta|^p d\xi)^{1/p} = \tfrac{|\bar{\gamma}_m|}{\sqrt{4\pi}}\|f * g_t\|_p.
\end{aligned} \tag{2.5}$$

Standard arguments imply that $\|f * g_t\|_p \to \|f\|_p$ as $t \to \infty$ (see [23], p. 62). Therefore,

$$\lim_{t\to\infty} t^{(\frac{m+1}{2}-\frac{1}{2p})}\|\partial_x^m E(t)\|_p = \frac{|\bar{\gamma}_m|}{\sqrt{4\pi}}\|\partial_\xi^m(e^{-\xi^2/4})\|_p\ .$$

Now we show that the convergence order is increased if $\bar{\gamma}_m = 0$. Consider the following integrals given inductively by

$$E_k(x) = \int_{-\infty}^{x} E_{k-1}(y)dy, \qquad k > m. \tag{2.6}$$

Suppose that $\lim_{x\to\infty} E_k(x) = 0$ for all $k > m$. Then, $|E_k(x)|$ decays exponentially for $|x|$ large and, therefore, after applying the integration by parts $k-m$ times with proper inductive arguments, one obtains

$$(-1)^{k-m}(k-m)! \int_{-\infty}^{\infty} E_k(x)dx = \int_{-\infty}^{\infty} x^{k-m} E_m(x)dx = 0.$$

On the other hand, by the Weierstrass Approximation Theorem, there exists a sequence of polynomials P_n such that

$$P_n(x) \to E_m(x) \qquad \text{as} \qquad n \to \infty$$

uniformly on any bounded domain $[-L, L]$. Therefore, we obtain

$$\|E_m\|_2^2 = \int E_m^2(x)dx = \lim_{n\to\infty} \int P_n(x)E_m(x)dx = 0.$$

Hence, if the initial value E_m is not a trivial one, there exists $k_0 > m$ such that $\lim_{x\to\infty} E_k(x) = 0$ for all $m \le k \le k_0$ and $\bar\gamma_{k_0} := \lim_{x\to\infty} E_{k_0+1}(x) \neq 0$. The exponential decay of $|E_{k_0}(x)|$ implies its integrability and hence $\bar\gamma_{k_0} < \infty$.

Let $\tilde E(x,t)$ be a solution with $E_{k_0}(x)$ as its initial value. Then clearly $\partial_x^m E = \partial_x^{k_0} \tilde E$ and hence

$$\lim_{t\to\infty} t^{(\frac{k_0+1}{2}-\frac{1}{2p})} \|\partial_x^m E\|_p = \lim_{t\to\infty} t^{(\frac{k_0+1}{2}-\frac{1}{2p})} \|\partial_x^{k_0} \tilde E\|_p = \frac{|\bar\gamma_{k_0}|}{\sqrt{4\pi}} \|\partial_\xi^{k_0}(e^{-\xi^2/4})\|_p \, .$$

Therefore, if $\bar\gamma_m = 0$, we obtain higher decay order. Summing up, we have the following result.

Lemma 2.1 *Let $E(x,t)$ be the solution of the heat equation with a nontrivial continuous initial value $E_m(x)$ satisfying the exponential decay in (2.1). Then*

$$t^{\frac{m+1}{2}} \|\partial_x^m E(t)\|_\infty \le \frac{\|\partial_\xi^m (e^{-\xi^2/4})\|_\infty}{\sqrt{4\pi}} \int |E_m(x)|dx. \tag{2.7}$$

Let E_k's be given inductively by (2.6). Then there exists $k_0 \ge m$ such that $\lim_{x\to\infty} E_k(x) = 0$ for $m \le k \le k_0$ and $0 \neq \lim_{x\to\infty} E_{k_0+1}(x) < \infty$, and

$$\lim_{t\to\infty} t^{(\frac{k_0+1}{2}-\frac{1}{2p})} \|\partial_x^m E\|_p = \frac{\|\partial_\xi^{k_0}(e^{-\xi^2/4})\|_p}{\sqrt{4\pi}} |\lim_{x\to\infty} E_{k_0+1}(x)| \, , \quad 1 \le p \le \infty. \tag{2.8}$$

Suppose that $\int E_m(x)dx = 0$. Then, the convergence order in (2.8) implies that $\lim_{t\to\infty} t^{(\frac{m+1}{2}-\frac{1}{2p})} \|\partial_x^m E\|_p = 0$. Hence, we may simply say that

$$\lim_{t\to\infty} t^{(\frac{m+1}{2}-\frac{1}{2p})} \|\partial_x^m E\|_p = \frac{\|\partial_\xi^m (e^{-\xi^2/4})\|_p}{\sqrt{4\pi}} \Big| \int E_m(x)dx \Big| \, , \quad 1 \le p \le \infty, \tag{2.9}$$

which is a weaker statement than (2.8). In the followings we use the convergence order in (2.9) for the simplicity of statements. If the optimal convergence order is concerned and $\int E_m(x)dx = 0$, then we may refer to (2.8). It is well known that the solution of the heat equation converges to zero with convergence order $O(t^{-1/2})$. Lemma 2.1 implies that the decay order of its derivatives increases by $\frac{1}{2}$ after each differentiations. The estimate (2.8) indicates that this decay order is sharp since it gives the correct power and the correct coefficient.

2.2 Moments and convergence order as $t \to \infty$

In this section we show that the decay rates of the m-th order derivative in (2.7)–(2.9) are naturally transferred to the convergence order of an approximation to the solution. For a given solution $u(x,t)$, consider the k-th order moment $\bar{\gamma}_k(t)$ given by

$$\bar{\gamma}_k(t) = \int x^k u(x,t)dx, \qquad k = 0, 1, 2, \cdots, \quad t \geq 0.$$

We can easily show how does the moment $\bar{\gamma}_k(t)$ evolve.

Lemma 2.2 *Let $u(x,t)$ be the solution of the heat equation and $\bar{\gamma}_k(t)$ be the k-th order moment. Then,*

$$\frac{d}{dt}\bar{\gamma}_k(t) = \begin{cases} 0\ , & k = 0 \ \text{ or } \ 1, \\ k(k-1)\bar{\gamma}_{k-2}(t), & k \geq 2. \end{cases} \tag{2.10}$$

PROOF. For $k = 0$, (2.10) is equivalent to the conservation of mass. For $k = 1$, since $u_t = u_{xx}$, the integration by parts gives

$$\bar{\gamma}_1'(t) = \int x u_t dx = \int x u_{xx} dx = [x u_x - u]_{-\infty}^{\infty} = 0.$$

Similarly, for $k \geq 2$, we obtain

$$\begin{aligned} \bar{\gamma}_k'(t) &= \textstyle\int x^k u_t dx = \int x^k u_{xx} dx \\ &= [x^k u_x - k x^{k-1} u]_{-\infty}^{\infty} + \textstyle\int k(k-1) x^{k-2} u dx = k(k-1)\bar{\gamma}_{k-2}(t). \qquad \square \end{aligned}$$

This lemma shows that even numbered moments and odd numbered ones evolve separately. More explicitly, one may obtain

$$\begin{aligned} \bar{\gamma}_{2n}(t) &= \textstyle\sum_{k=0}^{n} \frac{(2n)!}{(n-k)!(2k)!} t^{n-k} \bar{\gamma}_{2k}(0), \\ \bar{\gamma}_{2n+1}(t) &= \textstyle\sum_{k=0}^{n} \frac{(2n+1)!}{(n-k)!(2k+1)!} t^{n-k} \bar{\gamma}_{2k+1}(0). \end{aligned}$$

If $\bar{\gamma}_k(0) = 0$ for all $0 \le k \le n$, then $\bar{\gamma}_k(t) = 0$ for all $0 \le k \le n$, $\bar{\gamma}_k(t) = \bar{\gamma}_k(0)$ for $k = n+1, n+2$, $\bar{\gamma}_k(t)$ is linear for $k = n+3, n+4$, $\bar{\gamma}_k(t)$ is quadratic for $k = n+5, n+6$, and so on.

Let $v(x,t)$ be an approximation solution of the exact one $u(x,t)$. Since the difference $e(x,t) = v(x,t) - u(x,t)$ is also a solution to the heat equation, the moments of $e(x,t)$ will be always zero if they are initially zero. Hence, it is natural to expect a higher convergence order by matching the moments of the approximation solution to that of the exact one.

Lemma 2.3 *If an integrable function $E_0(x)$ has an exponential decay for $|x|$ large as in (1.3) and zero moments up to $(m-1)$-th order, i.e.,*

$$\int_{-\infty}^{\infty} E_0(x)dx = \int_{-\infty}^{\infty} xE_0(x)dx = \cdots = \int_{-\infty}^{\infty} x^{m-1}E_0(x)dx = 0, \quad n > 0, \tag{2.11}$$

then there exists $E_m \in W^{m,1}(\boldsymbol{R})$ such that

$$\partial_x^m E_m(x) = E_0(x). \tag{2.12}$$

PROOF. Consider a sequence of functions defined inductively by

$$E_k(x) = \int_{-\infty}^{x} E_{k-1}(y)dy, \quad 0 < k \le m.$$

First we show that

$$\int_{-\infty}^{\infty} E_k(x)dx = 0 \qquad \text{and} \qquad E_k(x) \to 0 \text{ exponentially as } |x| \to \infty \tag{2.13}$$

for $k = 0, 1, \cdots, m-1$. It suffices to show (2.13) for $k = l < m$ under the assumption that (2.13) holds for all $k = 0, 1, \cdots, l-1$. Note that it is clearly satisfied for $k = 0$. Since $\int_{-\infty}^{\infty} E_{l-1}(x)dx = 0$ and $E_{l-1}(x) \to 0$ exponentially as $|x| \to \infty$, its integral $E_l(x)$ also decays exponentially as $|x| \to \infty$. Using the fact that E_k decays exponentially fast for all $0 \le k \le l$, we obtain

$$\int_{-\infty}^{\infty} E_l(x)dx = (-1)^l \int_{-\infty}^{\infty} \frac{x^l}{l!} E_0(x)dx = 0$$

employing the integration by parts and then (2.11). So (2.13) holds for $k = l$. Hence, (2.13) holds for all $0 \le k \le m-1$. Then (2.12) is clearly satisfied. $\square$

The convergence order of the approximation is obtained as a corollary of Lemmas 2.1 and 2.3.

Theorem 2.4 *Let $u(x,t)$ and $v(x,t)$ be the solutions of the heat equation with their initial values $u_0(x)$ and $v_0(x)$, respectively. Suppose that the initial difference $E_0(x) := u_0(x) - v_0(x)$ has a compact support $\subset [-L, L]$ and has zero moments up to $(m-1)$-th order as in (2.11). Then,*

$$t^{\frac{m+1}{2}} \|u(t) - v(t)\|_\infty \le \frac{\|\partial_\xi^m (e^{-\frac{1}{4}\xi^2})\|_\infty}{\sqrt{4\pi}} \int \Big|E_m(x)\Big| dx, \tag{2.14}$$

and, for $1 \le p \le \infty$,

$$\lim_{t\to\infty} t^{(\frac{m+1}{2} - \frac{1}{2p})} \|u(t) - v(t)\|_p = \frac{\|\partial_\xi^m (e^{-\frac{1}{4}\xi^2})\|_p}{\sqrt{4\pi}} \Big| \int E_m(x) dx \Big|, \tag{2.15}$$

where $E_m(x) \in W^{m,1}(\boldsymbol{R})$ be the function satisfying (2.12).

PROOF. Let $E(x,t)$ be the solution of the heat equation with its initial value $E_m(x)$. Then, clearly, $\partial_x^m E(x,t)$ is the solution of the heat equation with its initial value $\partial_x^m E_m(x) = E_0(x)$. Hence, $\partial_x^m E(x,t) = e(x,t) \equiv u(x,t) - v(x,t)$, and (2.14) and (2.15) follow from Lemma 2.1. $\Box$

Remark 2.5 *In this section we have considered convergence orders as $t \to \infty$ with a fixed $n > 0$. However the relation (2.3), for example, provides certain convergence information as $n \to \infty$ with a fixed $t > 0$, too. To obtain a convergence order as $n \to \infty$ we need to specify $E_m(x)$ corresponding to our approximation $\phi_n(x,t)$, which will be considered in Section 6.*

3 Positive solutions and truncated moment problem

Consider a linear combination of heat kernels

$$\phi_n(x,t) \equiv \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{-(x-c_i)^2/(4t)}. \tag{3.1}$$

We use the $2n$ freedom of choices in ρ_i's and c_i's to control the first $2n$ moments of the approximation. Introduce a notation γ_k to denote the initial moments, i.e.,

$$\gamma_k \equiv \int x^k u_0(x) dx, \qquad k = 0, 1, 2, \cdots. \tag{3.2}$$

Let $\mathbf{r}_k$ be the column n-vector and $\mathbf{A}$ be the $n \times n$ Hankel matrix given by

$$\begin{aligned} \mathbf{r}_k &= (\gamma_k, \gamma_{k+1}, \cdots, \gamma_{k+n-1})^t, \qquad && k = 0, 1, \cdots \\ \mathbf{A} &\equiv (a_{ij}) = (\gamma_{i+j}), && i, j = 0, 1, \cdots, n-1. \end{aligned} \tag{3.3}$$

Since $\phi_n(x,t) \to \sum_{i=1}^n \rho_i \delta_{c_i}(x)$ as $t \to 0$, the difference between the initial value and its approximation is

$$E_0(x) \equiv u_0(x) - \sum_{i=1}^n \rho_i \delta_{c_i}(x),$$

where $\delta_{c_i}(x)$ is the Dirac-delta measure centered at c_i, i.e., $\delta_{c_i}(x) = \delta(x - c_i)$. Hence, the zero moment conditions in (2.11) can be written as

$$\int \sum_{i=1}^n x^k \rho_i \delta_{c_i}(x)\, dx = \int x^k u_0(x)\, dx (\equiv \gamma_k), \qquad 0 \le k \le 2n-1, \tag{3.4}$$

or, in a matrix form, as

$$\begin{pmatrix} 1 & \cdots & 1 \\ c_1 & \cdots & c_n \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ \cdot & \cdots & \cdot \\ c_1^{2n-1} & \cdots & c_n^{2n-1} \end{pmatrix} \begin{pmatrix} \rho_1 \\ \cdot \\ \cdot \\ \rho_n \end{pmatrix} = \begin{pmatrix} \gamma_0 \\ \gamma_1 \\ \cdot \\ \cdot \\ \cdot \\ \gamma_{2n-1} \end{pmatrix}. \tag{3.5}$$

After eliminating all ρ_i's (see e.g. Section 4.3), we obtain n-equations involving c_i's only:

$$\mathbf{A}\Psi = \mathbf{r}_n, \tag{3.6}$$

where the column vector $\Psi = (\psi_0, \cdots, \psi_{n-1})^t$ is given by

$$\psi_0 = (-1)^{n+1} \Pi c_i, \quad \psi_1 = (-1)^n \sum_{j=1}^n \Pi_{i \neq j} c_i, \quad \cdots \quad, \psi_{n-1} = \sum_{i=1}^n c_i. \tag{3.7}$$

Consequently,

$$g_n(x) := x^n - \sum_{j=0}^{n-1} \psi_j x^j = (x - c_1)(x - c_2) \cdots (x - c_n). \tag{3.8}$$

Hence, if the initial zero moment conditions (3.4) are satisfied, then c_i's are zero points of the polynomial $g_n(x)$, where its coefficients are given as a solution of (3.6).

To show the existence and the uniqueness of the approximation we need to show that the Hankel matrix in (3.6) is nonsingular. Then there exists $\psi_j, j = 0, \cdots, n-1$ which satisfies (3.6) uniquely. The next step is to show that the polynomial $g_n(x)$ in (3.8) has n distinct real zeros $c_1 < \cdots < c_n$. Then ρ_i's are given by solving the Vandermonde given by the first n-equations in (3.5), i.e.,

$$\begin{pmatrix} 1 & 1 & \cdots 1 \\ c_1 & c_2 & \cdots c_n \\ \cdot & \cdot & \cdots\cdot \\ \cdot & \cdot & \cdots\cdot \\ \cdot & \cdot & \cdots\cdot \\ c_1^{n-1} & c_2^{n-1} & \cdots c_n^{n-1} \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \\ \cdot \\ \cdot \\ \cdot \\ \rho_n \end{pmatrix} = \begin{pmatrix} \gamma_0 \\ \gamma_1 \\ \cdot \\ \cdot \\ \cdot \\ \gamma_{n-1} \end{pmatrix}. \tag{3.9}$$

It is well known that the Vandermonde matrix is nonsingular if c_i's are all different. Then, we can easily check that c_i's and ρ_i's also satisfies the next n-equations in (3.5).

Suppose that the initial value $u_0(x)$ is positive. Then, the uniqueness and the existence is resolved by the theory for the moment problem (see [1,3]). In the followings we introduce this technique briefly for the completeness and the later use in the paper. Consider

$$\Psi^t \mathbf{A} \Psi = \sum_{i,j=0}^{n-1} \psi_i \psi_j \gamma_{i+j} = \int \sum_{i,j=0}^{n-1} \psi_i x^i \psi_j x^j u_0(x) dx = \int \Big(\sum_{k=0}^{n-1} \psi_k x^k \Big)^2 u_0(x) dx.$$

Since the integrand $(\sum_{k=0}^{n-1} \psi_k x^k)^2 u_0(x)$ is nonnegative, we have $\Psi^t \mathbf{A} \Psi \geq 0$. Furthermore, $\Psi \mathbf{A} \Psi^t = 0$ if and only if $(\sum_{k=0}^{n-1} \psi_k x^k)^2 u_0(x) = 0$ for all $x \in \boldsymbol{R}$. For $\Psi \neq 0$, the polynomial $\sum_{k=0}^{n-1} \psi_k x^k$ has at most $n-1$ zeros and, therefore, $\Psi \mathbf{A} \Psi^t > 0$ if the support of the initial value u_0 consists of at least n points. Hence, we may conclude that the Hankel matrix $\mathbf{A} \equiv (\gamma_{i+j})_{i,j=0}^{n-1}$ is nonsingular (originally done by Hamburger).

To show that $g_n(x)$ has n-distinct real zeros, consider a linear functional S defined on the space of polynomials $r(x) = \sum_{i=0}^{l} r_i x^i$ by

$$S(r) := r_0 \gamma_0 + \cdots + r_l \gamma_l.$$

Then,

$$S(r^2) = S\Big(\sum_{i,j=0}^{l} r_i r_j x^{i+j}\Big) = \sum_{i,j=0}^{l} r_i r_j \gamma_{i+j} > 0.$$

Suppose that $r(x) \geq 0$. Then the degree of the polynomial $r(x)$ is even and there exist two polynomials p, q such that $r(x) = p^2(x) + q^2(x)$ (see e.g. [2; p.2]). So $S(r) = S(p^2) + S(q^2) > 0$.

Since $\mathbf{A}$ is nonsingular, there exists an n-vector $\Psi = (\psi_0, \cdots, \psi_{n-1})$ uniquely so that $\mathbf{A}\Psi = \mathbf{r}_n$, i.e.,

$$\sum_{j=0}^{n-1} \psi_j \mathbf{r}_j = \mathbf{r}_n,$$

or

$$\gamma_{n+k} - \sum_{j=0}^{n-1} \psi_j \gamma_{j+k} = 0, \quad k = 0, 1, \cdots, n-1. \tag{3.10}$$

Considering the polynomial $g_n(x)$ and the definition of the functional $S(r)$, we can easily check that (3.10) implies

$$S(g_n x^k) = 0, \qquad k = 0, 1, \cdots, n-1. \tag{3.11}$$

Suppose that $g_n(x)$ never changes its sign. Then, $g_n(x) \geq 0$ and, hence, $S(g_n) > 0$, which contradicts to (3.11). Suppose that $g_n(x)$ changes its sign at points $c_1, \cdots, c_l$ only. Then $g_n(x)(x - c_1)\cdots(x - c_l) \geq 0$ and $S(g_n(x)(x - c_1)\cdots(x - c_l)) > 0$. On the other hand, if $l < n$, then the linearity of the functional $S(r)$ together with (3.11) implies that $S(g_n(x)(x - c_1)\cdots(x - c_l)) = 0$. Hence, we obtain that $g_n(x)$ has n-distinct real roots, say $c_1 < \cdots < c_n$.

Now we show that there exist ρ_i's that solve (3.5) in a unique way, i.e.,

$$\sum_{i=1}^{n} \rho_i c_i^l = \gamma_l, \quad l = 0, 1, \cdots, 2n-1. \tag{3.12}$$

Since c_i's are all different, there exists a unique solution for the Vandermonde (3.9), i.e., (3.12) is satisfied for all $0 \leq l < n$. Now we complete the proof using inductive arguments. Let $0 \leq k \leq n-1$. We will show that the identity in (3.12) holds for $l = n + k$ under the assumption that it holds for all $0 \leq l < n + k$. First observe that, since c_i's are zero points of $x^k g_n(x), k \geq 0$,

$$c_i^{n+k} = \sum_{j=0}^{n-1} \psi_j c_i^{j+k} \qquad \text{for any} \quad 1 \leq i \leq n,\ k \geq 0.$$

Using the relations (3.10) and (3.12) for $l < n + k$, we obtain

$$\gamma_{n+k} = \sum_{j=0}^{n-1} \psi_j \gamma_{j+k} = \sum_{j=0}^{n-1} \psi_j \sum_{i=1}^{n} \rho_i c_i^{j+k} = \sum_{i=1}^{n} \rho_i \sum_{j=0}^{n-1} \psi_j c_i^{j+k} = \sum_{i=1}^{n} \rho_i c_i^{n+k}.$$

Hence, (3.12) holds by the induction.

In summary, the proof of the existence and the uniqueness of the solution to the problem (3.5) consists of three steps. The invertibility of the Hankel matrix $\mathbf{A}$ in (3.6) and the existence of n-distinct real roots c_i's of g_n are the first two. The latter depends on the positive definiteness of the matrix $\mathbf{A}$ which is easily proved for positive initial value $u_0(x)$. On the other hand, after obtaining c_i's, finding ρ_i's that satisfy (3.5) does not require the positivity. It depends only on the recursive structure of the problem. The following theorem is now clear from Theorem 2.4:

Theorem 3.1 *Let $u(x,t)$ be the solution of the heat equation with its initial value $u_0(x)$. If $u_0(x)$ is nonnegative (or nonpositive), there exist $\rho_i, c_i, i = 1, \cdots, n$ such that, for $\phi_n(x,t) \equiv \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{-(x-c_i)^2/(4t)}$,*

$$\lim_{t\to\infty} t^{n+\frac{p-1}{2p}} \|u(t) - \phi_n(t)\|_p = \frac{\|\partial_\xi^{2n}(e^{-\frac{1}{4}\xi^2})\|_p}{\sqrt{4\pi}} \Big| \int E_{2n}(x)dx \Big|, \tag{3.13}$$

where $1 \le p \le \infty$ and $E_{2n}(x) \in W^{2n,1}(R)$ is the $2n$-th order antiderivative of $E_0(x) = u(x,0) - \phi_n(x,0)$ given in Lemma 2.3. Furthermore, such a function $\phi_n(x,t)$ is unique.

Remark 3.2 *Several softwares such as Maple can solve (3.5). However, since the problem is highly nonlinear, it takes very long time even for small n. Therefore, even for the computational purpose, one need to follow the steps of the proof to construct the approximation $\phi_n(x)$.*

4 General initial value

In this section we consider a general initial value which may have sign changes. Then the existence and the uniqueness theory of the previous section is not applicable since it is for positive solutions only. In this section we observe that the existence and uniqueness may fail for a general solution.

4.1 Approximation with a heat kernel

For the case $n = 1$, the approximation $\phi_1(x,t) = \frac{\rho_1}{\sqrt{4\pi t}}\, e^{-(x-c_1)^2/(4t)}$ is given by

$$\rho_1 = \gamma_0, \qquad c_1\,\rho_1 = \gamma_1. \tag{4.1}$$

If $\gamma_0 \neq 0$, c_1 is uniquely decided by $c_1 = \gamma_1/\gamma_0$, i.e., c_1 is the *center of the mass* of the initial mass distribution u_0. The convergence order in Theorem 2.4 is written as

$$\lim_{t\to\infty} t^{(\frac{3}{2}-\frac{1}{2p})}\|u(t)-\phi_1(t)\|_p = \bar{\gamma}_2\|\partial_\xi^2(e^{-\frac{1}{4}\xi^2})\|_p/\sqrt{4\pi}, \quad 1 \le p \le \infty,$$

where $\bar{\gamma}_2 = \int_{-\infty}^{\infty}\int_{-\infty}^{x}\int_{-\infty}^{y}|u_0(z)-\rho_1\delta_{c_1}(z)|dzdydx$.

Now consider a singular case $\gamma_0 = 0$. Then the possible approximation is $\phi_1 \equiv 0$. If $\gamma_1 = 0$, then the equation for the first moment is satisfied for any $c_1 \in \boldsymbol{R}$ and hence we obtain the above convergence order which is equivalent to the decay rate $u(x,t)$. If $\gamma_1 \neq 0$, (4.1) has no solution and hence we do not obtain the convergence order of $O(t^{(\frac{1}{2p}-\frac{3}{2})})$ for t large.

4.2 Approximation with two heat kernels

The double heat kernel solution $\phi_2(x,t) = \sum_{i=1}^{2}\frac{\rho_i}{\sqrt{4\pi t}}\, e^{-(x-c_i)^2/(4t)}$ that approximates the solution $u(x,t)$ is obtained by solving

$$\begin{aligned} \rho_1 + \rho_2 \quad &= \gamma_0, \qquad & \rho_1 c_1 + \rho_2 c_2 &= \gamma_1, \\ \rho_1 c_1^2 + \rho_2 c_2^2 &= \gamma_2, \qquad & \rho_1 c_1^3 + \rho_2 c_2^3 &= \gamma_3. \end{aligned}$$

We may simplify the equation by eliminating ρ_i's and obtain two equations of the form $\mathbf{A}\Psi = \mathbf{r}_2$ or

$$\begin{pmatrix} \gamma_0 & \gamma_1 \\ \gamma_1 & \gamma_2 \end{pmatrix}\begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix} = \begin{pmatrix} \gamma_2 \\ \gamma_3 \end{pmatrix}.$$

First we need to check the invertibility of the Hankel matrix. Its determinant is the variant of the initial value u_0 if it is a probability distribution, i.e.,

$$|\mathbf{A}| \equiv \gamma_0\gamma_2 - \gamma_1^2. \tag{4.2}$$

If $|\mathbf{A}| \neq 0$, ψ_i's can be solved using the Cramer's rule, and c_i's are zeros of a quadratic function

$$g_2(x) = x^2 + \frac{\gamma_1\gamma_2 - \gamma_0\gamma_3}{|\mathbf{A}|}x + \frac{\gamma_1\gamma_3 - \gamma_2^2}{|\mathbf{A}|}.$$

Hence, the centers c_1, c_2 are given by

$$c_{1,2} = \frac{(\gamma_0\gamma_3 - \gamma_1\gamma_2) \pm \sqrt{D}}{2|\mathbf{A}|}, \qquad c_1 < c_2, \tag{4.3}$$

under two assumptions,

$$|\mathbf{A}| \neq 0, \quad D := (\gamma_1\gamma_2 - \gamma_0\gamma_3)^2 - 4(\gamma_0\gamma_2 - \gamma_1^2)(\gamma_1\gamma_3 - \gamma_2^2) > 0. \tag{4.4}$$

After obtaining c_i's, the problem (3.5) is easily solved and gives

$$\rho_1 = \frac{\gamma_0 c_2 - \gamma_1}{c_2 - c_1}, \qquad \rho_2 = \frac{\gamma_0 c_1 - \gamma_1}{c_1 - c_2}. \tag{4.5}$$

From Theorem 2.4 we may conclude that, if $D > 0$ and $|\mathbf{A}| \neq 0$, then

$$\lim_{t\to\infty} t^{(\frac{5}{2}-\frac{1}{2p})}\|u(x,t) - \phi_2(x,t)\|_p \leq \bar{\gamma}_4\|\partial_\xi^4(e^{-\frac{1}{4}\xi^2})\|_p/\sqrt{4\pi}, \quad 1 \leq p \leq \infty, \tag{4.6}$$

where $\bar{\gamma}_4 = \int\int_{-\infty}^{x}\int_{-\infty}^{y}\int_{-\infty}^{z}\int_{-\infty}^{v}\Big|u_0(w) - \rho_1\delta_{c_1}(w) - \rho_2\delta_{c_2}(w)\Big|dwdvdzdydx.$

Example 4.1 *Consider an initial value*

$$U_k(x) = \begin{cases} -1, & -2k-0.5 < x < -k-0.5, \quad k+0.5 < x < 2k+0.5, \\ 1, & -k-0.5 \leq x \leq k+0.5, \\ 0, & \text{otherwise}, \end{cases} \tag{4.7}$$

where $k > 0$. Let $\gamma_{i,k}$ be the i-th moments of the function U_k, i.e.,

$$\gamma_{i,k} := \int x^i U_k(x)dx, \quad i = 0, 1, \cdots.$$

Then we have $\gamma_{0,k} = 1$ and, since U_k are even functions, $\gamma_{i,k} = 0$ for odd i's. Hence, $|A|$ and D in (4.4) are

$$|A| = \gamma_{2,k}, \qquad D = 4(\gamma_{2,k})^3.$$

One may easily compute that $\gamma_{2,0} = 1/12$, $|A| = \gamma_{2,k_2} = 0$ *for*

$$k_2 \equiv 0.5(\sqrt[3]{2} - 1)/(2 - \sqrt[3]{2}),$$

and $D = \gamma_{2,k}^3 \leq 0$ *if and only if* $k \geq k_2$*. From this example we may observe that Hankel matrix can be singular and even the regularity of the matrix does not guarantee the existence of* $\phi_2(x,t)$ *that satisfies (4.6).*

4.3 Approximation with three heat kernels

To demonstrate how to obtain the simplified problem (3.6) from (3.5) its derivation is included in the followings for the case $n = 3$. Then (3.5) reads

$$\begin{aligned}
\rho_1 + \rho_2 + \rho_3 \quad\quad &= \gamma_0, \\
\rho_1 c_1 + \rho_2 c_2 + \rho_3 c_3 &= \gamma_1, \\
\rho_1 c_1^2 + \rho_2 c_2^2 + \rho_3 c_3^2 &= \gamma_2, \\
\rho_1 c_1^3 + \rho_2 c_2^3 + \rho_3 c_3^3 &= \gamma_3, \\
\rho_1 c_1^4 + \rho_2 c_2^4 + \rho_3 c_3^4 &= \gamma_4, \\
\rho_1 c_1^5 + \rho_2 c_2^5 + \rho_3 c_3^5 &= \gamma_5.
\end{aligned} \tag{4.8}$$

Multiply c_1 to the k-th equation and subtract $(k+1)$-th one from it for $k = 1, \cdots, 5$ and obtain 5 equations without ρ_1, i.e.,

$$\begin{aligned}
\rho_2(c_1 - c_2) \quad + \rho_3(c_1 - c_3) \quad &= \gamma_0 c_1 - \gamma_1, \\
\rho_2(c_1 - c_2)c_2 + \rho_3(c_1 - c_3)c_3 &= \gamma_1 c_1 - \gamma_2, \\
\rho_2(c_1 - c_2)c_2^2 + \rho_3(c_1 - c_3)c_3^2 &= \gamma_2 c_1 - \gamma_3, \\
\rho_2(c_1 - c_2)c_2^3 + \rho_3(c_1 - c_3)c_3^3 &= \gamma_3 c_1 - \gamma_4, \\
\rho_2(c_1 - c_2)c_2^4 + \rho_3(c_1 - c_3)c_3^4 &= \gamma_4 c_1 - \gamma_5.
\end{aligned}$$

Do the similar process two more times and obtain three equations without ρ_i's,

$$\begin{aligned}
0 &= \gamma_0 c_1 c_2 c_3 - \gamma_1(c_1 c_2 + c_2 c_3 + c_3 c_1) + \gamma_2(c_1 + c_2 + c_3) - \gamma_3, \\
0 &= \gamma_1 c_1 c_2 c_3 - \gamma_2(c_1 c_2 + c_2 c_3 + c_3 c_1) + \gamma_3(c_1 + c_2 + c_3) - \gamma_4, \\
0 &= \gamma_2 c_1 c_2 c_3 - \gamma_3(c_1 c_2 + c_2 c_3 + c_3 c_1) + \gamma_4(c_1 + c_2 + c_3) - \gamma_5,
\end{aligned}$$

which are identical to (3.6)–(3.7) with $n = 3$, i.e.,

$$\begin{pmatrix} \gamma_0 & \gamma_1 & \gamma_2 \\ \gamma_1 & \gamma_2 & \gamma_3 \\ \gamma_2 & \gamma_3 & \gamma_4 \end{pmatrix} \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \end{pmatrix} = \begin{pmatrix} \gamma_3 \\ \gamma_4 \\ \gamma_5 \end{pmatrix},$$

where $\psi_0 = c_1c_2c_3, \psi_1 = -(c_1c_2 + c_2c_3 + c_3c_1)$ and $\psi_2 = c_1 + c_2 + c_3$.

The determinant of the Hankel matrix,

$$|\mathbf{A}| = \gamma_0\gamma_2\gamma_4 + 2\gamma_1\gamma_2\gamma_3 - \gamma_2^3 - \gamma_0\gamma_3^2 - \gamma_1^2\gamma_4,$$

should not be zero for the existence and uniqueness of the solution to the problem (4.8). If $|\mathbf{A}| \neq 0$, then ψ_i are given by Cramer's rule, i.e.,

$$\begin{aligned} \psi_0 &= (2\gamma_3\gamma_2\gamma_4 + \gamma_3\gamma_1\gamma_5 - \gamma_3^3 - \gamma_2^2\gamma_5 - \gamma_4^2\gamma_1)/|\mathbf{A}|, \\ \psi_1 &= (\gamma_2\gamma_5\gamma_1 + \gamma_0\gamma_4^2 + \gamma_3^2\gamma_2 - \gamma_3\gamma_1\gamma_4 - \gamma_4\gamma_2^2 - \gamma_0\gamma_3\gamma_5)/|\mathbf{A}|, \\ \psi_2 &= (\gamma_0\gamma_2\gamma_5 + \gamma_3^2\gamma_1 + \gamma_2\gamma_4\gamma_1 - \gamma_0\gamma_3\gamma_4 - \gamma_3\gamma_2^2 - \gamma_1^2\gamma_5)/|\mathbf{A}|, \end{aligned}$$

and c_i's are zeros of third order polynomial,

$$g_3(x) = x^3 - \psi_2x^2 - \psi_1x - \psi_0. \tag{4.9}$$

So the solvability of the problem (4.8) is equivalent to the existence of three distinct real roots $c_1 < c_2 < c_3$ of (4.9). The convergence order in Theorem 2.4 gives the asymptotic convergence order:

$$\lim_{t\to\infty} t^{(\frac{7}{2}-\frac{1}{2p})}\|u(x,t) - \phi_3(x,t)\|_p \leq \bar{\gamma}_6\|\partial_\xi^6(e^{-\frac{1}{4}\xi^2})\|_p/\sqrt{4\pi}, \quad 1 \leq p \leq \infty, \tag{4.10}$$

where $\phi_3(x,t) = \frac{1}{\sqrt{4\pi t}}\sum_{i=1}^3 \rho_i e^{-(x-c_i)^2/(4t)}$ and

$$\bar{\gamma}_6 = \int \int_{-\infty}^{x} \int_{-\infty}^{y} \int_{-\infty}^{z} \int_{-\infty}^{v} \int_{-\infty}^{w} \int_{-\infty}^{u} \Big|u_0(\tau) - \sum_{i=1}^{3} \rho_i\delta_{c_i}(\tau)\Big| d\tau du dw dv dz dy dx.$$

Consider Example 4.1 for the approximation ϕ_3. Since $\gamma_{0,k} = 1$ and $\gamma_{1,k} = \gamma_{3,k} = \gamma_{5,k} = 0$, we obtain

$$|A| = \gamma_{2,k}(\gamma_{4,k} - \gamma_{2,k}^2), \quad \psi_1 = \gamma_{4,k}/\gamma_{2,k}, \quad \psi_0 = \psi_2 = 0.$$

Hence, if

$$|\mathbf{A}| \neq 0 \quad \text{and} \quad \psi_1 > 0,$$

then $g_3(x)$ has three distinct real roots,

$$c_1 = -\sqrt{\psi_1}, \quad c_2 = 0, \quad c_3 = \sqrt{\psi_1}.$$

One may show that $\gamma_{4,k} > 0$ if and only if $0 < k < k_4 := 0.5(\sqrt[5]{2}-1)/(2-\sqrt[5]{2})$. Therefore, if $k_4 < k < k_2$, then $\psi_1 < 0$ and the existence of $\phi_3(x,t)$ satisfying (4.10) is not guaranteed. This example shows that the solvability of (3.5) is not obvious for sign changing initial value $u_0(x)$.

5 Approximation of general sign changing solutions

Now consider a general sign changing initial value. Since the initial value $u_0(x)$ satisfies (1.3), there exists $C > 0$ such that $v_0(x) := u_0(x) + \frac{C}{\sqrt{4\pi}} e^{-x^2/4} \geq 0$. Then nonnegative function v_0 satisfies (1.3) and hence we may apply the theory in Section 3. Let ρ_i's and c_i's be the solutions of the moment problem with initial value $v_0(x)$. Then, the solution $u(x,t)$ can be approximated by

$$u(x,t) \sim \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{-(x-c_i)^2/(4t)} - \frac{C}{\sqrt{4\pi(t+1)}} e^{-x^2/4(t+1)}. \tag{5.1}$$

Since the auxiliary part of the approximation is the solution with the extra initial value added to $u_0(x)$, the convergence order of this approximation is same as the one in (1.7). This example shows that we may obtain the same convergence order for general sign-changing solutions by simply adding an extra term.

On the other hand, if the grid points are preassigned, $c_i = \bar{c}_i$, then we have the freedom in choosing the weights ρ_i's only. These ρ_i's are simply obtained by solving the first n equations in (3.5), where the corresponding matrix is Vandermonde matrix, i.e.,

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ \bar{c}_1 & \bar{c}_2 & \cdots & \bar{c}_n \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \bar{c}_1^{n-1} & \bar{c}_2^{n-1} & \cdots & \bar{c}_n^{n-1} \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \\ \cdot \\ \cdot \\ \cdot \\ \rho_n \end{pmatrix} = \begin{pmatrix} \gamma_0 \\ \gamma_1 \\ \cdot \\ \cdot \\ \cdot \\ \gamma_{n-1} \end{pmatrix}. \tag{5.2}$$

The Vandermonde determinant $\Pi_{1\le i<j\le n}(\bar c_j-\bar c_i)$ is not zero if $\bar c_i$ are all different. So (5.2) is solvable and we may construct an approximation

$$\eta_n(x,t):=\sum_{i=1}^n\frac{\rho_i}{\sqrt{4\pi t}}e^{-(x-\bar c_i)^2/(4t)}. \tag{5.3}$$

Then $\eta_n(\cdot,t)$ converges to $u(\cdot,t)$ having order

$$\|u(t)-\eta_n(t)\|_p=O(t^{(\frac{1}{2p}-\frac{n+1}{2})})\qquad\text{as}\quad t\to\infty,$$

since $\lim_{t\to 0}\eta_n(x,t)$ has zero moments upto $(n-1)$-th order.

6 Convergence as $n\to\infty$ with a fixed $t>0$

In this section we discuss about the convergence of the approximation $\phi_n(x,t)$ to the solution $u(x,t)$ as $n\to\infty$ with a fixed $t>0$. We are not going to pursue a rigorous proof for that and the discussions in this section are rather intuitive and hilarious.

In this section we consider a geometric convergence order such as

$$\beta_n(t):=\frac{\|u(t)-\phi_n(t)\|_\infty}{\|u(t)-\phi_{n+1}(t)\|_\infty}\to 1+4\frac{t}{v}(\equiv\beta(t/v))\quad\text{as}\quad n\to\infty, \tag{6.1}$$

where $v>0$ may depend on the initial value $u_0(x)$. First this convergence order implies that the error decays to zero for any fixed $t>0$ as $n\to\infty$. Furthermore, the convergence order is somewhat extreme. For example if $t>v/4$, then the approximation error is reduced by half if one more heat kernel is employed.

Set the approximation error as

$$e_n(x,t)=u(x,t)-\phi_n(x,t).$$

Consider a sequence of functions

$$E_k^n(x)=\int_{-\infty}^x E_{k-1}^n(y)dy,\qquad k=1,2,\cdots,2n,$$

where

$$E_0^n(x):=e_n(x,0)=u_0(x)-\sum_{i=1}^n\rho_i\delta(x-c_i).$$

Notice that the upper index 'n' is to denote that it is related to the approximation $\phi_n(x,t)$ and the lower index k indicates that it is the k-th order antiderivative of the initial approximation. Then, from (2.3), we obtain

$$(\sqrt{t})^{2n+1}\|e_n(t)\|_\infty = \frac{\bar{\gamma}_{2n}}{\sqrt{4\pi}}\sup_\xi |\int \partial_\xi^{2n}(e^{-\zeta^2/4})\sqrt{t}E_{2n}^n(\sqrt{t}(\xi-\zeta))/\bar{\gamma}_{2n}d\zeta|, \tag{6.2}$$

where $\bar{\gamma}_{2n} := \int_{-\infty}^{\infty} E_{2n}^n(x)dx < \infty$.

One interesting observation is that, for n large, $E_{2n}^n(x)$ has a Gaussian like structure. The following conjecture can be easily observed numerically. However, we do not have its proof.

Conjecture 6.1 *There exist $c \in \boldsymbol{R}$ and $v > 0$ which may depend on the initial value $u_0(x)$ and satisfy*

$$\|\frac{1}{\sqrt{v\pi}}e^{\frac{-(x-c)^2}{v}} - \frac{1}{\bar{\gamma}_{2n}}E_{2n}^n(x)\|_\infty \to 0 \quad as \quad n \to \infty. \tag{6.3}$$

where $\bar{\gamma}_{2n} := \int_{-\infty}^{\infty} E_{2n}^n(x)dx$. Furthermore,

$$\frac{\bar{\gamma}_{2n}}{\bar{\gamma}_{2(n+1)}}\frac{\|D_x^{2n}e^{\frac{-x^2}{v}}\|_\infty}{\|D_x^{2n+2}e^{\frac{-x^2}{v}}\|_\infty} \to 1 \quad as \quad n \to \infty. \tag{6.4}$$

The $(2n-1)$th order derivative of $E_{2n}^n(x)$ is $E_1^n(x)$ which is at most of order $O(1/n)$, which does not make any difference in the geometric convergence order such as (6.1). Hence we may treat it as of order $O(1)$. Note that $\bar{\gamma}_{2n}$ is obtained after integrating $E_0^n(x)$ $2n$-times and hence its order should be the reciprocal of the order of $\|D_x^{2n}(e^{\frac{-x^2}{v}})\|_\infty$, which is the $2n$-th derivative of the Gaussian. Hence (6.4) is natural from (6.3). Furthermore, for $\xi = x/\sqrt{v}$,

$$\|D_x^{2n}(e^{\frac{-x^2}{v}})\|_\infty = \|D_\xi^{2n}(e^{-\xi^2})(\xi_x)^{2n}\|_\infty = \frac{1}{v^n}\|D_\xi^{2n}(e^{-\xi^2})\|_\infty.$$

Under Conjecture 6.1, one also has for $n > 0$ large that

$$\begin{aligned}
&\sup_\xi \Big| \int D_y^{2n}(e^{-y^2/4})\ \sqrt{t}E_{2n}^n(\sqrt{t}(x-y))/\bar{\gamma}_{2n}dy\Big| \\
&\qquad\qquad \cong \frac{1}{\sqrt{v\pi t}}\sup_x \Big| \int D_y^{2n}(e^{-y^2/4})e^{-\frac{(x-y-c/\sqrt{t})^2}{v/t}}dy\Big| \\
&\qquad\qquad = \frac{1}{\sqrt{v\pi t}}\Big| \int D_y^{2n}(e^{-y^2/4})e^{-\frac{y^2}{v/t}}dy\Big| =: A(n, v/t).
\end{aligned}$$

Notice that due to the symmetry of $D_x^{2n}(e^{-x^2/4})$ and $e^{-\frac{x^2}{v/t}}$ the supremum is obtained at $x - c/\sqrt{t} = 0$. Then we obtain from the relations (6.2) and (6.4) that

$$t^{-1}\frac{\|e_n(t)\|_\infty}{\|e_{n+1}(t)\|_\infty} \cong \frac{\bar{\gamma}_{2n}}{\bar{\gamma}_{2(n+1)}}\frac{A(n,v/t)}{A(n+1,v/t)} \cong \frac{v^n}{v^{n+1}}\frac{\|D_x^{2n+2}(e^{-x^2})\|_\infty}{\|D_x^{2n}(e^{-x^2})\|_\infty}\frac{A(n,v/t)}{A(n+1,v/t)}.$$

One can easily check that

$$\frac{\|D_x^{2n+2}(e^{-x^2})\|_\infty}{\|D_x^{2n}(e^{-x^2})\|_\infty} = 4n+2, \qquad \frac{A(n,v/t)}{A(n+1,v/t)} = \frac{4+v/t}{4n+2},$$

using a mathematical software such as Maple or by hand. Therefore, we obtain the convergence order in (6.1), i.e.,

$$\frac{\|e_n(t)\|_\infty}{\|e_{n+1}(t)\|_\infty} \cong t\frac{1}{v}(4n+2)\frac{4+v/t}{4n+2} = 1 + 4\frac{t}{v} \quad \text{for } n \text{ large.}$$

Notice that $c \in \boldsymbol{R}$ in (6.3) does not make any difference in the convergence order. The factor that decides the geometric convergence rate is the variance factor v of the limit function $\frac{1}{\sqrt{v\pi}}e^{-x^2/v}$. It seems that the variance factor v depends on the initial value $u_0(x)$ and it will be discussed more in Section 7.2.

Remark 6.2 *For $n > 0$ small, $E_{2n}^n(x)/\bar{\gamma}_{2n}$ is not close enough to the Gaussian and the arguments above are not valid. Therefore, one can expect the convergence order only after such a stage. Then it is natural to ask how large n should be. The answer depends on the initial value. Clearly, if $u_0(x)$ itself is like a gaussian, then such an $n > 0$ can be relatively small. In other case the corresponding $n > 0$ could be larger than that.*

7 Numerical examples

In this section we test the convergence orders numerically for $t > 0$ large and for $n > 0$ large. These tests confirm the convergence orders obtained in the previous sections. This section consists of four subsections. The first two are for $t \to \infty$ and for $n \to \infty$ limits. In the third one we test the behavior of an alternative approach in (7.8) as $n \to \infty$. In the last subsection we do numerical tests for Conjecture 6.1.

There are two difficulties in observing the theoretical convergence order for $t > 0$ large. First the convergence rate for small time $0 < t \ll 1$ is a lot lower than the theoretical one for $t > 0$ large. So we need to wait a certain amount of time to observe the theoretical convergence order. On the other hand, since the convergence order is so high, the approximation error at the right moment can be as small as of order 10^{-36} or 10^{-64} (see Tables 1 and 2). So we should employ enough precisions in its computation to obtain meaningful numerical results.

The second difficulty which is more restrictive is in computing the solution $u(x,t)$. To compute the decay order of $\|u(x,t) - \phi_n(x,t)\|_\infty$ reasonably, we should obtain the exact value of $u(x,t)$ or compute it with a smaller error than the actual approximation error. However, it is impossible to do the integration in (1.1) numerically with such a small error. (In this sense the approximation $\phi_n(x,t)$ is more exact than the exact formula in (1.1).) To avoid such a difficulty, we consider two examples with exact solutions. In the numerical tests of following subsections we employ these examples only.

Example 7.1 (Example with a single hump) *Consider the solution of*

$$u_t = u_{xx}, \quad u(x,0) = K(x,t_0), \quad x \in \boldsymbol{R},\ t > 0, \tag{7.1}$$

where $K(x,t)$ is the heat kernel

$$K(x,t) = \frac{1}{\sqrt{4\pi t}} e^{-x^2/4t}.$$

Then the exact solution is simply $u(x,t) = K(x,t+t_0)$ and the variance of the initial value is $var = 2t_0$. This rather simple example let us observe certain convergence behavior very clearly.

Example 7.2 (Example with double humps) *Consider the solution of*

$$u_t = u_{xx}, \quad u(x,0) = \frac{1}{2}[K(x+1,t_0) + K(x-1,t_0)], \quad x \in \boldsymbol{R},\ t > 0. \tag{7.2}$$

Then the solution is simply $u(x,t) = \frac{1}{2}[K(x+1,t+t_0) + K(x-1,t+t_0)]$ and the variance of the initial value is $var = 1 + 2t_0$.

7.1 Numerical tests for the long time asymptotics

The approximation

$$\phi_n(x,t) \equiv \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{\frac{-(x-c_i)^2}{4t}} \tag{7.3}$$

Table 1

The error $e_n(x,t) = u(x,t) - \phi_n(x,t)$ and the convergence order α_n in (7.5) have been computed for Examples 7.1 and 7.2 with $n = 4, 8$ and $t + 0 = 1$. We observe that $\alpha_n(t) \to -(n + \frac{1}{2})$ as $t \to \infty$.The norms in all tables are L^∞-norms.

	Example 7.1				Example 7.2			
t	$\|e_4(t)\|$	$\alpha_4(t)$	$\|e_8(t)\|$	$\alpha_8(t)$	$\|e_4(t)\|$	$\alpha_4(t)$	$\|e_8(t)\|$	$\alpha_8(t)$
0.1	2.17e-01,	0.7	1.13e-01,	1.0	2.24e-01,	0.8	1.30e-01,	0.9
0.2	1.13e-01,	0.9	2.98e-02,	1.9	1.33e-01,	0.8	4.57e-02,	1.5
0.4	3.48e-02,	1.7	3.34e-03,	3.2	5.30e-02,	1.3	7.27e-03,	2.7
0.8	6.24e-03,	2.5	1.38e-04,	4.6	1.21e-02,	2.1	4.27e-04,	4.1
1.6	6.81e-04,	3.2	2.21e-06,	6.0	1.60e-03,	2.9	9.09e-06,	5.6
3.2	5.12e-05,	3.7	1.72e-08,	7.0	1.37e-04,	3.5	8.57e-08,	6.7
6.4	3.03e-06,	4.1	8.40e-11,	7.7	8.79e-06,	4.0	4.68e-10,	7.5
12.8	1.56e-07,	4.3	3.13e-13,	8.1	4.73e-07,	4.2	1.86e-12,	8.0
25.6	7.48e-09,	4.4	1.01e-15,	8.3	2.31e-08,	4.4	6.18e-15,	8.2
51.2	3.44e-10,	4.4	3.01e-18,	8.4	1.08e-09,	4.4	1.88e-17,	8.4
102.4	1.55e-11,	4.5	8.66e-21,	8.4	4.89e-11,	4.5	5.44e-20,	8.4
204.8	6.93e-13,	4.5	2.44e-23,	8.5	2.19e-12,	4.5	1.54e-22,	8.5

constructed in Section 3 converges to the exact solution $u(x,t)$ with order

$$\|u(t) - \phi_n(t)\|_\infty = O(t^{-\frac{2n+1}{2}}) \quad \text{as} \quad t \to \infty. \tag{7.4}$$

In Table 1 the error $e_n(x,t) = u(x,t) - \phi_n(x,t)$ and the convergence order α_n have been computed for $n = 4, 8$ as doubling the time from $t = 0.1$ to $t = 204.8$. The convergence order of the approximation has been measured by computing

$$\alpha_n(t) \sim \frac{\ln(\|e_n(t/2)\|_\infty / \|e_n(t)\|_\infty)}{\ln(1/2)}. \tag{7.5}$$

(Note that we always measure the error in L^∞-norm. However, in tables we use the notation $\|\cdot\|$ for the norm for the sake of saving space.)

From the table one may clearly observe that the convergence order $\alpha_n(t)$ converges to the optimal convergence order in (7.4) as $t \to \infty$. We may say that the optimal convergence order is obtained in a finite time of order $O(1)$. One can find similar behavior from the Example 7.2.

Table 2
The error $e_n(x,t) = u(x,t) - \phi_n(x,t)$ and the geometric convergence rate $\beta_n(t)$ in (6.1) have been computed for Examples 7.1 and 7.2 with $t = 1, 10$ and $t_0 = 1$. We may observe convergence rate in Section 6.

	Example 7.1				Example 7.2			
n	$\|e_n(1)\|$	$\beta_n(1)$	$\|e_n(10)\|$	$\beta_n(10)$	$\|e_n(1)\|$	$\beta_n(1)$	$\|e_n(10)\|$	$\beta_n(10)$
2	2.8e-02	2.91	2.0e-04	20.84	4.28e-02	2.48	3.83e-04	15.83
3	9.6e-03	2.96	9.5e-06	20.92	1.72e-02	2.49	2.32e-05	16.53
4	3.2e-03	2.98	4.5e-07	20.95	6.7e-03	2.57	1.36e-06	17.06
7	1.2e-04	2.99	4.9e-11	20.98	3.67e-04	2.66	2.47e-10	17.89
10	4.5e-06	3.0	5.3e-15	20.99	1.89e-05	2.71	4.09e-14	18.35
13	1.7e-07	3.0	5.8e-19	21.0	9.35e-07	2.74	6.45e-18	18.65
16	6.1e-09	3.0	6.2e-23	21.	4.45e-08	2.76	9.65e-22	18.86
19	2.3e-10	3.0	6.7e-27	21.0	2.08e-09	2.78	1.41e-25	19.02
22	8.4e-12	3.0	7.3e-31	21.0	9.65e-11	2.79	2.02e-29	19.15
25	3.1e-13	3.0	7.9e-35	21.0	4.36e-12	2.8	2.85e-33	19.26
46	2.97e-23	3.0	1.35e-62	21.0	1.38e-21	2.85	2.25e-60	19.70
49	1.1e-24	3.0	1.46e-66	21.0	5.95e-21	2.86	2.94e-64	19.74

7.2 Numerical tests for $n \to \infty$ limits

Now we are going to check the convergence order for n large with a fixed $t > 0$. Consider the geometric convergence ratio

$$\beta_n(t) := \|e_{n-1}(t)\|_\infty \Big/ \|e_n(t)\|_\infty.$$

In Table 2 the error $\|e_n(t)\|_\infty$ and this ratio are computed for Examples 7.1 and 7.2 at two instances with $t = 1$ and $t = 10$ as increasing n from $n = 2$ to $n = 25$. One can clearly observe certain geometric convergence order as in (6.1). In both examples we can clearly see that $10(\beta_n(1) - 1) \sim (\beta_n(10) - 1)$, which indicates that the corresponding constant $v > 0$ in (6.1) which decides the geometric convergence ratio does not depend on the time $t > 0$.

From the test for Example 7.1 one can clearly see that $\beta_n(1) \to 3$ and $\beta_n(10) \to 21$ as $n \to \infty$. In both of the cases the corresponding v is $v = 2$ which is the variance of the initial value $var = 2(\equiv 2t_0)$. The convergence pattern for Example 7.2 is somewhat different. First the convergence speed of the ratio $\beta_n(t)$ is slow. It seems due to the complexity of the structure of the initial value. At the moment $n = 49$ the corresponding variance index is $v = 2.15$ which is still decreasing and already smaller than the variance of the initial value $u_0(x)$ which is $var = 3(\equiv 1 + 2t_0)$. It seems that the factor that decides the geometric convergence rate is the tail of the initial value for $|x|$ large. However, we do not clearly understand the relation yet.

7.3 Approximation using derivatives of the Gaussian

Duoandikoetzea and Zuazua [8] suggested a different approach based on a summation of derivatives of the heat kernel,

$$\psi_{2n}(x,t) \equiv \sum_{i=0}^{2n-1} \frac{\gamma_i}{(i!)\sqrt{4\pi t}} \frac{\partial^i}{\partial x^i} e^{-x^2/(4t)}, \tag{7.6}$$

and proved the optimal convergence order,

$$\|u(t) - \psi_{2n}(t)\|_\infty = O\Big(t^{-\frac{2n+1}{2}}\Big) \quad \text{as} \quad t \to \infty. \tag{7.7}$$

This result has been extended to general linear parabolic equations with periodic coefficients in [22]. (Note that the original multi-dimensional result is rewritten in one dimensional version here for an easier comparison.) The asymptotic convergence order in (7.7) indicates that ψ_{2n} is also a good approximation of the solution $u(x,t)$ for t large. In this section we observe that $\|u(t) - \psi_{2n}(t)\|_\infty$ may diverge as $n \to \infty$.

We may write $\psi_{2n}(x,t)$ in (7.6) as

$$\psi_{2n}(x,t) = \sum_{i=0}^{2n-1} \frac{-\gamma_i}{2(i!)} \Big(\frac{-1}{2\sqrt{t}}\Big)^{n+1} H_i\Big(\frac{x}{2\sqrt{t}}\Big) e^{-x^2/(4t)}, \tag{7.8}$$

where $H_i(x)$ is the Hermite polynomial of order i. In Table 3 the approximation error and the geometric convergence ratio β_n are given for Example 7.1. To denote the relation between the initial value and the convergence ratio more clearly, we set

$$\beta_{2n}(t,t_0) := \|e_{2n-2}(t)\|_\infty \Big/ \|e_{2n}(t)\|_\infty, \tag{7.9}$$

where $e_{2n}(x,t) = u(x,t) - \psi_{2n}(x,t)$.

Table 3
The error $e_n(x,t) = u(x,t) - \psi_{2n}(x,t)$ and the geometric convergence rate $\beta_n(t,t_0)$ in (7.9) have been computed numerically for Example 7.1 with $t_0 = 10$ and $t = 1, 10, 100$. We may observe the convergence rate in (7.10).

2n	$\|e_{2n}(1)\|$	$\beta_{2n}(1,10)$	$\|e_{2n}(10)\|$	$\beta_{2n}(10,10)$	$\|e_{2n}(100)\|$	$\beta_{2n}(100,10)$
4	1.21e+00	0.1623821	1.85e-02	1.4142136	9.77e-05	13.4400610
6	9.37e+00	0.1295695	1.50e-02	1.2335625	8.11e-06	12.0475285
8	7.88e+01	0.1188625	1.29e-02	1.1610328	7.08e-07	11.4555359
14	5.74e+04	0.1089029	9.66e-03	1.0825322	5.40e-10	10.7781946
20	4.73e+07	0.1058095	8.05e-03	1.0553099	4.54e-13	10.5307485
26	4.12e+10	0.1043095	7.04e-03	1.0415615	3.99e-16	10.4026370
32	3.69e+13	0.1034247	6.34e-03	1.0332791	3.60e-19	10.3243276
38	3.38e+16	0.1028412	5.81e-03	1.0277462	3.31e-22	10.2715121
44	3.13e+19	0.1024275	5.39e-03	1.0237896	3.07e-25	10.2334861
50	2.93e+22	0.1021190	5.06e-03	1.0208199	2.88e-28	10.2048012

One may observe that $\beta_{2n}(1,10) \to 0.1$, $\beta_{2n}(10,10) \to 1$ and $\beta_{2n}(100,10) \to 10$ as $n \to \infty$. This observation leads us to another conjecture

$$\lim_{n\to\infty} \frac{\|u(t) - \psi_{2n}(t)\|_\infty}{\|u(t) - \psi_{2n+2}(t)\|_\infty} = \frac{t}{t_0} \ . \tag{7.10}$$

This relation indicates that the approximation error increases exponentially if $t < t_0$ and hence $\psi_{2n}(x,t)$ is meaningful for $t > t_0$ only.

7.4 Numerical test for Conjecture 6.1

The geometric convergence rate (6.1) for n large has been obtained under Conjecture 6.1 and observed numerically in Section 7.2. Notice that the conjecture itself is of an independent interest which has no direct relation with the heat equation. In this section we test the limits (6.3) and (6.4) in the conjecture.

In Table 4 the uniform norm of the difference in (6.3) and the ratio in (6.4) are given for Examples 7.1 and 7.2. In both of the cases we took $v = 2t_0$. The results for Example 7.1 show the convergence more clearly. In particular the test for (6.4) shows that the ratio is identically one if the initial value $u_0(x)$ is the Gaussian.

Table 4
We may observe conjectures in (6.3) and (6.4) numerically. In this table those conjectures are tested using Examples 7.1 and 7.2 with $t_0 = 1$ and $v = 2t_0$.

	$\|\frac{1}{\sqrt{2t_0\pi}}e^{\frac{-x^2}{2t_0}} - \frac{1}{\bar{\gamma}_{2n}}E^n_{2n}(x)\|$		$\frac{\bar{\gamma}_{2n-2}}{\bar{\gamma}_{2n}}\frac{\|D_x^{2n-2}e^{-x^2/2t_0}\|}{\|D_x^{2n}e^{-x^2/2t_0}\|}$	
n	Example 7.1	Example 7.2	Example 7.1	Example 7.2
2	2.233e-02	4.378e-02	1.0	0.7500000
3	2.070e-02	3.675e-02	1.0	0.7826087
4	1.631e-02	3.547e-02	1.0	0.8070175
5	1.387e-02	3.353e-02	1.0	0.8237512
6	1.207e-02	3.194e-02	1.0	0.8369731
7	1.070e-02	3.054e-02	1.0	0.8474264
8	9.675e-03	2.932e-02	1.0	0.8561101
9	8.743e-03	2.825e-02	1.0	0.8634099
10	8.016e-03	2.729e-02	1.0	0.8696921

The columns of the table for Example 7.2 also show similar convergence behaviors. However, the speed of its convergence seems a lot slower. In fact it is not even clear that taking $v = 2t_0$ is the correct one for the case of Example 7.2. Since $2t_0$ is the variance of Example 7.1, we also tried $2t_0 + 1$ which is the variance of Example 7.2. However, we could not obtain the convergence and $v = 2t_0$ seems a better choice. It also seems that the v in (6.3) depends on the structure of the initial value $u_0(x)$ for $|x|$ large.

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