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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 linear combinations of n heat kernels to approximate solutions to the heat equation. We show that such approximations are 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 positive solutions of the heat equation such approximations are achieved using the theory of truncated moment problems. For general sign-changing solutions these type of approximations are obtained by simply adding an auxiliary heat kernel. Furthermore, inspired by numerical computations, we conjecture that such approximations converge geometrically as $n \to \infty$ for any fixed $t > 0$.

Key words. heat equation, moments, asymptotics convergence rates, approximation of an integral formula, heat kernel

AMS subject classifications. 35K05, 78M05, 41A10

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1. Introduction.

It is well known that

$$u(x,t) = \int \frac{u_0(c)}{\sqrt{4\pi t}} e^{\frac{-(x-c)^2}{4t}} dc \tag{1.1}$$

is the physically meaningful solution to the heat equation

$$u_t = u_{xx}, \quad u(x,0) = u_0(x) \in L^1(\boldsymbol{R}), \qquad x, u \in \boldsymbol{R}, \quad t > 0, \tag{1.2}$$

where, for simplicity, the initial value $u_0(x)$ is assumed to be continuous. In this paper, we shall refer to (1.1) as the solution of the heat equation (1.2) for the sake of brevity. If a general L^1 initial value is considered, no asymptotic convergence order to a fundamental solution is expected in L^1-norm. Hence, the asymptotic convergence order is usually studied under suitable restrictions on its initial value $u_0(x)$ for $|x|$ large.

Since the analysis of this paper is based on the *moments* of the solution, the initial value $u_0(x)$ is required to have finite moments up to certain order, say, $2n$. We set $x^{2n}u_0(x) \in L^1(\boldsymbol{R})$ and the moments of the initial value $u_0(x)$ as

$$\gamma_k := \int x^k u_0(x)dx < \infty, \qquad k = 0, 1, \ldots, 2n. \tag{1.3}$$

For example, if the initial value has an algebraic decay order higher than $2n+1$ for $|x|$ large, i.e., for $\varepsilon > 0$,

$$u_0(x) = O\left(|x|^{-(2n+1+\varepsilon)}\right) \quad \text{as} \quad |x| \to \infty, \tag{1.4}$$

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then the moments are well defined up to order $2n$. In the study of asymptotics the initial value is frequently assumed to have the order that a fundamental solution has for $|x|$ large. For the heat equation case the fundamental solution is the Gaussian and the corresponding decay order is $u_0(x) = O(e^{-x^2})$ as $|x| \to \infty$. Hence, the moment γ_k is defined for all order $k \geq 0$.

One may do the integration in the explicit formula (1.1) only approximately, even though the integration gives the exact value of the solution. In numerical computations finding an efficient way to compute such an integration has been an important issue. From this point of view, it seems useful to consider its approximation in a simpler form. Duoandikoetxea and Zuazua [9] showed that the following linear combination of derivatives of the Gaussian

$$\psi_{2n}(x,t) \equiv \sum_{i=0}^{2n-1} \frac{(-1)^i \gamma_i}{(i!)\sqrt{4\pi t}}\, \partial_x^i \left(e^{\frac{-x^2}{4t}} \right) \tag{1.5}$$

approaches to the solution u with a convergence order of

$$\|u(t) - \psi_{2n}(t)\|_p = O\left(t^{\left(\frac{1}{2p} - \frac{2n+1}{2}\right)} \right) \quad \text{as} \quad t \to \infty \ \text{ for } \ 1 \leq p \leq \infty, \tag{1.6}$$

where $\|\cdot\|_p$ denotes the L^p-norm in the whole space $\boldsymbol{R}$ and ∂_x^i the ith order partial differentiation with respect to x. Note that the original multidimensional result is written in a one-dimensional (1D) version for an easier comparison. This asymptotic convergence order indicates that ψ_{2n} is a good approximation of the solution $u(x,t)$ for t large. However, it does not necessarily mean that ψ_{2n} is a good approximation as $n \to \infty$ with a fixed $t > 0$. In fact, Table 7.3 shows that this L^p-norm difference may diverge geometrically as $n \to \infty$ if the fixed time $t > 0$ is not large enough. This is not surprising since the high order derivatives of the Gaussian in (1.5) diverge as their orders increase.

In this article we consider a linear combination of "n" heat kernels

$$\phi_n(x,t) \equiv \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}}\, e^{\frac{-(x-c_i)^2}{4t}} \tag{1.7}$$

as an approximation to the solution $u(x,t)$. One may regard this summation as a discrete version of the integration in (1.1) by considering c_i's as grid points and ρ_i's as approximations of $u_0(c)dc$ in the interval (c_{i-1}, c_i). However, we employ these $2n$ degrees of freedom, ρ_i's and c_i's, to match the first $2n$ initial moments, i.e., to satisfy the following $2n$ moment equations:

$$\lim_{t \to 0} \int x^k \phi_n(x,t)dx = \gamma_k, \qquad k = 0, 1, \ldots, 2n-1. \tag{1.8}$$

If the initial value is positive, the theory of truncated moment problems [3] gives the solvability of this problem. Then ϕ_n and u share identical first $2n$ moments for all $t \geq 0$. Note that ψ_{2n} in (1.5) also has the same property, and Duoandikoetxea and Zuazua obtained the convergence order in (1.6) based on it. Hence, we may obtain the same convergence order for the approximation $\phi_n(x,t)$. In this paper, we actually go a little bit further and obtain the limit of $t^{\frac{2n+1}{2} - \frac{1}{2p}} \|u(t) - \phi_n(t)\|_p$ as $t \to \infty$. This convergence order is then improved in Lemma 2.3 for the case that this limit becomes zero. A multidimensional extension of this approach requires a theory of multidimensional truncated moment problems. One may find one from a recent work by Curto and Fialkow [4].

From a practical point of view, it is desirable if the solution u can be approximated by ϕ_n as $n \to \infty$ for a fixed $t > 0$. Indeed, our numerical examples in section 7.2 indicate the following geometric convergence order:

$$\frac{\|u(t) - \phi_n(t)\|_\infty}{\|u(t) - \phi_{n+1}(t)\|_\infty} \to 1 + 4\frac{t}{v} \quad \text{as} \quad n \to \infty, \tag{1.9}$$

where the constant $v > 0$ depends on the initial value $u_0(x)$. However, its proof has, thus far, eluded us; nevertheless, we will include a discussion of (1.9) in section 6.

This paper is organized as follows. First, in section 2, we compute the limit of $t^{(\frac{2n+1}{2} - \frac{1}{2p})}\|u(t) - \phi_n(t)\|_p$ as $t \to \infty$ under the assumption (1.8), which gives the convergence order in (1.6). A short introduction to the theory of truncated moment problems is given in section 3, which provides the existence and the uniqueness of ρ_i's and c_i's that solve (1.8). We remark that the theory is applicable for nonnegative initial values only (see [1, 3]). For general sign-changing solutions the existence and the uniqueness of such ρ_i's and c_i's do not hold. In section 4 we discuss this issue in detail for three cases with $n = 1, 2$, and 3. In section 5 we construct approximations for general sign-changing cases by adding an auxiliary heat kernel or by assigning c_i's independently. The conjectured geometric convergence order for large $n > 0$ is discussed in section 6. The asymptotic convergence orders as $t \to \infty$ or $n \to \infty$ are numerically tested in sections 7.1 and 7.2. The convergence of the alternative approach using ψ_{2n} and the conjectured statements in section 6 are numerically tested in sections 7.3 and 7.4.

In the study of nonlinear diffusion or convection, fundamental solutions which have the Dirac measure as their initial value, i.e., $u_0(x) = \delta(x)$, often serve as canonical solutions. The Barenblatt solutions, the diffusion waves, and the N-waves are well-known examples (see [23]). In the study of porous medium equations, the Barenblatt solution is used as an asymptotic profile and the convergence order of general solutions to this special one has been studied in various cases (see [2, 6] and references therein). The diffusion wave and the Gaussian are the asymptotics of convection-diffusion equations for diffusion dominant cases (see [10, 11, 12, 16]). For convection dominant cases (see [14]) and inviscid convection equations (see [5, 8, 13, 20]) or hyperbolic systems (see [7, 17, 18]), N-waves represent the asymptotic behavior, where N-waves can be understood as a special solution with initial value $u_0(x) = \lim_{\varepsilon\to 0}[a\delta(x-\varepsilon) - b\delta(x+\varepsilon)]$ with $a, b > 0$. Placing the Dirac measure at the center of mass, the optimal convergence order of $O(t^{\frac{1}{2p} - \frac{3}{2}})$ in L^p-norm (or of $O(t^{-1})$ in L^1-norm) has been obtained in several cases (see [2, 13, 15]). Therefore, the result of this paper can be viewed as an extreme case that exploits all of the moments of the initial value.

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 [15] for the special case $n = 1$. Considering that the Burgers equation has been used as a tool to study the asymptotic structure of the viscous systems of conservation laws (see, e.g., [19]), we hope the approach in this article may be useful for other general models.

2. Asymptotic convergence order. In this section, we show that the decay rate of a derivative of a solution is naturally transferred to the convergence order of our approximation. This connection will be made by assigning the moments of a solution to its approximation. Let $\gamma_k(t)$ be the kth order moment of a solution $u(x,t)$ at time $t \geq 0$, i.e.,

$$\gamma_k(t) = \int x^k u(x,t)dx, \qquad k = 0, 1, 2, \ldots, t \geq 0.$$

(Notice that we are slightly abusing the notation γ_k in (1.3) in the following couple of paragraphs.) We can easily show how the moment $\gamma_k(t)$ evolves as $t \to \infty$.

LEMMA 2.1. *Let $u(x,t)$ be the solution to the heat equation and $\gamma_k(t)$ be its kth order moment at time $t \geq 0$. Then*

$$\frac{d}{dt}\gamma_k(t) = \begin{cases} 0\ , & k = 0 \text{ or } 1, \\ k(k-1)\gamma_{k-2}(t), & k \geq 2. \end{cases}$$

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

$$\gamma_1'(t) = \int x u_t dx = \int x u_{xx} dx = [xu_x - u]_{-\infty}^{\infty} = 0.$$

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

$$\begin{aligned} \gamma_k'(t) &= \int x^k u_t dx = \int x^k u_{xx} dx \\ &= \left[x^k u_x - kx^{k-1}u\right]_{-\infty}^{\infty} + \int k(k-1)x^{k-2}u dx = k(k-1)\gamma_{k-2}(t). \qquad \square \end{aligned}$$

This lemma shows that even numbered moments and odd numbered ones evolve independently. One may explicitly write

$$\begin{aligned} \gamma_{2n}(t) &= \sum_{k=0}^{n} \frac{(2n)!}{(n-k)!(2k)!} t^{n-k} \gamma_{2k}(0), \\ \gamma_{2n+1}(t) &= \sum_{k=0}^{n} \frac{(2n+1)!}{(n-k)!(2k+1)!} t^{n-k} \gamma_{2k+1}(0). \end{aligned} \tag{2.1}$$

If $\gamma_k(0) = 0$ for all $0 \leq k \leq n$, then $\gamma_k(t) = 0$ for all $0 \leq k \leq n$, $\gamma_k(t) = \gamma_k(0)$ for $k = n+1, n+2$, $\gamma_k(t)$ is linear for $k = n+3, n+4$, $\gamma_k(t)$ 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 up to certain order if they are initially zero. Hence, it is natural to expect a higher convergence order by matching the moments of the approximation solution to those of the exact one. We proceed with our discussion in this respect.

LEMMA 2.2. *If $x^m E_0(x) \in L^1(\boldsymbol{R})$ and*

$$\int_{-\infty}^{\infty} x^k E_0(x) dx = 0 \quad \text{for all} \quad 0 \leq k < m, \tag{2.2}$$

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

$$\partial_x^m E_m(x) = E_0(x). \tag{2.3}$$

Proof. The proof was given by Duoandikoetxea and Zuazua [9] for the multidimensional case. Here we provide its 1D counterpart. Consider a sequence of functions defined inductively by

$$E_k(x) = \int_{-\infty}^{x} E_{k-1}(y)dy, \quad 0 < k \leq m. \tag{2.4}$$

First, we show that E_k's are well defined,

$$\int_{-\infty}^{\infty} E_k(x)dx = 0 \qquad \text{and} \qquad E_k(x) \to 0 \ \text{ as } |x| \to \infty \tag{2.5}$$

for $k = 0, 1, \ldots, m-1$. It suffices to show (2.5) for $k = l < m$ under the assumption that (2.5) holds for all $k = 0, 1, \ldots, l-1$. Note that it is clearly satisfied for $k = 0$. Since $\int_{-\infty}^{\infty} E_{l-1}(x)dx = 0$, the integral $E_l(x)$ also decays to zero as $|x| \to \infty$. Using the fact that E_k decays to zero as $|x| \to \infty$ for all $0 \leq k \leq l$, we obtain

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

using the integration by parts and then (2.2). Therefore, (2.5) holds for $k = l$ and, hence, for all $0 \leq k \leq m-1$. Since $x^m E_0(x) \in L^1(\boldsymbol{R})$, $E_m \in W^{m,1}(\boldsymbol{R})$ and (2.3) is satisfied. ∎

The existence of E_m satisfying (2.3) is the key observation to obtain the asymptotic convergence order. We now continue our discussion under the assumption that the initial value $E_0(x)$ satisfies (2.2) and $E_m(x)$ is its mth order antiderivative given in Lemma 2.2. However, the following discussions about the decay rate of derivatives of a solution can be considered independently. Let $E_m(x,t)$ be the solution to the heat equation with initial value $E_m(x,0) = E_m(x) \in W^{m,1}(\boldsymbol{R})$, i.e.,

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

The dissipation of the solution can be easily shown by introducing similarity variables:

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

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

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

and its mth order derivative is given by

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

Now consider the decay order of the mth order derivative of the solution $E_m(x,t)$. First, let $C_m := |\int E_m(y)dy|$ and consider the case $C_m \neq 0$. Then

$$\big(\sqrt{t}\big)^{m+1} |\partial_x^m E_m(x,t)| = \sqrt{t}\left|\partial_\xi^m \tilde{E}_m(\xi,t)\right| = \frac{C_m}{\sqrt{4\pi}} \left| \int f(\zeta) g_t(\xi-\zeta)d\zeta \right|, \tag{2.6}$$

where

$$g_t(\xi) = \sqrt{t} E_m\big(\sqrt{t}\xi\big)/C_m, \;\; f(\xi) = \partial_\xi^m \left(e^{-\xi^2/4}\right). \tag{2.7}$$

After taking the supremum on both sides of (2.6), one obtains

$$\left(\sqrt{t}\right)^{m+1}\|\partial_x^m E_m(t)\|_\infty \le \frac{C_m}{\sqrt{4\pi}}\left\|\partial_\xi^m\left(e^{-\xi^2/4}\right)\right\|_\infty .$$

If one takes $t\to\infty$ limit to (2.6), then

$$\lim_{t\to\infty}\left(\sqrt{t}\right)^{m+1}|\partial_x^m E_m(x,t)| = \frac{C_m}{\sqrt{4\pi}}|f(\xi)|.$$

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

$$\lim_{t\to\infty}\left(\sqrt{t}\right)^{m+1}\|\partial_x^m E_m(t)\|_\infty = \frac{C_m}{\sqrt{4\pi}}\left\|\partial_\xi^m\left(e^{-\xi^2/4}\right)\right\|_\infty .$$

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

$$\begin{aligned} t^{\left(\frac{m+1}{2}-\frac{1}{2p}\right)}\ & \|\partial_x^m E_m(t)\|_p \\ &= \left(\sqrt{t}\right)^{m+1}\left(\frac{1}{\sqrt{t}}\right)^{1/p}\left(\int|\partial_x^m E_m(x,t)|^p dx\right)^{1/p} \\ &= \left(\int\left|\left(\sqrt{t}\right)^{m+1}\partial_x^m E_m(x,t)\right|^p d\left(\frac{x}{\sqrt{t}}\right)\right)^{1/p} \\ &= \left(\int\left|\sqrt{t}\partial_\xi^m \tilde{E}_m(\xi,t)\right|^p d\xi\right)^{1/p} \\ &= \frac{C_m}{\sqrt{4\pi}}\left(\int\left|\int f(\zeta)g_t(\xi-\zeta)d\zeta\right|^p d\xi\right)^{1/p} = \frac{C_m}{\sqrt{4\pi}}\|f*g_t\|_p. \end{aligned} \tag{2.8}$$

Standard arguments imply that $\|f*g_t\|_p\to\|f\|_p$ as $t\to\infty$ (see [21, p. 62]). Therefore,

$$\lim_{t\to\infty} t^{\left(\frac{m+1}{2}-\frac{1}{2p}\right)}\|\partial_x^m E_m(t)\|_p = \frac{C_m}{\sqrt{4\pi}}\left\|\partial_\xi^m\left(e^{-\xi^2/4}\right)\right\|_p .$$

Now we consider the case that $C_m=0$. Then one can easily show that this limit is zero. In fact, we will improve the convergence order by working with higher order antiderivatives. Let

$$E_k(x)=\int_{-\infty}^x E_{k-1}(y)dy, \qquad k>m. \tag{2.9}$$

We can easily show that $\int_{-\infty}^\infty E_{k_0}(x)dx (=\lim_{x\to\infty}E_{k_0+1}(x)\,)\ne 0$ for some $k_0>m$. Suppose that $\int_{-\infty}^\infty E_k(x)dx=0$ for all $k>m$. Then $|E_k(x)|$ decays to zero for $|x|$ large, and, therefore, after integrating by parts k times with proper inductive arguments, one obtains

$$(-1)^k k!\int_{-\infty}^\infty E_k(x)dx = \int_{-\infty}^\infty x^k E_0(x)dx = 0.$$

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

$$P_n(x)\to E_0(x) \qquad \text{as} \qquad n\to\infty$$

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

$$\|E_0\|_2^2 = \int_{-L}^{L} E_0^2(x)dx = \lim_{n\to\infty} \int_{-L}^{L} P_n(x)E_0(x)dx = 0.$$

Hence, if the initial value E_0 is not a trivial one, there exists $k_0 > m$ such that $\lim_{x\to\infty} E_k(x) = 0$ for all $0 \le k \le k_0$ and $C_{k_0} := |\lim_{x\to\infty} E_{k_0+1}(x)| \neq 0$. If $E_0(x)$ decays with an algebraic order $k_0+1+\varepsilon$, $\varepsilon > 0$, for $|x|$ large, then $C_{k_0} < \infty$. However, C_{k_0} can be unbounded in general.

Let $E_{k_0}(x,t)$ be the solution with $E_{k_0}(x)$ as its initial value. Then, clearly, $\partial_x^m E_m = \partial_x^{k_0} E_{k_0} = E_0$ and, hence,

$$\lim_{t\to\infty} t^{\left(\frac{k_0+1}{2}-\frac{1}{2p}\right)} \|\partial_x^m E_m\|_p = \lim_{t\to\infty} t^{\left(\frac{k_0+1}{2}-\frac{1}{2p}\right)} \left\|\partial_x^{k_0} E_{k_0}\right\|_p = \frac{C_{k_0}}{\sqrt{4\pi}} \left\|\partial_\xi^{k_0} e^{\frac{-\xi^2}{4}}\right\|_p .$$

Therefore, if $C_m := |\int E_m(y)dy| = 0$, one obtains a higher decay order. Summing up, we obtain the following lemma.

Lemma 2.3. *Let $E_m(x,t)$ be the solution to the heat equation with a nontrivial initial value $E_m(x) \in W^{m,1}(\boldsymbol{R})$ and E_k's be given inductively by* (2.9). *Then there exists $k_0 \ge m$ such that $\lim_{x\to\infty} E_k(x) = 0$ for $0 \le k \le k_0$ and $0 \neq |\lim_{x\to\infty} E_{k_0+1}(x)|$, and, for $m \le k \le k_0$,*

$$\lim_{t\to\infty} t^{\left(\frac{k+1}{2}-\frac{1}{2p}\right)} \|\partial_x^m E_m(t)\|_p = \frac{\left\|\partial_\xi^k e^{-\xi^2/4}\right\|_p}{\sqrt{4\pi}} \left|\int E_k(x)dx\right| , \ 1 \le p \le \infty. \tag{2.10}$$

If $\int E_m(x)dx = 0$, then the limit in (2.10) implies that $\lim_{t\to\infty} t^{\left(\frac{m+1}{2}-\frac{1}{2p}\right)} \|\partial_x^m E_m\|_p = 0$. Hence, we may simply say that

$$\lim_{t\to\infty} t^{\left(\frac{m+1}{2}-\frac{1}{2p}\right)} \|\partial_x^m E_m(t)\|_p = \frac{\left\|\partial_\xi^m \left(e^{-\xi^2/4}\right)\right\|_p}{\sqrt{4\pi}} \left|\int E_m(x)dx\right| , \quad 1 \le p \le \infty, \tag{2.11}$$

which is a weaker statement than (2.10) is. Note that one may obtain the upper bound of the term $t^{\left(\frac{m+1}{2}-\frac{1}{2p}\right)} \|\partial_x^m E_m(t)\|_p$ using Young's inequality. In fact, the corresponding upper bound for the estimate ψ_{2n} was obtained in [9].

In the following, we take the convergence order in (2.11) for simplicity. If an optimal convergence order is concerned and $\int E_m(x)dx = 0$, then one may refer to (2.10). It is well known that an L^1 solution to the heat equation decays to zero with order $O(t^{-1/2})$. Lemma 2.3 says that the decay order of its derivative is increased by $\frac{1}{2}$ after each differentiation. The asymptotic convergence order between two solutions is now obtained as a corollary of previous lemmas.

Theorem 2.4. *Let $u(x,t)$ and $v(x,t)$ be solutions of the heat equation with initial values $u_0(x)$ and $v_0(x)$, respectively. Suppose that the initial difference $E_0(x) := u_0(x) - v_0(x)$ satisfies the assumptions in Lemma* 2.2. *Then, for $1 \le p \le \infty$,*

$$\lim_{t\to\infty} t^{\left(\frac{m+1}{2}-\frac{1}{2p}\right)} \|u(t) - v(t)\|_p = \frac{\left\|\partial_\xi^m \left(e^{-\frac{1}{4}\xi^2}\right)\right\|_p}{\sqrt{4\pi}} \left|\int E_m(x)dx\right|, \tag{2.12}$$

where $E_m \in W^{m,1}(\boldsymbol{R})$ is the one that satisfies $\partial_x^m E_m(x) = E_0(x)$.

Proof. Let $E_m(x,t)$ be the solution to the heat equation with initial value $E_m(x)$. Then $\partial_x^m E_m(x,t)$ is the solution to the heat equation with initial value $\partial_x^m E_m(x) = E_0(x)$. Hence, $\partial_x^m E_m(x,t)(= E(x,t)\,) = u(x,t) - v(x,t)$ and (2.12) follows from (2.11). ∎

Remark 2.5. In this section, we basically considered the convergence order of $\phi_n(x,t)$ ($\cong v(x,t)$) to $u(x,t)$ as $t \to \infty$ with a fixed $n > 0$. However, the relation (2.6), 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 problems. Consider a linear combination of heat kernels

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

The $2n$ freedom of choices in ρ_i's and c_i's are used to control the first $2n$ moments of the approximation. Remember that γ_k is to denote the initial kth moment, i.e.,

$$\gamma_k := \int x^k u_0(x) dx, \qquad k = 0, 1, \dots, 2n-1. \tag{3.2}$$

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

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

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

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

where $\delta_{c_i}(x)$ is the Dirac measure centered at c_i, i.e., $\delta_{c_i}(x) = \delta(x - c_i)$. Hence, the zero moment conditions in (2.2) 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 section 4.3), one may obtain n-equations involving c_i's only:

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

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

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

Consequently, we set

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

(Note that the coefficient of the leading order term is 1 and, hence, $g_n(x) \to \infty$ as $x \to \infty$.) Hence, if the initial moments in (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 should show that the Hankel matrix in (3.6) is nonsingular. Then there exists a unique column vector $\Psi = (\psi_0, \dots, \psi_{n-1})^t$ that satisfies (3.6). The next thing to show is 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.,

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

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 satisfy the last n-equations in (3.5).

For a general sign-changing initial value $u_0(x)$ the Hankel matrix $\mathbf{A}$ can be singular, and examples are given in section 4. However, if the initial value $u_0(x)$ is nonnegative, then the uniqueness and the existence are resolved by the theory for the moment problem (see [1, 3]). In the following, we assume $u_0(x) \geq 0$ and introduce this technique briefly for the completeness and the later use in this paper. Consider

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

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, $\Psi^t\mathbf{A}\Psi = 0$ 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, $\Psi^t\mathbf{A}\Psi > 0$ 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. (The proof is originally done by Hamburger.)

To show that $g_n(x)$ has n-distinct real zeros, consider a linear functional S on the space of polynomials defined by

$$S(r) := \sum_{i=0}^{l} r_i\gamma_i = r_0\gamma_0 + \cdots + r_l\gamma_l \quad \text{for} \quad r(x) = \sum_{i=0}^{l} r_i x^i.$$

Then, the same statements used for the positivity of $\Psi^t \mathbf{A} \Psi$ also show that

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

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 [1, p. 2]). So $S(r) = S(p^2) + S(q^2) > 0$.

Since $\mathbf{A}$ is nonsingular, there exists an n-vector $\Psi = (\psi_0, \ldots, \psi_{n-1})$ 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

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

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

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

Suppose that $g_n(x)$ never changes its sign. Then $g_n(x) \geq 0$ and, hence, $S(g_n) > 0$, which contradicts (3.11) with $k = 0$. Suppose that $g_n(x)$ changes its sign at points $c_1, \ldots, c_l$ 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.,

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

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 to the heat equation with initial value $u_0(x)$. If $u_0(x)$ is nonnegative (or nonpositive) and $x^{2n}u_0(x) \in L^1(\boldsymbol{R})$, then there exist $\rho_i, c_i, i = 1,\dots,n$, such that, for $\phi_n(x,t) \equiv \sum_{i=1}^n \frac{\rho_i}{\sqrt{4\pi t}}\, e^{-(x-c_i)^2/(4t)}$,*

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

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

Remark 3.2. The system (3.5) can be solved by commercial software such as Maple. However, since the problem is highly nonlinear, it takes a very long time even for small n. Therefore, even for the computational purpose, one needs to follow the steps of the proof to construct $\phi_n(x)$.

4. General initial value. In this section, we consider a general initial value which may change its sign. 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 single 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 obtained by solving

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

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

$$\lim_{t\to\infty} t^{\left(\frac{3}{2}-\frac{1}{2p}\right)} \|u(t)-\phi_1(t)\|_p = \frac{\left\|\partial_\xi^{2}\left(e^{-\frac{1}{4}\xi^2}\right)\right\|_p}{\sqrt{4\pi}} \left|\int_{-\infty}^{\infty} E_2(x)dx\right|, \quad 1 \le p \le \infty,$$

where $E_2(x)$ is the second order antiderivative of the initial error $E_0(x) := u_0(x) - \rho_1\delta_{c_1}(x)$ given by (2.4), i.e., $E_2(x) = \int_{-\infty}^{x}\int_{-\infty}^{y}(u_0(z)-\rho_1\delta_{c_1}(z))dzdy$.

Now consider the singular case $\gamma_0 = 0$. Then the approximation is simply $\phi_1 \equiv 0$. If $\gamma_1 = 0$, then the equation for the first moment is satisfied for any $c_1 \in \boldsymbol{R}$ and 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 we do not obtain a single heat kernel approximation ϕ_1 with the desirable convergence order $O(t^{(\frac{1}{2p}-\frac{3}{2})})$ 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

$$\begin{aligned} \rho_1 + \rho_2 \quad &= \gamma_0, \qquad & \rho_1c_1 + \rho_2c_2 &= \gamma_1,\\ \rho_1c_1^2 + \rho_2c_2^2 &= \gamma_2, \qquad & \rho_1c_1^3 + \rho_2c_2^3 &= \gamma_3. \end{aligned} \tag{4.2}$$

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

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

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

$$|\mathbf{A}| = \gamma_0\gamma_2 - \gamma_1^2.$$

If $|\mathbf{A}| \neq 0$, ψ_i's can be solved using 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

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

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

$$\lim_{t\to\infty} t^{\left(\frac{5}{2}-\frac{1}{2p}\right)}\|u(t) - \phi_2(t)\|_p \le \frac{\left\|\partial_\xi^4\left(e^{-\frac{1}{4}\xi^2}\right)\right\|_p}{\sqrt{4\pi}}\left|\int_{-\infty}^{\infty} E_4(x)dx\right|,\ 1 \le p \le \infty, \tag{4.6}$$

where $E_4(x)$ is the fourth order antiderivative of the initial error $E_0(x) := u_0(x) - \sum_{i=1}^{2}\rho_i\delta_{c_i}(x)$ given by (2.4).

Example 4.1. Consider an initial value

$$U_l(x) = \begin{cases} -1, & -2l - 0.5 < x < -l - 0.5,\ \ l + 0.5 < x < 2l + 0.5, \\ 1, & -l - 0.5 \le x \le l + 0.5, \\ 0, & \text{otherwise}, \end{cases} \tag{4.7}$$

where $l > 0$. Let $\gamma_{k,l}$ be the kth moments of the function $U_l(x)$, i.e.,

$$\gamma_{k,l} := \int x^k U_l(x)dx, \quad k = 0, 1, \ldots.$$

Then $\gamma_{0,l} = 1$ for all $l > 0$ and, since U_l is an even function, $\gamma_{k,l} = 0$ for $k = 1, 3, 5, \ldots$. Hence, $|A|$ and D in (4.4) are given by

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

One may easily check that $\gamma_{2,l} = 0$, if and only if

$$l = l_2 := 0.5\left(\sqrt[3]{2} - 1\right) / \left(2 - \sqrt[3]{2}\right),$$

and $D = 4(\gamma_{2,l})^3 > 0$, if and only if $l < l_2$. Hence, the moment problem (4.2) with the initial value $U_l(x)$ is solvable only for $l < l_2$. This example says that, even if the Hankel matrix is nonsingular, $\phi_2(x,t)$ that satisfies convergence order in (4.6) may not exist.

4.3. Approximation with three heat kernels. The derivation of (3.6) from (3.5) is not clear without some calculations. In the following, such a derivation is given for an example. For the case $n = 3$ the system (3.5) reads

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

Multiply c_1 to the kth equation and subtract $(k+1)$th one from it for $k = 1, \ldots, 5$ and obtain five 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:

$$\begin{aligned} 0 &= \gamma_0 c_1 c_2 c_3 - \gamma_1(c_1c_2 + c_2c_3 + c_3c_1) + \gamma_2(c_1 + c_2 + c_3) - \gamma_3, \\ 0 &= \gamma_1 c_1 c_2 c_3 - \gamma_2(c_1c_2 + c_2c_3 + c_3c_1) + \gamma_3(c_1 + c_2 + c_3) - \gamma_4, \\ 0 &= \gamma_2 c_1 c_2 c_3 - \gamma_3(c_1c_2 + c_2c_3 + c_3c_1) + \gamma_4(c_1 + c_2 + c_3) - \gamma_5, \end{aligned}$$

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 derivation is done for the case $n = 3$.

The determinant of the 3×3 Hankel matrix is given by

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

If $|\mathbf{A}| \neq 0$, then ψ_i are given by Cramer's rule:

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

The points c_i's are zeros of third order polynomial

$$g_3(x) = x^3 - \psi_2 x^2 - \psi_1 x - \psi_0. \tag{4.9}$$

Hence, 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:

$$\lim_{t\to\infty} t^{\left(\frac{7}{2}-\frac{1}{2p}\right)} \|u(t) - \phi_3(t)\|_p \le \frac{\left\|\partial_\xi^6 \left(e^{-\frac{1}{4}\xi^2}\right)\right\|_p}{\sqrt{4\pi}} \left|\int_{-\infty}^{\infty} E_6(x)dx\right|, \quad 1 \le p \le \infty, \tag{4.10}$$

where $E_6(x)$ is the sixth order antiderivative of the initial error $E_0(x) := u_0(x) - \sum_{i=1}^{3} \rho_i \delta_{c_i}(x)$ given by (2.4).

Consider the initial value given in Example 4.1. Since $\gamma_{1,l} = \gamma_{3,l} = \gamma_{5,l} = 0$ and $\gamma_{0,l} = 1$, we obtain

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

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 $\gamma_{4,l} > 0$ if and only if $0 < l < l_4 := 0.5(\sqrt[5]{2} - 1)/(2 - \sqrt[5]{2})$. Therefore, if $l_4 < l < l_2$, 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 values.

5. Approximation for sign-changing solutions. Now consider a general sign-changing initial value. First, consider the case that the initial value $u_0(x)$ decays for $|x|$ large with the order that the Gaussian has, i.e.,

$$u_0(x) = O\left(e^{-|x|^2}\right) \quad \text{as} \quad |x| \to \infty. \tag{5.1}$$

Then there exists $M > 0$ such that $v_0(x) := u_0(x) + \frac{M}{\sqrt{4\pi}} e^{-x^2/4} \ge 0$, and we may apply the theory in section 3 to the nonnegative function v_0. 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

$$u(x,t) \sim \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{-(x-c_i)^2/(4t)} - \frac{M}{\sqrt{4\pi(t+1)}} e^{-x^2/4(t+1)}. \tag{5.2}$$

Since the auxiliary part of the approximation is the exact solution with the extra initial value added to $u_0(x)$, the convergence order of this approximation is the same as the one in Theorem 3.1. 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, say, $c_i = \bar{c}_i$, 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 the Vandermonde matrix, i.e.,

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ \bar{c}_1 & \bar{c}_2 & \cdots & \bar{c}_n \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \bar{c}_1^{n-1} & \bar{c}_2^{n-1} & \cdots & \bar{c}_n^{n-1} \end{pmatrix} \begin{pmatrix} \rho_1 \\ \rho_2 \\ \cdot \\ \cdot \\ \cdot \\ \rho_n \end{pmatrix} = \begin{pmatrix} \gamma_0 \\ \gamma_1 \\ \cdot \\ \cdot \\ \cdot \\ \gamma_{n-1} \end{pmatrix}. \tag{5.3}$$

The Vandermonde determinant $\prod_{1\le i<j\le n}(\bar{c}_j - \bar{c}_i)$ is not zero if $\bar{c}_i$ are all different and, hence, (5.3) is solvable. Now construct a different kind of approximation:

$$\eta_n(x,t) := \sum_{i=1}^{n} \frac{\rho_i}{\sqrt{4\pi t}} e^{-(x-\bar{c}_i)^2/(4t)}. \tag{5.4}$$

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

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

since $\lim_{t\to 0}(\eta_n(x,t) - u_0(x))$ has zero moments up to $(n-1)$th order.

6. Convergence as $n \to \infty$ with fixed $t > 0$. In this section, we discuss the convergence of the approximation $\phi_n(x,t)$ to the solution $u(x,t)$ as $n \to \infty$ with a fixed $t > 0$. An interesting behavior of the approximation $\phi_n(x,t)$ that one may observe numerically is a geometric convergence order such as

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

where $v > 0$ depends on the initial value $u_0(x)$. (We do not have a proof of it. Hence, the statements here are rather conjectures.) This convergence order implies that the error decays to zero very fast as $n \to \infty$ for any fixed time $t > 0$. This convergence order is somewhat extreme. For example, if $t > v/4$, then the approximation error is reduced into half whenever just a single heat kernel is added.

Set the approximation error as

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

Consider a sequence of functions

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

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 E_k^n is related to the approximation $\phi_n(x,t)$ and the lower index k is to indicate that E_k^n is the kth order antiderivative of the initial approximation error $E_0^n(x)$. Then, from (2.6), one obtains

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

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

An interesting observation is that, for n large, $E_{2n}^n(x)$ has a Gaussian-like structure. The following has been observed numerically.

CONJECTURE 6.1. *Suppose that the initial value $u_0(x)$ is nonnegative and has finite moments up to any order. Then there exist $c \in \boldsymbol{R}$ and $v > 0$ such that*

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

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

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

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 C_{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 a natural conclusion if (6.3) is assumed. Furthermore, for $\xi = x/\sqrt{v}$,

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

Under Conjecture 6.1, the right-hand side of (6.2) can be approximated using $A(n, v/t)$ given by

$$\begin{aligned} \sup_x \left| \int D_y^{2n} \left(e^{-y^2/4} \right) \sqrt{t} E_{2n}^n \frac{\sqrt{t}(x-y)}{C_{2n}} dy \right| & \\ \cong \frac{\sqrt{t}}{\sqrt{v\pi}} \sup_x & \left| \int D_y^{2n} \left(e^{-y^2/4} \right) e^{-\frac{(x-y-c/\sqrt{t})^2}{v/t}} dy \right| \\ = \frac{\sqrt{t}}{\sqrt{v\pi}} & \left| \int D_y^{2n} \left(e^{-y^2/4} \right) e^{-\frac{y^2}{v/t}} dy \right| =: A(n, v/t). \end{aligned}$$

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

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

One can easily check that

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

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 another discussion about it will be included in section 7.2.

Remark 6.2. For $n > 0$ small, $E_{2n}^n(x)/C_{2n}$ is not close enough to the Gaussian and the arguments above do not apply. 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 cases, the corresponding $n > 0$ could be larger.

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 of the approximation $\phi_n(x,t)$. In the third one, we test the behavior of the alternative approach $\psi_{2n}(x,t)$ as $n \to \infty$. In the last one, 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 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 7.1 and 7.2). So we should employ enough precisions in the 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 $\|u(x,t) - \phi_n(x,t)\|_\infty$ accurately, we should obtain the exact value $u(x,t)$ or compute it with a smaller error than the actual approximation error. However, it seems impossible to do the integration in (1.1) numerically with such a small error. (In this sense, one may say that the approximation $\phi_n(x,t)$ is more exact than the exact formula in (1.1).) To avoid such a difficulty, we consider the following two examples with explicit solutions. In the following numerical tests we employ these examples.

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 illustrates 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 $var = 1 + 2t_0$.

Table 7.1

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 this and the following 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

Table 7.2

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 $t_0 = 1$. The ratio $\beta_n(t)$ converges to the limit in (6.1) quickly with $v = 2$ for Example 1 and slowly for Example 2.

	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

7.1. Numerical tests for the long time asymptotics. The approximation

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

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

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

In Table 7.1 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 measure the error in L^∞-norm in the following numerical examples and denote it by $\|\cdot\|$ in the tables to get it fitted in the tables.) From Table 7.1, one clearly observes that the convergence order $\alpha_n(t)$ approaches the optimal convergence order in (7.4) as $t \to \infty$. Notice that these numerical tests for $t \to \infty$ limits show similar patterns of the convergence for both Examples 7.1 and 7.2.

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 ratio

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

(The ratio $r = a_n/a_{n-1}$ is usually considered for a geometric sequence. Here we consider its reciprocal for easier comparison.) In Table 7.2, the error $\|e_n(t)\|_\infty$ and this ratio are computed for Examples 7.1 and 7.2 at two instances $t = 1$ and $t = 10$ with increasing n from $n = 2$ to $n = 25$. One can clearly observe a 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 cases, the corresponding v is $v = 2$ which is the variance of the initial value. The convergence pattern for Example 7.2 is 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 index v corresponding to the geometric convergence rate $\beta = 19.74$ is $v = 2.15$ and seems still decreasing. This value is already smaller than the variance of the initial value which is 3 and looks likely to converge to $v = 2$. It seems that the factor that decides the geometric convergence rate is not the variance but the tail of the initial value for $|x|$ large.

7.3. Approximation using derivatives of the Gaussian. We may write $\psi_{2n}(x,t)$ in (1.5) as

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

where $H_i(x)$ is the Hermite polynomial of degree i. In Table 7.3, the approximation error and the geometric convergence ratio β_n are given for Example 7.1. To make the relation between the initial value and the convergence ratio more clear, we set

$$\beta_{2n}(t,t_0) := \|e_{2n-2}(t)\|_\infty \Big/ \|e_{2n}(t)\|_\infty, \tag{7.7}$$

where $e_{2n}(x,t) = u(x,t) - \psi_{2n}(x,t)$ and $u_0(x) = K(x,t_0)$ with $t_0 = 10$.

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 a conjecture

$$\lim_{n\to\infty} \frac{\|u(t) - \psi_{2n}(t)\|_\infty}{\|u(t) - \psi_{2n+2}(t)\|_\infty} = \frac{t}{t_0}\ , \tag{7.8}$$

which indicates that the approximation error increases geometrically if $t < t_0$ and, hence, $\psi_{2n}(x,t)$ is meaningful for $t > t_0$ only. We may consider t_0 as the age of the initial value since $u_0(x) = K(x,t_0)$. This t_0 seems to be related to the time-shift t_* in [22]. Generally, one may call t_0 the age of a general initial value u_0 of the heat equation if $\lim_{n\to\infty} \frac{\|u(t_0)-\psi_{2n}(t_0)\|_\infty}{\|u(t_0)-\psi_{2n+2}(t_0)\|_\infty} = 1$.

Table 7.3

The error $e_n(x,t) = u(x,t) - \psi_{2n}(x,t)$ *and the geometric convergence rate* $\beta_n(t,t_0)$ *in* (7.7) *have been computed numerically for Example* 7.1 *with* $t_0 = 10$ *and* $t = 1, 10, 100$. *We may observe the convergence rate in* (7.8).

$2n$	$\|e_{2n}(1)\|$	$\beta_{2n}(1,10)$	$\|e_{2n}(10)\|$	$\beta_{2n}(10,10)$	$\|e_{2n}(100)\|$	$\beta_{2n}(100,10)$
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

Table 7.4

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* $v = 2t_0$.

	$\left\| \frac{1}{\sqrt{2t_0\pi}} e^{\frac{-x^2}{2t_0}} - \frac{1}{C_{2n}} E^n_{2n}(x) \right\|$		$\frac{C_{2n-2}}{C_{2n}} \frac{\left\| D_x^{2n-2} e^{-x^2/2t_0} \right\|}{\left\| D_x^{2n} e^{-x^2/2t_0} \right\|}$	
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

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. 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 7.4, 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 cases, we have taken $v = 2t_0$. The results for Example 7.1 show the convergence 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.

The columns for Example 7.2 also show similar convergence behavior. However, the speed of its convergence is 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, one may also try $2t_0 + 1$, which is the variance of Example 7.2. However, one cannot obtain the convergence, and $v = 2t_0$ seems a better choice. The computation is done up to $n = 10$ and that was our best. If computations with higher n are performed, we conjecture that the convergence to the unity will be more clearly observed.

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