Qualitative Properties of a Numerical Scheme for the Heat Equation

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Summary. In this paper we consider a classical finite difference approximation of the heat equation. We study the long time behaviour of the solutions of the considered scheme and various questions related to the fundamental solutions. Finally we obtain the first term in the asymptotic expansion of the solutions.

1 Introduction

The main goal of this paper is the study of the long time behaviour of classical finite difference approximations of the heat equation.

Let us consider the linear heat equation on the whole space

$$\begin{cases} u_t - \Delta u = 0 \ \text{ in } \mathbf{R}^d \times (0,\infty), \\ u(0,x) = \varphi(x) \text{ in } \mathbf{R}^d. \end{cases}$$

By means of Fourier's transform, solutions can be represented as the convolutions between the fundamental solutions and the initial data:

$$u(t) = G(t,\cdot) * \varphi,$$

where

$$G(t,x) = \frac{1}{(4\pi t)^{-d/2}} \mathrm{e}^{-\frac{|x|^2}{4t}} = \frac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \mathrm{e}^{\mathrm{i}x\cdot\xi} \mathrm{e}^{-|\xi|^2 t} \mathrm{d}\xi.$$

The smoothing effect of the fundamental solutions $G(t,x)$ yields to the following behaviour of the solution (cf. [3], Ch. 3, p. 44):

$$\|u(t)\|_{L^p(\mathbf{R}^d)} \le C(p,q)\, t^{-d/2\,(1/q-1/p)} \|\varphi\|_{L^q(\mathbf{R}^d)}, \quad t>0,\ p \ge q. \tag{1}$$

A finer analysis is given in [4], where the authors consider initial data which decay polynomially at infinity. Duoandikoetxea & Zuazua [4] study how the mass of the solution is distributed as $t \to \infty$. They prove the existence of a positive constant $c = c(p,q,d)$ such that for any q and p satisfying $1 \le q < d/(d-1)$, $d \ge 2$ ($1 \le q < \infty$ for $d=1$), $q \le p < \infty$,

$$\left\| u(t,\cdot) - \left(\int_{\mathbf{R}^d} \varphi(x)\mathrm{d}x \right) G(t,\cdot) \right\|_{L^p(\mathbf{R}^d)} \le c\, t^{-\frac{1}{2}-\frac{d}{2}(\frac{1}{q}-\frac{1}{p})} \| |x|\varphi \|_{L^q(\mathbf{R}^d)} \tag{2}$$

holds for all $t > 0$ and $\varphi \in L^1(\mathbf{R}^d)$ with $|x|\varphi(x) \in L^q(\mathbf{R}^d)$.

Let us consider the classical finite-difference scheme:

$$\begin{cases} \dfrac{du^h}{dt} = \Delta_h u^h,\ t > 0, \\ \\ u^h(0) = \varphi^h. \end{cases} \tag{3}$$

Here u^h stands for the infinite unknown vector $\{u^h_{\mathbf{j}}\}_{\mathbf{j}\in\mathbf{Z}^d}$, $u^h_{\mathbf{j}}(t)$ being the approximation of the solution u at the node $x_{\mathbf{j}} = \mathbf{j}h$, and Δ_h is the classical second order finite difference approximation of Δ:

$$(\Delta_h u^h)_{\mathbf{j}} = \frac{1}{h^2}\sum_{k=1}^{d}(u^h_{\mathbf{j}+e_k} + u^h_{\mathbf{j}-e_k} - 2u^h_{\mathbf{j}}).$$

This scheme is widely used and satisfies the classical properties of consistency and stability which imply L^2-convergence (cf. [7], Ch. 13, p. 292).

It is interesting to know whenever the properties of the continuous problem are preserved by the numerical scheme. In the following we are concerned with the spatial shape of the discrete solution for large times. To do that we introduce the spaces $l^p(h\mathbf{Z}^d)$:

$$l^p(h\mathbf{Z}^d) = \left\{ \{u_{\mathbf{j}}\}_{\mathbf{j}\in\mathbf{Z}^d} : \|u\|^p_{l^p(h\mathbf{Z}^d)} = h^d \sum_{\mathbf{j}\in\mathbf{Z}^d} |u_{\mathbf{j}}|^p < \infty \right\}$$

and study the behaviour of $l^p(h\mathbf{Z}^d)$-norms of the solutions as $t \to \infty$.

The main tool in our analysis is the semi-discrete Fourier transform (SDFT):

$$\widehat{u}(\xi) = h^d \sum_{\mathbf{j}\in\mathbf{Z}^d} \mathrm{e}^{-\mathrm{i}\mathbf{j}\cdot\xi h}\, u_{\mathbf{j}}\,,\ \xi \in \left[-\frac{\pi}{h}, \frac{\pi}{h}\right]^d$$

and its inverse

$$u_{\mathbf{j}} = \frac{1}{(2\pi)^d}\int_{[-\pi/h,\pi/h]^d} \widehat{u}(\xi)\mathrm{e}^{\mathrm{i}\mathbf{j}\cdot\xi h}\mathrm{d}\xi,\ \mathbf{j} \in \mathbf{Z}^d.$$

We refer to [5] and [10] for a survey on this subject. By means of SDFT we compute the solutions of equation (3) in a similar way as in the continuous case, writing them as a convolution of a fundamental solution $K^{d,h}_t$ and the initial datum. This allows us to obtain decay rates of the solution in different $l^q - l^p$ norms analogous to (1). All the estimates are uniform with respect to the step size, h. This proves a kind of $l^q - l^p$ stability of our scheme:

Theorem 1. *Let $1 \leq q \leq p \leq \infty$. Then there exists a positive constant $c(p,q,d)$ such that*

$$\|u^h(t)\|_{l^p(h\mathbf{Z}^d)} \leq c(p,q,d)\, t^{-d/2\,(1/q-1/p)} \|\varphi^h\|_{l^q(h\mathbf{Z}^d)}$$

for all $t > 0$, uniformly in $h > 0$.

A similar approach in the case of the transport equation has been studied by Brenner and Thomée [2] and Trefethen [11]. They introduce a finite difference approximation and give conditions which guarantee the l^p-stability of the scheme.

Next we prove that the fundamental solutions $K_t^{d,h}$ of equation (3) are related to the modified Bessel function $I_\nu(x)$:

$$(K_t^{d,h})_{\mathbf{j}} = \left(\frac{\exp(-\frac{2t}{h^2})}{\pi h}\right)^d \prod_{k=1}^{d} I_{j_k}\left(\frac{2t}{h^2}\right),\ \mathbf{j} = (j_1, j_2, \ldots, j_d) \in \mathbf{Z}^d. \quad (4)$$

This property proves the positivity and various properties regarding the monotonicity of the discrete kernel $K_t^{d,h}$.

Finally, we consider the weighted space $l^1(h\mathbf{Z}^d, |x|)$ and obtain the first term in the asymptotic expansion of the discrete solution. The weighted spaces $l^p(h\mathbf{Z}^d, |x|)$, $1 \leq p < \infty$ are defined as follows:

$$l^p(h\mathbf{Z}^d, |x|) = \Big\{ \{u_{\mathbf{j}}\}_{\mathbf{j}\in\mathbf{Z}^d} : \|u\|^p_{l^p(h\mathbf{Z}^d,|x|)} = h^d \sum_{\mathbf{j}\in\mathbf{Z}^d} |u_{\mathbf{j}}|^p |\mathbf{j}h|^p < \infty \Big\}.$$

The following theorem gives us the first term of the asymptotic expansion of the solution u^h:

Theorem 2. *Let $p \geq 1$. Then there exists a positive constant $c(p,d)$ such that*

$$\left\| u^h(t) - \left(h \sum_{\mathbf{j}\in\mathbf{Z}^d} \varphi^h_{\mathbf{j}} \right) K_t^{d,h} \right\|_{l^p(h\mathbf{Z}^d)} \leq c(p,d)\, t^{-1/2-d/2\,(1-1/p)} \|\varphi^h\|_{l^1(h\mathbf{Z}^d,|x|)}$$

for all $\varphi^h \in l^1(h\mathbf{Z}^d, |x|)$ and $t > 0$, uniformly in $h > 0$.

This shows that for t large enough the solution behaves as the fundamental solution. In contrast with (2) our result is valid only for the initial data in the weighted space $l^1(h\mathbf{Z}, |x|)$. The extension of this result to general initial data, i.e. in $l^q(h\mathbf{Z}, |x|)$, $1 < q < p$, remains an open problem. In [6] we consider the first $k \geq 1$ terms of the asymptotic expansion of the discrete solution and obtain a similar result.

2 Proof of the Results

By means of SDFT we obtain that $\widehat{u}^h$ satisfies the following ODE:

$$\frac{d\widehat{u}^h}{dt}(t,\xi)=-\frac{4}{h^2}\sum_{k=1}^{d}\sin^2\left(\frac{\xi_k h}{2}\right)\widehat{u}^h(t,\xi),\ t>0,\ \xi\in\left[-\frac{\pi}{h},\frac{\pi}{h}\right]^d.$$

In the Fourier space, the solution $\widehat{u}^h$ reads

$$\widehat{u}^h(t,\xi)=\mathrm{e}^{-tp_h(\xi)}\widehat{\varphi}^h(\xi),\ \xi\in\left[-\frac{\pi}{h},\frac{\pi}{h}\right]^d,$$

where the function $p_h:[-\pi/h,\pi/h]^d\to\mathbf{R}$ is given by

$$p_h(\xi)=\frac{4}{h^2}\sum_{k=1}^{d}\sin^2\left(\frac{\xi_k h}{2}\right). \tag{5}$$

The solution of equation (3) is given by a discrete convolution between the fundamental solution $K_t^{d,h}$ and the initial datum:

$$u^h(t)=K_t^{d,h}*\varphi^h.$$

The inverse SDFT of the function $\mathrm{e}^{-tp_h(\xi)}$ gives us the following representation of the fundamental solution $K_t^{d,h}$:

$$(K_t^{d,h})_{\mathbf{j}}=\frac{1}{(2\pi)^d}\int_{[-\pi/h,\pi/h]^d}\mathrm{e}^{-tp_h(\xi)}\mathrm{e}^{\mathrm{i}\mathbf{j}\cdot\xi h}\mathrm{d}\xi,\ \mathbf{j}\in\mathbf{Z}^d.$$

We point out that for any $\mathbf{j}=(j_1,j_2,\dots,j_d)\in\mathbf{Z}^d$ the kernel $K_t^{d,h}$ can be written as the product of one-dimensional kernels $K_t^{1,h}$:

$$(K_t^{d,h})_{\mathbf{j}}=\prod_{k=1}^{d}(K_t^{1,h})_{j_k}. \tag{6}$$

A simple change of variables in the explicit formula of $K_t^{1,h}$ relates it with the modified Bessel functions:

$$(K_t^h)_j=\frac{\exp(-\frac{2t}{h^2})}{\pi h}I_j\left(\frac{2t}{h^2}\right),\ j\in\mathbf{Z}.$$

Separation of variables formula (6) proves (4). We recall that the modified Bessel's function $I_\nu(x)$ is positive for any positive x. Also for a fixed x, the map $\nu\to I_\nu(x)$ is even and decreasing on $[0,\infty)$ (cf. [8], Ch. II, p. 60). These properties prove that the kernel $K_t^{d,h}$ has the following properties:

Theorem 3. *Let $t>0$ and $h>0$. Then*
i) For any $\mathbf{j}=(j_1,j_2,\dots,j_d)\in\mathbf{Z}^d$

$$(K_t^{d,h})_{\mathbf{j}}=\left(\frac{\exp(-\frac{2t}{h^2})}{\pi h}\right)^d\prod_{k=1}^{d}I_{j_k}\left(\frac{2t}{h^2}\right).$$

ii) For any $\mathbf{j} \in \mathbf{Z}^d$*, the kernel* $(K_t^{d,h})_{\mathbf{j}}$ *is positive.*
iii) The map $j \in \mathbf{Z} \mapsto (K_t^{1,h})_j$ *is increasing for* $j \leq 0$ *and decreasing for* $j \geq 0$*.*
iv) For any $\mathbf{a} = (a_1, a_2, \dots, a_d) \in \mathbf{Z}^d$ *and* $\mathbf{b} = (b_1, b_2, \dots, b_d) \in \mathbf{Z}^d$ *satisfying*

$$|a_1| \leq |b_1|, |a_2| \leq |b_2|, \dots, |a_d| \leq |b_d|,$$

the following holds

$$(K_t^{d,h})_{\mathbf{b}} \leq (K_t^{d,h})_{\mathbf{a}}.$$

The long time behaviour of the kernel $K_t^{d,h}$ is similar to the one of its continuous counterpart.

Theorem 4. *Let* $p \in [1, \infty]$*. Then there exists a positive constant* $c(p,d)$ *such that*

$$\|K_t^{d,h}\|_{l^p(h\mathbf{Z}^d)} \leq c(p,d)\, t^{-d/2\,(1-1/p)} \tag{7}$$

holds for all positive times t*, uniformly on* $h > 0$*.*

Once Theorem 4 is proved, Young's inequality provides the decay rates of the solutions of equation (3) as stated in Theorem 1.

Proof (of Theorem 4). A scaling argument shows that $(K_t^{d,h})_{\mathbf{j}} = (K_{t/h^2}^{d,1})_{\mathbf{j}}$, reducing the proof to the case $h = 1$.

In the sequel we consider the band limited interpolator of the sequence $K_t^{d,1}$ (cf. [12], Ch. I, p. 13):

$$K_*^d(t,x) = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{e}^{\mathrm{i}x\cdot\xi} \mathrm{e}^{-tp_1(\xi)} \mathrm{d}\xi. \tag{8}$$

In [9] the authors prove the existence of a positive constant A such that for any function f with its Fourier transform supported in the cube $[-\pi,\pi]^d$ the following holds:

$$\sum_{\mathbf{j}\in\mathbf{Z}^d} |f(\mathbf{j})|^p \leq A^d \int_{\mathbf{R}^d} |f(x)|^p \mathrm{d}x,\ p \geq 1. \tag{9}$$

This reduces (7) to similar estimates on the $L^p(\mathbf{R}^d)$-norm of K_*^d. The interpolator K_*^d satisfies

$$\|D^\alpha K_*^d(t,\cdot)\|_{L^p(\mathbf{R})} \leq c(\alpha,p,d)\, t^{-|\alpha|/2-d/2\,(1-1/p)} \tag{10}$$

for any multiindex $\alpha = (\alpha_1, \dots, \alpha_d)$ and $1 \leq p \leq \infty$. Using (5) and (8), we reduce (10) to the one dimensional case. We consider the cases $p = 1$ and $p = \infty$. The general case, $1 < p < \infty$, follows by the Hölder inequality. The case $p = \infty$ easily follows by the rough estimate:

$$\|D^\alpha K_*^1(t,\cdot)\|_{L^\infty(\mathbf{R}^d)} \leq \frac{1}{2\pi} \int_{-\pi}^{\pi} |\xi|^\alpha \exp\left(-4t\sin^2\frac{\xi}{2}\right) \mathrm{d}\xi \leq c(\alpha)\, t^{-(\alpha+1)/2}.$$

Finally, we apply Carlson-Beurling's inequality (cf. [1] and [2]):

$$\|\widehat{a}\|_{L^1(\mathbf{R})} \leq (2\|a\|_{L^2(\mathbf{R})}\|a'\|_{L^2(\mathbf{R})})^{1/2}$$

to the function $a(\xi) = |\xi|^\alpha \exp(-4t\sin^2\xi/2)$. We obtain the existence of a positive constant C such that for all $t>0$,

$$\|K^1_*(t)\|_{L^1(\mathbf{R})} \leq C.$$

This proves Theorem 4. □

Now we sketch the proof of Theorem 2.

Proof (of Theorem 2). First, a scaling argument reduces the proof to the case $h=1$. We consider the cases $p=1$ and $p=\infty$, the other cases follow by interpolation. The solution $u^1(t)$ of equation (3) is given by:

$$u^1_{\mathbf{j}}(t) = (K^{d,1}_t * \varphi^1)_{\mathbf{j}} = \sum_{\mathbf{n}\in\mathbf{Z}^d} (K^{d,1}_t)_{\mathbf{j}-\mathbf{n}}\varphi^1_{\mathbf{n}}.$$

Let us introduce the sequence $\{a_{\mathbf{j}}(t)\}_{\mathbf{j}\in\mathbf{Z}^d}$ as follows

$$\begin{aligned} a_{\mathbf{j}}(t) &= \Big(u^1(t) - K^{d,1}_t \sum_{\mathbf{n}\in\mathbf{Z}^d}\varphi^1_{\mathbf{n}}\Big)_{\mathbf{j}} = u^1_{\mathbf{j}}(t) - (K^{d,1}_t)_{\mathbf{j}} \sum_{\mathbf{n}\in\mathbf{Z}^d}\varphi^1_{\mathbf{n}} \\ &= \sum_{\mathbf{n}\in\mathbf{Z}^d}(K^{d,1}_t)_{\mathbf{j}-\mathbf{n}}\varphi^1_{\mathbf{n}} - (K^{d,1}_t)_{\mathbf{j}}\sum_{\mathbf{n}\in\mathbf{Z}^d}\varphi^1_{\mathbf{n}} \\ &= \sum_{\mathbf{n}\in\mathbf{Z}^d}\varphi^1_{\mathbf{n}}\Big((K^{d,1}_t)_{\mathbf{j}-\mathbf{n}} - (K^{d,1}_t)_{\mathbf{j}}\Big). \end{aligned}$$

In the sequel we denote by c a constant that may change from one line to another. It remains to prove that

$$\sup_{\mathbf{j}\in\mathbf{Z}^d}|a_{\mathbf{j}}(t)| \leq c\,t^{-(d+1)/2}\,\|\varphi^1\|_{l^1(\mathbf{Z}^d,|x|)} \tag{11}$$

and

$$\sum_{\mathbf{j}\in\mathbf{Z}^d}|a_{\mathbf{j}}(t)| \leq c\,t^{-1/2}\,\|\varphi^1\|_{l^1(\mathbf{Z}^d,|x|)}.$$

The Taylor formula applied to the function K^d_* gives us

$$K^d_*(t,\mathbf{j}-\mathbf{n}) - K^d_*(t,\mathbf{j}) = \int_0^1 \sum_{|\alpha|=1} D^\alpha K^d_*(t,\mathbf{j}-s\mathbf{n})(-\mathbf{n})^\alpha \mathrm{d}s.$$

As a consequence, for any $\mathbf{j}\in\mathbf{Z}^d$ the sequence $a_{\mathbf{j}}(t)$ satisfies

$$\begin{aligned}|a_{\mathbf{j}}(t)| &\leq \sum_{\mathbf{n}\in\mathbf{Z}^d} |\varphi^1_{\mathbf{n}}| \sum_{|\alpha|=1} \int_0^1 |\mathbf{n}^\alpha||D^\alpha K^d_*(t,\mathbf{j}-s\mathbf{n})|\mathrm{d}s \\ &\leq c \sum_{\mathbf{n}\in\mathbf{Z}^d} |\varphi^1_{\mathbf{n}}||\mathbf{n}| \sum_{|\alpha|=1} \int_0^1 |D^\alpha K^d_*(t,\mathbf{j}-s\mathbf{n})|\mathrm{d}s \\ &= c \sum_{\mathbf{n}\in\mathbf{Z}^d} |\varphi^1_{\mathbf{n}}||\mathbf{n}| \sum_{|\alpha|=1} b^\alpha_{\mathbf{j},\mathbf{n}}(t). \end{aligned} \tag{12}$$

To prove inequality (11), which corresponds to $p=\infty$, it is sufficient to show that

$$b^\alpha_{\mathbf{j},\mathbf{n}}(t) \leq c\,t^{-(d+1)/2}$$

for all indices α with $|\alpha|=1$. Inequality (10) shows that

$$b^\alpha_{\mathbf{j},\mathbf{n}}(t) \leq \|D^\alpha K^d_*(t)\|_{L^\infty(\mathbf{R}^d)} \leq c\,t^{-|\alpha|/2-d/2} = c\,t^{-(d+1)/2}.$$

Now let us consider the case $p=1$. We sum on $\mathbf{j}\in\mathbf{Z}^d$ in inequality (12) and obtain:

$$\begin{aligned}\sum_{\mathbf{j}\in\mathbf{Z}^d} |a_{\mathbf{j}}(t)| &\leq \sum_{\mathbf{j}\in\mathbf{Z}^d}\sum_{\mathbf{n}\in\mathbf{Z}^d} |\varphi^1_{\mathbf{n}}||\mathbf{n}| \sum_{|\alpha|=1} b^\alpha_{\mathbf{j},\mathbf{n}}(t) \\ &= \sum_{\mathbf{n}\in\mathbf{Z}^d} |\varphi^1_{\mathbf{n}}||\mathbf{n}| \sum_{|\alpha|=1}\sum_{\mathbf{j}\in\mathbf{Z}^d} b^\alpha_{\mathbf{j},\mathbf{n}}(t).\end{aligned}$$

It remains to prove that

$$\sum_{\mathbf{j}\in\mathbf{Z}^d} b^\alpha_{\mathbf{j},\mathbf{n}}(t) \leq c\,t^{-1/2} \tag{13}$$

for all $\mathbf{n}\in\mathbf{Z}^d$ and for any multiindex α with $|\alpha|=1$. Using the separation of variables, we get for all $\mathbf{j}=(j_1,\ldots,j_d)\in\mathbf{Z}^d$ and $\mathbf{n}=(n_1,\ldots,n_d)\in\mathbf{Z}^d$,

$$b^\alpha_{\mathbf{j},\mathbf{n}}(t) = \int_0^1 \prod_{k=1}^d |D^\alpha K^1_*(t,j_k-sn_k)|\mathrm{d}s$$

and hence,

$$\begin{aligned}\sum_{\mathbf{j}\in\mathbf{Z}^d} b^\alpha_{\mathbf{j},\mathbf{n}}(t) &= \int_0^1 \prod_{k=1}^d \left(\sum_{j_k\in\mathbf{Z}} |D^{\alpha_k} K^1_*(t,j_k-sn_k)|\right)\mathrm{d}s \\ &\leq \sup_{s\in\mathbf{R}} \prod_{k=1}^d \left(\sum_{j_k\in\mathbf{Z}} |D^{\alpha_k} K^1_*(t,j_k-s)|\right).\end{aligned}$$

We prove that each term in the last product is dominated by $t^{-\alpha_k/2}$ and consequently the product will be bounded by $t^{-|\alpha|/2}$. Applying (9) to the function $K^1_*(t,\cdot-s)$, each of the above sum satisfies

$$\sum_{j_k \in \mathbf{Z}} |D^{\alpha_k} K^1_*(t, j_k - s)| \leq c \int_{\mathbf{R}} |D^{\alpha_k} K^1_*(t, x - s)| \mathrm{d}x$$
$$= c \int_{\mathbf{R}} |D^{\alpha_k} K^{1,1}_*(t, x)| \mathrm{d}x \leq c\, t^{-|\alpha_k|/2}.$$

This proves inequality (13) and finishes the proof of Theorem 2. □

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