VARIABLE TIME STEPS OPTIMIZATION OF L_ω STABLE CRANK-NICOLSON METHOD.

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Abstract. We study the optimization of Crank-Nicolson method, also known as Euler second order trapezoidal rule [4] for ordinary differential equations. The Crank-Nicolson method for the numerical integration of the first order ordinary differential equations is A stable, but it is not L stable. This means that the stability region coincides exactly with negative half-plane $z : \Re z \leq 0$, but the stability function $|R(z)|$ tends to 1 rather than zero as $\Re z \to -\infty$. This causes unexpected oscillatory behavior of the numerical solution of stiff differential equations. In order to avoid this problem, we optimize the stability property of the stability function. Variable steps within the sequence of steps by Crank-Nicolson method allow us to obtain different stability functions and formulate optimization problem for roots and poles of the stability function. The optimal solution of this problem is the classical rational Zolotarev function. The appropriate selection the sequence of step-sizes eliminates oscillatory behavior of the numerical solution.

Key words. rational functions, ordinary differential equations, Crank-Nicolson, Zolotarev problem

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1. Introduction. We consider Crank-Nicolson method, also known as Euler second order trapezoidal rule [4], for solving stiff ordinary differential equations, which may arize as the result of descretization of parabolis partial differential equation. Under appropriate smoothness assumptions, the Crank-Nicolson method has second order accuracy. But for stiff ordinary differential equations, the numerical solution can be very different from the solution of the exact problem. We demonstrate this with the example of heat equation,

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2}, \\ u(x,0) &= u^0(x), \\ u(0,t) &= u(1,t) = 0, \end{aligned} \tag{1.1}$$

where $x \in [0,1]$ and $t > 0$.

The exact solution of this problem can be found by the method of separation of variables [15] as,

$$\begin{aligned} u(x,t) &= \sum_{k=1}^{\infty} c_k e^{-\lambda_k t} \varphi_k(x), \\ \varphi_k(x) &= \sqrt{2} \sin \pi k x, \end{aligned} \tag{1.2}$$

where

$$\lambda_k = k^2 \pi^2,$$

$$c_k = (u^0(x), \varphi_k(x))_{L_2} = \int_0^1 u^0(x) \varphi_k(x) dx$$

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$$||u(x,t)||_{L_2}^2 = \sum_{k=1}^{\infty} c_k^2 e^{-2\lambda_k t}.$$

Because eigenfunctions are normalized $||\varphi_k(x)||_{L_2} = 1$, we can obtain a bound on the L_2 norm of the solution

$$||u(x,t)||_{L_2}^2 \le e^{-2\lambda_1 t} \sum_{k=1}^{\infty} c_k^2 = e^{-2\lambda_1 t} ||u^0(x)||_{L_2}^2,$$

or

$$||u(x,t)||_{L_2} \le e^{-\lambda_1 t} ||u^0(x)||_{L_2}, \tag{1.3}$$

for any $t \ge 0$. Because $\lambda_{k+1} > \lambda_k$ the harmonics corresponding to larger k decreases faster. Thus for sufficiently large t we can make the approximation

$$u(x,t) \approx c_1 e^{-\lambda_1 t} \varphi_1(x), \quad c_1 \ne 0, \tag{1.4}$$

for sufficiently large t. In order to approximate (1.1) we use method of lines with uniform grid $\Delta x = 1/(n+1)$. We divide the interval $[0,1]$ by n points $\{x_i\}_1^n$ and use method of lines [8] to approximate heat equation. Now the values $u_i, \quad i = 1, \dots, n$ are solutions of semidiscretization of the heat equation (1.1) at points $x_i = i\Delta x, \quad i = 1, \dots, n$, which satisfy system of n ordinaty diferential equations

$$\frac{du_i}{dt} = (u_{i+1} - 2u_i + u_{i-1})/\Delta x^2, i = 1, \dots, n. \tag{1.5}$$

This is homogeneous system of linear ordinary differential equations

$$\frac{du}{dt} = -Au, \quad u(t_0) = u^0,$$

where A is $n \times n$ three diagonal matrix with elements $a_{i,i\pm1} = -1/\Delta x^2$ and $a_{i,i} = 2/\Delta x^2$. The matrix A has complete set of eigen vectors and eigen values

$$\begin{aligned}
\lambda_k^{\Delta x} &= \frac{4}{\Delta x^2} \sin^2 \frac{\pi \Delta x k}{2}, \\
(\varphi_k^{\Delta x})_i &= \sqrt{2} \sin \pi k x_i, \\
c_k^{\Delta x} &= (y^0, \varphi_k^{\Delta x}), \\
(y, v) &= \sum_{k=1}^{n} y_i v_i \Delta x, \\
||y|| &= \sqrt{(y,y)}.
\end{aligned}$$

We use superscript Δx in order to indicate that eigenvectors, $\varphi_k^{\Delta x}$, and eigenvalues, $\lambda_k^{\Delta x}$, of the matrix A analogue of eigenvectors and eigenvalues of the differential problem (1.1) obtained by finite difference approximation with spatial step Δx. We can use the method of separation of variables in order to find solution of the equation (1.5)

$$u_i(t) = \sum_{k=1}^{n} c_k e^{\lambda_k^{\Delta x} t} \varphi_k^{\Delta x}. \tag{1.6}$$

The eigen values λ_k have the following properties

$$\lambda_k^{\Delta x} + \lambda_{n+1-k}^{\Delta x} = \frac{4}{\Delta x^2}.$$

If $k > [(m+1)/2]$ the value $\Delta_k = \lambda_k^{\Delta x} - \lambda_{k-1}^{\Delta x} = \lambda_{n+2-k}^{\Delta x} - \lambda_{n+1-k}^{\Delta x}$ is decreasing when k is increasing. Consequently, $\lambda_k^{\Delta x}$ are not grownig like eigen values of exact solution of PDE $\pi^2 k^2$ for the large k, but we observe fast decreasing of the rate of grows of $\lambda_k^{\Delta x}$. It means that $\lambda_k^{\Delta x}$ are not approximating $\pi^2 k^2$ anymore and, as time grows, the appropriate terms in expantion of the numerical solution becomes unrealisticly large and they can be considered as gurbage.

In order to reduce an influence of these terms we use special sequence of Crank-Nicolson steps. Let us consider one step of of Crank-Nicolson method for solution of semidiscret problem

$$\frac{y^{j+1} - y^j}{\tau} = -A\frac{y^{j+1} + y^j}{2}, \qquad (1.7)$$
$$y_i^0 = u^0(x_i), \quad i = 1, \ldots, n$$

where y^j is a vector with components $\{y_i^j\}_{i=1}^n$ is the numerical solution of the problem (1.5) after time step j at the point x_i: $y_i^j \approx u(x_i, t_j)$. We can use the method of separation of variables in order to find solution of the numerical scheme [8]

$$y^j = \sum_{k=1}^{n} c_k q_k^j \varphi_k^{\Delta x}, \qquad (1.8)$$

where

$$q_k = \frac{1 - 0.5\tau\lambda_k^{\Delta x}}{1 + 0.5\tau\lambda_k^{\Delta x}}.$$

Using the fact of ortho-normality of eigenvectors $(\varphi_k^{\Delta x}, \varphi_l^{\Delta x}) = \delta_{kl}$,

$$||y^j||^2 = \sum_{k=1}^{n} c_k^2 q_k^{2j} \le \rho^{2j}||y^0||^2,$$

or

$$||y^j|| \le \rho^j ||y^0||, \qquad (1.9)$$

where $\rho = \max_{1 \le k \le n} |q_k|$.

Formally Crank-Nicolson method has second order accuracy if τ approaches to zero. But we want to analyze the solution for realistic values τ typically used for numerical computations. Properties similar to (1.3) and (1.4) for numerical solution have the form

$$y^j = y(x_i, t_j) \approx c_1 q_1^j \varphi_1^{\Delta x}, \quad c_1 \ne 0. \qquad (1.10)$$

Because q_k is a decreasing sequence, the condition (1.10) can be satisfied if $|q_1| > |q_n|$. For example if

$$\tau < \tau_0 = \frac{2}{\sqrt{\gamma_1 M}}, \qquad (1.11)$$

where γ_1 and M maximum and minimum eigenvalues of the matrix A. In the example of the semidiscrete heat equation (1.5) the step $\tau_0 \approx \frac{\Delta x}{\pi}$. We call this an asymptotically stable numerical scheme. This problem have been widely discussed in literature e.g. [12, 3, 5].

If condition (1.11) is not satisfied, the numerical solution can be destroyed by modes corresponding large k.

Because q_k is approximately -1 for sufficientlt large τ and k the Crank-Nicolson method increases relative fraction of garbage components, especially for nonlinear problems. This circumstance can change solution dramatically for $t \to \infty$, and that is why we choose special sequence of steps to remove garbage components rather than approximate them.

The difference between the numerical and the exact solution is shown in Fig. 5.1 (c). Variable time steps [10, 9, 14, 13, 1] allow to improve stability of the explicit methods. In this article we propose the algorithm which uses Crank-Nicolson method with variable time steps. The special choice of the sequence of steps increases the average step size of the Crank-Nicolson method while preserving the property of asymptotical stability (1.3), (1.4).

2. Crank-Nicolson method for nonlinear equations. We analyze numerical solution of the system of ordinary differential equations

$$\frac{dy}{dt} = f(y,t), \tag{2.1}$$

where y and $f(y,t)$ are vectors of the length n. We define one step of the numerical method as a result of m steps of the Chrank-Nicolson method. The total step size, which is the sum of steps of each individual method is $\tau = \sum_{i=1}^{m} h_i$. The composition of these steps can be considered as a composition Runge-Kutta method

$$\begin{aligned} v^0 &= y^0, \\ v^{j+1} &= v^j + h_{j+1} f\left(\sum_{k=1}^{j} h_k + \tfrac{h_{j+1}}{2}, \tfrac{v^{j+1}+v^j}{2}\right), \quad j = 0, \ldots, m-1 \\ y^1 &= v^m, \quad t^1 = t^0 + \tau. \end{aligned} \tag{2.2}$$

We mainly restrict our consideration to the case of functions $f(y,t)$ with the Jacobian

$$J(x_1, \ldots, x_n) = \begin{bmatrix} \frac{\partial f_1(y,t)}{\partial y^1} & \cdots & \frac{\partial f_1(y,t)}{\partial y_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_n(y,t)}{\partial y_1} & \cdots & \frac{\partial f_n(y,t)}{\partial y_n} \end{bmatrix}$$

satisfying the following conditions:

1. $J(u,t)$ has set of eigenvectors $\{\varphi_i(t)\}_1^n$ and eigenvalues $\{\lambda_i(t)\}_1^n$ for all t, which form complete basis in R^n,
2. the eigenvalues are real $\lambda_i = \Re\lambda_i$,
3. the solutions of two equations

$$\begin{aligned} \frac{dy}{dt} &= f(y,t), \\ \frac{dz}{dt} &= f(y^n,t^n) + J(y^n,t^n)(z - y^n), \end{aligned} \tag{2.3}$$

satisfy $||y(t) - z(t)|| < C\tau^3$ uniformly for $t \in [t^n, t^{n+1}]$. Here C is a constant, independent of t, and $||y(t)|| = \max_{1<i<n} \max_{t^j<t<t^{j+1}} |y_i(t)|$.

In order to prove second order accuracy of the methods (2.2) we use the theorem which gives us an estimation of the global error of the numerical method after m steps ([4], II.3 pp.160-161)

THEOREM 2.1. *Let U be a neighborhood $\{(t, y(t))|t_0 \le t \le t_1\}$ where $y(t)$ is the exact solution of the (2.1). Suppose that in U*

$$||\frac{\partial f}{\partial y}|| \le L \ or \ \mu(\frac{\partial f}{\partial y}) \le L,$$

where μ is logarithmic norm and that the local error estimates $||e_i|| \le Ch_i^{p+1}$ are valid in U. Then the global error can be estimated by

$$||E|| \le h^p \frac{C'}{L}(\exp(L(t_1 - t_0))),$$

where $h = \max h_i$,

$$C' = \begin{cases} C, & if \quad \Lambda \ge 0, \\ C\exp(\Lambda h), & if \quad L < 0. \end{cases},$$

and h is small enough for the numerical solution to remain in U. For $L \to 0$ the estimate tends to $h^p C(t_1 - t_0)$

Because the method (2.2) is just a sequence of steps of Crank-Nicolson method with $p = 2$ and $h \le \tau = (t_1 - t_0)$ the error estimate becomes $||E|| \le C\tau^3$, which proves the following theorem.

THEOREM 2.2. *Suppose that ordinary differential equation 2.1 satisfies conditions from the previous theorem, then the method (2.2) has second order accuracy*

$$||y(t_1) - y_1|| \le C\tau^3,$$

where $\tau = \sum_{i=1}^{m} h_i$.

In order to formulate optimization problem, we use linear stability analysis. We consider homogeneous system of linear ordinary differential equations

$$\frac{du}{dt} = -Au, \quad u(t_0) = u^0, \tag{2.4}$$

where the matrix A is the Jacobian $-J(y^n, t^n)$. We use the fact that the linearized equation (2.3) approximates the non-linear ODE equation on the interval $[t^n, t^{n+1}]$. The difference of the solution y^n and disturbed $\tilde{y^n}$ solution $u = \tilde{y^n} - y^n$ of the linear ODE (2.3) satisfies (2.4) and we can use this equation in order to investigate properties of the numerical solution. As before, we assume that eigen values $\lambda_i \in [0, M]$, where $M = \sup_i \lambda_i$, and eigenvectors φ_i form basis in R^n,

$$h_i > 0, \quad h = \max_i h_i, \quad \delta = \frac{1-\omega}{1+\omega}, \quad cou = 2/M. \tag{2.5}$$

Now we suppose that we know value h, which guarantees predefined accuracy of the method (2.2) for $m = 1$. We use the method (2.2) for solution of the problem (2.4)

$$u^1 = \prod_{i=1}^{m}(I + 0.5h_i A)^{-1}(I - 0.5h_i A)u^0, \tag{2.6}$$

$$\tau = \tau(M, \omega) = \sum_{i=1}^{m} h_i. \tag{2.7}$$

We shall compare the expansions for numerical and exact solutions. The expansion for the numerical solution u^1 and u^0

$$u^1 = \sum_{j=1}^{n} c_j \left(\prod_{i=1}^{m} \frac{1 - 0.5h_i\lambda_j}{1 + 0.5h_i\lambda_j} \right) \varphi_j = \sum_{j=1}^{n} c_j R_m(\lambda_j)\varphi_j, \tag{2.8}$$
$$u^0 = \sum_{j=1}^{n} c_j\varphi_j,$$

where

$$R_m(\lambda) = \prod_{i=1}^{m} \frac{1 - 0.5h_i\lambda}{1 + 0.5h_i\lambda}, \tag{2.9}$$

$$R_m(0) = 1, \quad R'_m(0) = \tau = -\sum_{i=1}^{m} h_i, \quad h_i > 0 \tag{2.10}$$

and the expansion for the exact solution of (2.4) is

$$u(\tau) = \sum_{j=1}^{n} c_j e^{-\lambda_j \tau}\varphi_j. \tag{2.11}$$

If we compare (2.11) and (2.8) we can see that scheme (2.2) better approximates modes with small eigenvalues λ_j. If steps $\{h_i\}_1^m$ are too large the approximation of modes with large eigenvalues λ_j is very different from the exact solution, because $R_m(\lambda_j)$ can be close to ± 1, but the exact solution for these modes close to 0. That is the reason of the oscillating behavior of the numerical solution shown in Fig. 5.1 (c).

3. Stability function of the Crank-Nicolson method. In order to avoid this problem we choose steps $\{h_i\}_{i=1}^m$ such that stability function be less than some predefined parameter $1 > \omega > 0$. But the function (2.9) equals to one $R_m(0) = 1 > \omega$ in the origin and it approximates exponential function, which means we can not make it less than ω on the whole interval $[0, M]$. At the same time the function $R_m(\lambda)$ is monotonically decreasing and equals zero at $\frac{2}{\max\limits_{i=1,\ldots,m} h_i}$. This means that there is a point γ within the interval $[0, \frac{2}{\max\limits_{i=1,\ldots,m} h_i}]$, where $R_m(\gamma) = \omega$. We will construct rational function, such that it stays within the interval $R_m(\lambda) \in [-\omega, \omega]$ if $\lambda \in [\gamma, M]$.

DEFINITION 3.1. *We call the function (2.9) $L_\omega[0, M]$ stable if $h >$ cou and the function $R_m(\lambda)$ is monotonically decreasing non-negative function in $[0, \gamma]$ and*

$$\omega \geq \max_{\lambda \in [\gamma, M]} |R_m(\lambda)|, \quad 1 \geq \max_{\lambda \in [0, \gamma]} |R_m(\lambda)| \geq \omega, \tag{3.1}$$

where $0 < \omega < 1$, and $0 < \gamma < M$.

We use term $L_\omega[0, M]$ to outline similarity with L stability of Runge-Kutta methods. Now we are ready to formulate optimization problem for construction $L_\omega[0, M]$ stable method (2.2): Given m, ω, let us define $\bar{h} = h(m, \omega)$ as a maximum possible value when inequalities (3.1) are still valid. And let us define $\bar{\tau} = \bar{\tau}(m, \omega) = \max\limits_i h$. Now, we can change variables

$$z = \lambda/M, \quad z_i = h_i 2M, \quad \eta = \gamma/M, \quad 0 \leq \eta \leq 1, \quad \bar{z} = \bar{h}/(2M), \tag{3.2}$$

so that function (2.9) becomes

$$R_m(z) = \prod_{i=1}^{m} \frac{1 - z_i z}{1 + z_i z}. \tag{3.3}$$

Let us consider two simple cases.

1. Let $m = 1$. We can determine $\bar{z}$ from the equation

$$R_1(1) = \frac{1 - \bar{z}}{1 + \bar{z}} = -\omega,$$

and $\bar{z}$ becomes

$$\bar{z} = \frac{1}{\delta}, \quad \bar{h} = \frac{cou}{\delta}, \quad \bar{\tau} = \frac{cou}{\delta}, \tag{3.4}$$

where δ has been defined in (2.5). The value $\bar{\eta}$ can be found from the equation

$$\frac{(1 - \bar{z}\bar{\eta})}{(1 + \bar{z}\bar{\eta})} = \omega,$$

$$\bar{\eta} = \delta^2, \quad \bar{\gamma} = \delta^2 M. \tag{3.5}$$

Consequently, we can use the method (2.2) if $h \leq \bar{h} = \bar{h}(1, \omega)$, $m = 1$, $h_1 = h$, and $\tau = \tau(1, \omega) = h$.

2. In the second case $m = 2$ the function $\bar{R}_2(z)$ becomes

$$\bar{R}_2(z) = \frac{1 - pz + q^2 z^2}{1 + pz + q^2 z^2}, \tag{3.6}$$

where $p = (z_1 + z_2), q^2 = z_1 z_2$, and we can find $\bar{z}$ from the equations

$$\begin{aligned} \min_{z \in [0,1]} \bar{R}_2(z) &= \bar{R}_2(\tilde{z}) = -\omega, \\ \bar{R}_2(1) &= \omega, \end{aligned}$$

and $\tilde{z} = 1/q$ because $\bar{R}_2'(\tilde{z}) = 0$. In this case the first equation becomes $(2q - p)/(2q + p) = -\omega$, and $p = 2q/\delta$. Making use of the second equation, obtain quadratic equation for p

$$\begin{aligned} q^2 - 2q/\delta^2 + 1 &= 0, \\ \tfrac{\delta^2 (1-\omega) p^2}{4} - (1 + \omega)p + 1 - \omega &= 0. \end{aligned}$$

Where the solution of this equaton is

$$\begin{aligned} q &= (1 + \sqrt{1 - \delta^4})/\delta^2, \\ p &= \tfrac{2(1+\omega)}{(1-\omega)^2}((1 + \omega)^2 + 2\sqrt{2\omega(1 + \omega^2)}), \end{aligned}$$

and $p = 2(1 + \sqrt{1 - \delta^4})/\delta^3$, $\bar{z} = z_1 = p(1 + \sqrt{1 - \delta^2})/2$, $\quad z_2 = p(1 - \sqrt{1 - \delta^2})$, and $\bar{h}$ becomes

$$\bar{h} = h_1 = z_1 cou, \quad h_2 = z_2 cou, \quad \bar{\tau} = 2pcou. \tag{3.7}$$

Similarly, the value $\bar{\eta}$ satisfies the equation $(\bar{\eta}q)^2 - 2(\bar{\eta}q)/\delta^2 + 1 = 0$ and $\bar{\eta}q = (1 - \sqrt{1-\delta^4})/\delta^2$, and finally

$$\bar{\eta} \quad = \quad \delta^4(1+\sqrt{1-\delta^4})^{-2}. \tag{3.8}$$

So, we have shown that we can use method (2.2) if $h \le \bar{h}(2,\omega)$, $m = 2$ and $h = h_1$.

Now, let us consider possible cases in more details. Let $\tilde{h}$ is a root of the equation $(\frac{1-\tilde{h}M/2}{1+\tilde{h}M/2})^2 = \omega$, then we can take $h_1 = h$ and h_2 as a root of the equation $\frac{1-hM/2}{1+hM/2} \cdot \frac{1-h_2M/2}{1+h_2M/2} = \omega$ if $\tilde{h} \le h \le \bar{h}$, and finally we have

$$\frac{\tau(2,\omega)}{2} \ge \tau(1,\omega).$$

If $h < \tilde{h}$, we assume that $h_1 = h_2 = h$ and we have $\frac{\tau(2,\omega)}{2} \ge \tau(1,\omega)$, $h > \bar{h}(1,\omega)$, $\tau_2(2,\omega)/2 = \tau(1,\omega)$ if $h < \bar{h}(1,\omega)$.

3. Now we analyse the case $m \ge 3$, $r = cou/h < \delta^3/((1+\sqrt{1-\delta^2})(1+\sqrt{1-\delta^4}))$. Consider Zolotarev rational function dergree m

$$Z_m(z) = \prod_{i=1}^{m} \frac{1-\bar{z}_i z}{1+\bar{z}_i z}, \tag{3.9}$$

where

$$\bar{z}_i = 1/dn\left(\frac{2(m-i)+1}{2m}K(\eta^{'}),\eta^{'}\right), \quad i = 1,\ldots,m, \tag{3.10}$$

where $dn(u,k)$ is Jacobi elliptic function, $K(k)$ is elliptic integral, k is module, $k^{'} = \sqrt{1-k^2}$, $\eta^{'} = \sqrt{1-\eta^2}$, $K' = K(k')$, and nome $q = q(k) = \exp(-\pi\frac{K(k^{'})}{K(k)})$.

For the further analysis, we need the following properties of the functions $dn(u,\eta), K(k)$

$$\begin{aligned} dn(-u,\eta) = dn(u,\eta), \quad dn(K(\eta^{'}),\eta^{'}) = \eta, \\ dn(u+K(\eta^{'}),\eta^{'}) = \eta/dn(u,\eta^{'}), \quad dn(0,\eta^{'}) = 1. \end{aligned} \tag{3.11}$$

If k is close to zero we can use the following properties $K(k) \approx \pi/2, K(k^{'}) \approx \ln\frac{4}{k^{'}}$. The values $\bar{z}_i^{-1}$ are roots of the function $Z_m(z)$, $\bar{z}_i^{-1} \in [\eta,1], \eta < \bar{z}_1^{-1} < \bar{z}_2^{-1} < \ldots < \bar{z}_m^{-1} < 1, \bar{z}_1^{-1} \to \eta$ if $m \to \infty$.

The function $Z_m(z)$ has Chebyshev alternation property of $m+1$ points on the interval $[\eta,1]$, and this is the function of the least deviation from zero among rational functions (3.3), with the value of deviation from zero $E_m = E_m(\eta)$. The appropriate theorem was proved by Zolotarev [20, 6]

THEOREM 3.2. *The rational function (3.3) degree m is the function of the least deviation from zero*

$$\min_{\{z_i\}_1^m} \max_{[\eta,1]} |R_m(\lambda)| = E_m(\eta), \tag{3.12}$$

in the uniform $C[\eta,1]$ norm on the interval $[\eta,1]$, $0 < \eta < 1$, if and only if the parameters of the function are (3.10).

This rational function has $m+1$ points $\{\tilde{z}_i\}_1^{m+1}$, $0 < \tilde{z}_i < \tilde{z}_{i+1} \le 1$ such that $R_m(z)$ equals its local maximum value $E_m(\eta)$ with alternaiting sign

$$R_m(\tilde{z}_i) = (-1)^{i-1}E_m(\eta). \tag{3.13}$$

We will use this function for computation of the parameters of the numerical method (2.2), so in order to clarify relationship between Zolotarev rational function (3.9) and Zolotarev function for the interval $[a, M]$ we provide the following definition Let $\eta = \frac{a}{M}$, where a is a positive value $0 < a < M$.

DEFINITION 3.3 (2). *We call the function (2.9) with parameters*

$$h_i = h_i(\eta, m) = \tilde{h}_i^m / M, \quad i = 1, \dots, m, \tag{3.14}$$

where $\eta = a/M$ *and*

$$\tilde{h}_{m-i+1}^m = \frac{2}{dn\left(\frac{2i-1}{2m} K'(\eta), \eta'\right)}, \quad i = 1, \dots, m, \tag{3.15}$$

as Zolotarev rational function for the interval $[a, M]$.

Because Zolotarev rational function is monotonically decreasing function in the interval $[0, \tilde{\lambda}_1]$ it satisfies conditions of $L_\omega[0, M]$ stability if $\omega \geq E_m(\eta)$. Now we want to find parameters η and degree m such that sum of steps satisfies (2.7), $E_m(\eta) \leq \omega$ and m as low as possible.

Because the function $E_m(\eta)$ is continuous and monothonically decreasing function of η, and $E_m(0) = 1$ $E_m(1) = 0$, there are inverse functions $\eta = \eta_m(E_m)$, $\eta(0) = 1$, $\eta(1) = 0$ and $\bar{z}_1^{-1} = \bar{z}_1^{-1}(E_m)$. If we define

$$\mu^{1/2} = \frac{1 - \eta^{1/2}}{1 + \eta^{1/2}}, \quad \mu_1 = \sqrt{1 - \mu^2}, \quad q = q(\mu) = \exp\left(-\pi \frac{K(\mu_1)}{K(\mu)}\right), \tag{3.16}$$

then

$$E_m = 2q^{m/4} \prod_{n=1}^{\infty} (1 + q^{mn})^{(-1)^n}.$$

And we obtain

$$\frac{2q^{m/4}}{1 + q^{m/2}} \leq \frac{2q^{m/4}}{1 + q^m} \leq E_m \leq \frac{2q^{m/4}(1 + q^{2m})}{1 + q^m} \leq 2q^{m/4}. \tag{3.17}$$

Let $0 < \omega \leq 1, \eta = \eta_m(\omega), \eta \leq \nu \leq 1$, and define $F_m(\omega, \nu)$ as a class of rational functions (3.3), which satisfy $0 \leq \bar{z}_i \leq \nu^{-1}, i = 1, \dots, m$, and $\max_{\nu \leq t \leq 1} |\bar{R}_m(z)| \leq \omega$.

We use the following theorem in order to define algorithm for determination of variable time steps.

THEOREM 3.4. $\sup_{F_m(\omega,\nu), \eta \leq \nu \leq 1} |\bar{R}_m'(0)| = -Z_m'(0) = 2 \sum_{i=1}^m \bar{z}_i.$

The formula for $\bar{z}_1$ can be rewritten as follow

$$\bar{z}_1 = 1/dn\left((1 - \frac{1}{2m})K(\eta'), \eta'\right) = dn\left(\frac{1}{2m}K(\eta'), \eta'\right)/\eta, \tag{3.18}$$

or

$$\eta = \bar{z}_1^{-1} g_m(\eta), \quad g_m(\eta) = g(\eta, m) = dn(\frac{1}{2m}K(\eta'), \eta'). \tag{3.19}$$

The function $g_m(\eta)$ monotonically increases on $[0, 1]$ and $g_m(0) = 0$, $g_m(1) = 1$, $g_m{}'(1) = 0$, $g_m{}'(0) = \infty$, $g_m(\eta) > \eta$, $g_m''(\eta) < 0$ if $0 < \eta < 1$. The graphs of the functions $g_3(\eta)$ and η are plotted on the Fig. 3.2.

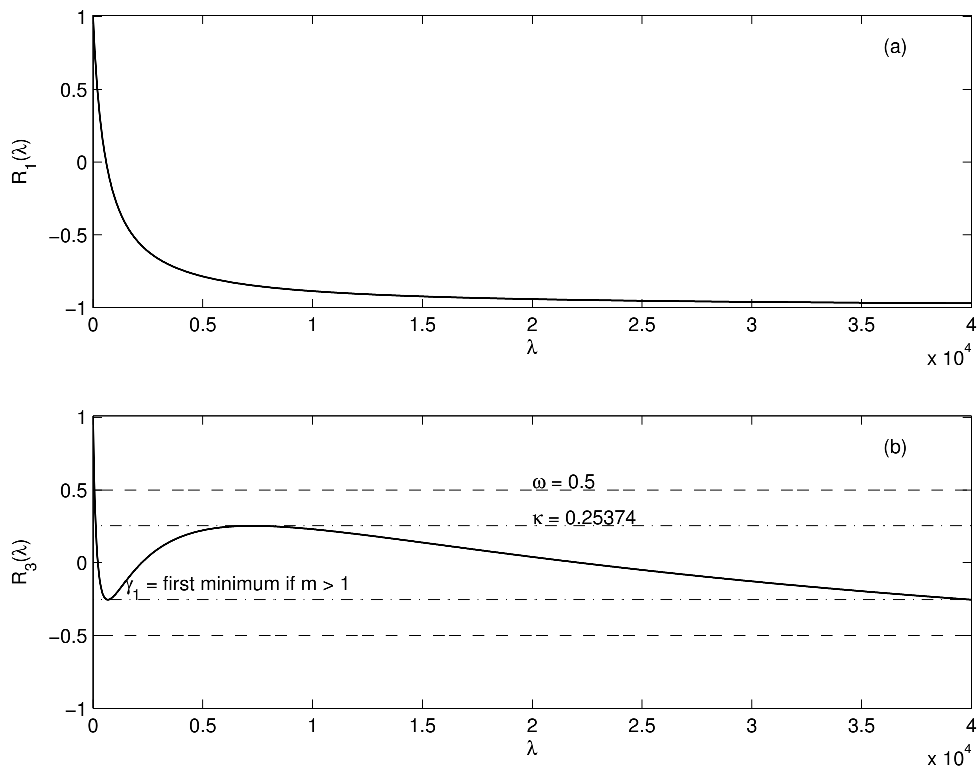

FIG. 3.1. *Rational function used by Crank-Nicolson method with constant step size $h = \Delta x(a)$. Optimal Zolotarev function degree $m = 3$ for $\omega = 0.5$ and $\tau = \Delta x$ (b).*

Because of monotonicity the equation (3.19) has only one solution on $[0, 1]$ if $m \geq 3$, $0 \leq z_1^{-1} \leq \delta$. At the vicinity of this solution the following inequality holds $0 < \bar{z}_1^{-1} g_m^{'}(\eta) < 1$. Given $0 < \bar{z}_1^{-1} = r = cou/h < \delta^3 < 1, m \geq 3$ we can use the method of successive approximations in order to find η from the equation (3.19)

$$\eta^{k+1} = r g_m(\eta^k), \quad k = 0, 1, \ldots. \tag{3.20}$$

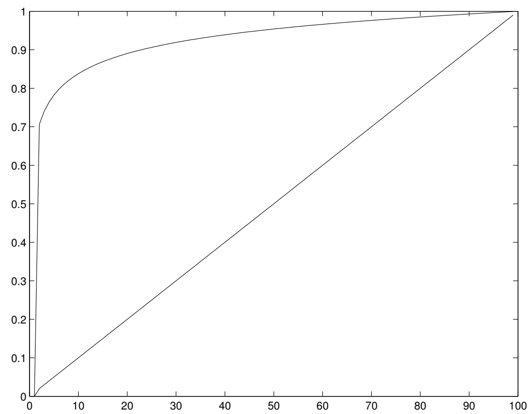

FIG. 3.2. *Function $g_m(\eta)$ and η.*

As an initial guess we can take upper estimate $\eta^0 = \delta^2$, or more precisely $\eta^0 = \delta^4(1+\sqrt{1-\delta^4})^{-2}$. The sequence η^k converges monotonically from above to the solution of the equation (3.19). The upper m_1 and lower m_2 estimates for the minimal m, which guarantees that inequality $E_m \le \omega$ is valid, can be found by mean of the inequalities (3.17)

$$2q^{m_1/4}(\mu) = \omega, \qquad \frac{2q^{m_2/4}}{1+q^{m_2/2}} = \omega,$$

or equivalently

$$m_j = m_j(\eta) = -\frac{4\ln\omega_j K(\mu)}{\pi K(\mu_1)}, \qquad \frac{m_1}{m_2} = \frac{\ln\omega_1}{\ln\omega_2} \tag{3.21}$$

where $\omega_1 = \omega/2$, $\omega_2 = \omega/(1+\sqrt{1-\omega^2})$.

Substitution of these values into equation (3.19) instead of m gives the solution $\tilde{\eta}_j, j = 1, 2$, and finally we can find μ_j, μ_{1j}, q_j from the equation (3.16) and upper and lower bounds for m. The estimation of the upper m_1 and lower m_2 bounds can be improved by means of inequality (3.17), if we take value ω_i to be minimal roots of the equations $2x(1+x^8) - \omega(1+x^4) = 0$, $x^4 - 2x/\omega + 1 = 0$. If value η is close to zero one can use asymptotic formula for $K(\mu), K(\mu_1) : K(\mu) \approx \pi/2$, $K(\mu_1) \approx \ln\frac{4}{\mu_1}$, and obtain

$$m_j \approx -\frac{8\ln\omega_j}{\pi^2}\ln\frac{4}{\mu_1}. \tag{3.22}$$

The value of $\tau_m(\eta)$ of Zolotarev rational function for the interval $[M\eta, M]$ equals $\tau_m(\eta) = \sum\limits_{i=1}^{m} h_i = \sigma_m(\eta)cou = 2\sigma_m(\eta)/M$, where

$$(3.23) \qquad \sigma_m(\eta) = \sum_{i=1}^{m} \bar{z}_i = \sum_{i=1}^{m} \frac{1}{dn\left(\frac{2(m-i)+1}{2m}K(\eta'),\eta'\right)}, \qquad \tau_m(\eta) = \sigma_m(\eta)cou.$$

So, let us estimate the value $\sigma_m(\eta)$.

THEOREM 3.5. *The value $\sigma_m(\eta) = \sigma_m(\eta)$ of Zolotarev rational function for the interval equals*

$$(3.24) \qquad \sigma_m(\eta) = 0.5M\sum_{i=1}^{m} h_i = m\frac{K'_{2m}k_{2m}}{K'\eta},$$

where $\eta' = \sqrt{1-\eta^2}$, $K_{2m} = K(k_{2m})$, $K'_{2m} = K(k'_{2m})$, $k_{2m} = \sqrt{1-(k'_{2m})^2}$, *where* $k'_{2m} = \eta^{2m}\prod\limits_{r=1}^{m} C^2_{2r-1}$, *where* $C_r = sn^2\left(\frac{rK'}{2m},\eta\right)$, *is elliptic integral, and* $sn(x,y)$ *is elliptic sinus.*

The value $\sigma_m(\eta)$ is bounded by

$$(3.25) \quad \frac{\pi m}{2K'\eta}\left(1+4\sum_{p=1}^{2n}\frac{(-1)^p q^{2mp}(\eta')}{1+q^{4mp}(\eta')}\right) > \sigma_m(\eta)$$
$$> \frac{\pi m}{2K'\eta}\left(1+4\sum_{p=1}^{2n+1}\frac{(-1)^p q^{2mp}(\eta')}{1+q^{4mp}(\eta')}\right),$$

for any n.

Proof. Let us consider expansion for the function (3.24) [19]

$$\sigma_m(\eta) = \sum_{i=1}^{m} nd\left(\frac{2i-1}{2m}K'(\eta),\eta'\right)$$
$$= \sum_{i=1}^{m}\left(\frac{\pi}{2K'\eta} + \frac{2\pi}{K'\eta}\sum_{l=1}^{\infty}\frac{(-1)^l q^l(\eta')\cos\frac{2i-1}{2m}\pi l}{1+q^{2l}(\eta')}\right),$$

where $nd(x,y) = (dn(x,y))^{-1}$. Because of the absolute convergence of the series for any q except $q=1$, when $\eta' = 1$ and $\eta = 0$, we can exchange sums over the m and l

$$\sigma_m(\eta) = \left(\frac{\pi}{2K'\eta}m + \frac{2\pi}{K'\eta}\sum_{l=1}^{\infty}\frac{(-1)^l q^l(\eta')}{1+q^{2l}(\eta')}\sum_{i=1}^{m}\cos\frac{2i-1}{m}\pi l\right),$$

The last sum can be simplified using the property

$$\sum_{i=1}^{m}\cos\frac{2i-1}{2m}\pi l = \begin{cases} 0, & \text{if } l \neq 2pm \quad p = 1,2,\ldots \\ (-1)^p m, & \text{if } l = 2pm, \quad p = 1,2,\ldots \end{cases}$$

$$\sigma_m(\eta) = \left(\frac{\pi}{2K'\eta}m + \frac{2\pi}{K'\eta}\sum_{l=1}^{\infty}\frac{(-1)^l q^l(\eta')}{1+q^{2l}(\eta')}(-1)^p m\delta_{l,2pm}\right) =$$
$$\left(\frac{\pi}{2K'\eta}m + \frac{2\pi m}{K'\eta}\sum_{p=1}^{\infty}\frac{(-1)^p q^{2mp}(\eta')}{1+q^{4mp}(\eta')}\right)$$

(3.26)

TABLE 3.1

The value $\tau(0.01)M/m = 2\sigma(0.01)$ and it's estimate via the inequality (3.26) for even and odd values n.

	m=1	m=2	m=3	m=4	m=5	m=6	m=7	m=8
$n = 0$	52.4334	52.4334	52.4334	52.4334	52.4334	52.4334	52.4334	52.4334
$n = 2$	21.2558	44.9547	50.9464	52.1453	52.3778	52.4227	52.4313	52.433
$n = 4$	20.0466	44.9444	50.9463	52.1453	52.3778	52.4227	52.4313	52.433
$n = 6$	20.0017	44.9444	50.9463	52.1453	52.3778	52.4227	52.4313	52.433
$M\frac{\tau_m(0.01)}{m}$	20.	44.9444	50.9463	52.1453	52.3778	52.4227	52.4313	52.433
$n = 5$	19.991	44.9444	50.9463	52.1453	52.3778	52.4227	52.4313	52.433
$n = 3$	19.7581	44.944	50.9463	52.1453	52.3778	52.4227	52.4313	52.433
$n = 1$	13.4888	44.6663	50.9357	52.1449	52.3778	52.4227	52.4313	52.433

In order to estimate the last series we use expantion for $nd(z,\bar{k})$ function

$$nd(z,\bar{k}) = \frac{\pi}{2\sqrt{1-\bar{k}^2}\bar{K}(\bar{k})} + \frac{2\pi}{\sqrt{1-\bar{k}^2}\bar{K}(\bar{k})}\sum_{p=1}^{\infty}\frac{(-1)^j\bar{q}^j(\bar{k})}{1+\bar{q}^{2j}(\bar{k})}\cos\frac{\bar{k}\pi z}{\bar{K}(\bar{k})}.$$

If we set $z = 0$ and use property $nd(0,\bar{k}) = 1$ we obtain

$$1 = \frac{\pi}{2\sqrt{1-\bar{k}^2}\bar{K}(\bar{k})} + \frac{2\pi}{\sqrt{1-\bar{k}^2}\bar{K}(\bar{k})}\sum_{p=1}^{\infty}\frac{(-1)^j\bar{q}^j(\bar{k})}{1+\bar{q}^{2j}(\bar{k})}.$$

or

$$\sum_{p=1}^{\infty}\frac{(-1)^j\bar{q}^j(\bar{k})}{1+\bar{q}^{2j}(\bar{k})} = \frac{\sqrt{1-\bar{k}^2}\bar{K}(\bar{k})}{2\pi} - \frac{1}{4}. \tag{3.27}$$

If we set $\bar{q}(\bar{k}) = q^{2m}(\eta') = \exp -\pi\frac{2mK}{K'}$ the left hand side of the expression (3.27) formally equals to the last sum at (3.26). The nome $q^{2m}(\eta') = \exp -\pi\frac{2mK}{K'}$ corresponds to the second principal $2m^{th}$ degree transformation ([2], p.214) with the ratio of elliptic integrals $\frac{K_{2m}}{K'_{2m}} = 2m\frac{K}{K'}$ and appropriate module k_{2m}. Consequently, if we set $k'_{2m} = \bar{k}$ and $k_{2m} = \sqrt{1-k'^{2}_{2m}}$ and $K'_{2m} = \bar{K}(\bar{k})$ the (3.27) becomes

$$\sum_{p=1}^{\infty}\frac{(-1)^p q^{2mp}(\eta')}{1+q^{4mp}(\eta')} = \frac{K'_{2m}k_{2m}}{2\pi} - \frac{1}{4},$$

which we substitute to (3.26) and finally obtain

$$\sigma_m(\eta) = \left(\frac{\pi}{2K'\eta}m + \frac{2\pi m}{K'\eta}\left(\frac{K'_{2m}k_{2m}}{2\pi} - \frac{1}{4}\right)\right) = \frac{mK'_{2m}k_{2m}}{K'\eta}.$$

Because $q(\eta')$ is always positive the series (3.26) has terms with alternating sign, and each even and odd term gives us upper or lower estimate for $\sigma_m(\eta)$ respectively. □

The value $\tau_m(\eta)M/m = 2\sigma_m(\eta)/m$ $(n = \infty)$ and an example of the inequality (3.26) is provided in Table 3.

Because computation of elliptic integrals is slow we can use approximation for the steps via the formula [12, 16, 17, 18]

$$h_i(\eta, m) \approx \frac{(1+2\theta)(1+\theta^{\sigma_i})}{\theta^{\sigma_i/2}(1+\theta^{1-\sigma_i}+\theta^{1+\sigma_i})M}, \quad i=1,\dots,m>1 \tag{3.28}$$

$$h(\eta, 1) = \frac{2}{\sqrt{\eta}M} \text{ if } m=1, \tag{3.29}$$

where $\theta = \frac{1}{16}\eta^2(1+0.5\eta^2)$, $\sigma = \frac{2i-1}{2m}, i=1,\dots,m$.

Let us estimate the ratio of the average stepsize and maximal stepsize $S = \frac{\sigma_m(\eta)}{m\bar{z}_1}$. Because values η, $K(\eta^{'})$ are increasing and values $\eta^{'}, q(\eta^{'})$ are decreasing for a given $\bar{z}_1$ and increasing m, then the value S is decreasing. The upper estimate for $\bar{\tau}_m/\bar{h}$ can be obtained using inequality

$$\bar{\tau}_m/\bar{h} = mS < \frac{\pi m}{2K(\eta^{'})dn(\frac{1}{2m}K(\eta^{'}),\eta^{'})} = \ln(2/\omega)p(\omega,\eta), \tag{3.30}$$

where

$$p(\omega,\eta) = \frac{2K(\mu)}{K(\mu_1)K(\eta^{'})dn(\frac{1}{2m_1}K(\eta^{'}),\eta^{'})}.$$

Numerical computations of this value gives estimate $0 < p(\omega,\eta) \le p(\omega,0) < 0.33 + 5.27\omega$, and finally we obtain

$$\bar{\tau}_m < (0.35+5.25\omega)\ln(2/\omega)\bar{h}. \tag{3.31}$$

Now we can formulate optimizatin problem. There are several possible formulations. In the first approach, we consider Runge-Kutta method (2.2) which is composed of several internal steps. And given maximal sum of internal steps $\tau_{max} = \tau = \sum\limits_1^m h_i$ we find appropriate m and sequence of internal steps $\{h_i\}_1^m$ in order to garantee $L_{omega}[0,M]$ stability. Plus, it is reasonable to fund such m that for given τ amount of computational work in the Runge-Kutta method (2.2) to be as low as possible, which means that we want the number of stages m to be as small as possible:

Given τ and $0<\omega<1$, find minimal m and sequence $\{h_i\}_1^m$ which satisfies (2.7) such that the function (2.9) is $L_\omega[0,M]$ stable.

Another approach, which we adopt here, is based on the fact that the error of approximation can be evaluated in terms of the maximal step size $h = \max\limits_i h_i$, and given maximal sum of internal steps τ_{max}, we can take $\tau_{max} = \max\limits_i h_i$. In this case we formulate the optimization problem as following

Given h and $0<\omega<1$ find minimal m and sequence $\{h_i\}_1^m$ such that the function (2.9) is $L_\omega[0,M]$ stable and τ is as large as possible.

We search for solution of this problem in the class of Zolotarev rational functions.

The method (2.2) has order $o(\tau^2)$. Suppose we can estimate maximum possible step τ_{max} which assures predefined computational error. Several methods can be used for evaluation τ_{max}, but we do not discuss this issue in this article. We prefer to use step size estimation technique based on embedded formulas [4, 5]. Given τ_{max} we can find optimal parameters m and η of Zolotarev function. In order to do that we can use two equations

$$\bar{z}_1 cou = h \tag{3.32}$$

$$E_m \leq \omega \tag{3.33}$$

Starting from $m = 1$ we solve the first equations for η, then verify the second condition (3.33). If it is not valid we take $m + 1$ and use the same algorithm. As soon as m and η have been defined we can find sequence $\{h_i\}_{i=1}^m$, which defines $L_{\omega_m}[0, M]$ stable method, which has maximum mean step size τ/m in the class of Zolotarev rational functions 3.14. The steps $\{h_i\}_{i=1}^m$ are enumerated in descending order. But for practical reasons it is better to change the sequence of steps in order to make a large step followed by a small step. In this case the intermediate stability function obtained after several steps, rather than complete sequence of steps, can possess Chebyshev alternation or almost Chebyshev alternation [12]. This new enumeration is better for solution of nonlinear problems as well as linear problems with time dependent matrix $A = A(t)$. In order to obtain such optimal order of steps one can use principal transformation of elliptic functions. We show only idea of the enumeration algorithm. Let $m = 3n$, then $Z_{3n}(z) = Z_n(z)Q2n(z)$, where $Z_n(z)$ is formed by parameters $2(m-i)+1$ which are divisible by 3. This is the first group of parameters. If n is also divisible by 3, we continue similarly by extracting second group of parameters ans so on.

4. Computation of parameters of numerical method. In the previous section we have defined the algorithm of determination of parameters of the numerical method (2.2). The implementation of each step of the method (2.2) is the same as implementation of Crank-Nicolson scheme, which is widely described in the literature. In this section we consider algorithm for the fast computation of the variable steps of the method (2.2).

Suppose we have some estimation for the value M and total step-size of the next step of the method τ_{max}. Estimation for M can be obtained by several methods including direct computations, norm evaluation of the Jacobian matrix, via Gershgorin theorem or non-linear power method proposed by B.P.Sommeijer, L.F.Shampine and J.G.Verwer [14].

Let us describe the algorithm of comutation of steps h_i. If $m = 1, 2$ steps are defined by the formulas (3.4), (3.7). Now we consider the case $m \geq 3, r = cou/h < \delta^3/((1+\sqrt{1-\delta^2})(1+\sqrt{1-\delta^4}))$. Firstly, we find m_1 from the system (3.32) and (3.33), with initial guess $\eta^0 = \delta^4(1+\sqrt{1-\delta^4})^{-2}$. The iterates m_1^{k+1}, η^{k+1} can be calculated using the following strategy: given η^k define $\mu^k, \mu1^k$ (3.16) and

$$m_1^{k+1} = m_1(\eta^k), \quad \eta^{k+1} = rg(\eta^k, m_1^{k+1})$$

Secondly, we define m_2 using similar approach. After m_1 and m_2 have been defined we have few numbers from the interval $[m_2, [m_1]+1]$. By solving (3.19) using iterates (3.20) we find minimal m and appropriate η for which conditions (3.4), (3.7) are valid. Then given m, η we obtain $\bar{z}_i$ and h_i, which are enumerated in descending order, and estimate (3.30) for $\bar{\tau}_m(\eta)$.

We use algorithm described in the previous section to determine degree of Zolotarev function m and steps $\{h_i\}_{i=1}^m$. In the theorem 2.7 we derive expression $\tau_m(\eta)$ in terms of elliptic integrals. But computation of elliptic integrals is slow and that is the reason we use approximation for the steps via the formula (3.29) and (3.29) [12, 16, 17, 18]. As soon as steps have been calculated the verification of the second inequality in (3.33) is also simple, because the value $E_m(\eta) \approx |R_m(M)|$.

5. Numerical experiments. We conducted a numerical experiment computing the heat equation (1.1) via method of lines (1.5) with initial and boundary conditions below

$$u(x,0) = \begin{cases} 0, & 0 \geq x \geq 1/3, \\ 1, & 1/3 < x < 2/3, \\ 0 & 2/3 \geq x \geq 1 \end{cases} \tag{5.1}$$
$$u(0,1) = u(1,t) = 0$$

We compare results of computations by $m = 3$ steps of Crank-Nicolson method with constant step size τ/m Fig. 5.1(c) and the results of computations by numerical method (2.2) with appropriately chosen number of stages m and steps (3.29) presented on the Fig. 5.1(d). with parameters η and m satisfying

$$\tau = \Delta x = \sum_{i=1}^{m} h_i(a, M, m),$$
$$\omega \geq |R_m(M)|$$

The dash line on the Fig. 5.1(c) and Fig. 5.1(d) is an exact solution of the heat equations. The comparison of the solutions Fig. 5.1(c) and Fig. 5.1(d) clearly demonstrates that oscillations of the Crank-Nicolson method with the constant step size disappears in Crank-Nicolson method with optimally chosen variable steps. The plot on the Fig. 5.2 shows the decay of Fourier coefficients for method with constant steps Fig. 5.2(b) and optimally chosen variable steps Fig. 5.2(c). Comparison of the distribution of Fourier harmonics of initial values Fig. 5.2(a) and constant step solution Fig. 5.2(b) shows that high harmonics are not decaying properly, but solution with variable steps shows decay of the large harmonics as it should occur for the exact solution of the heat equation.

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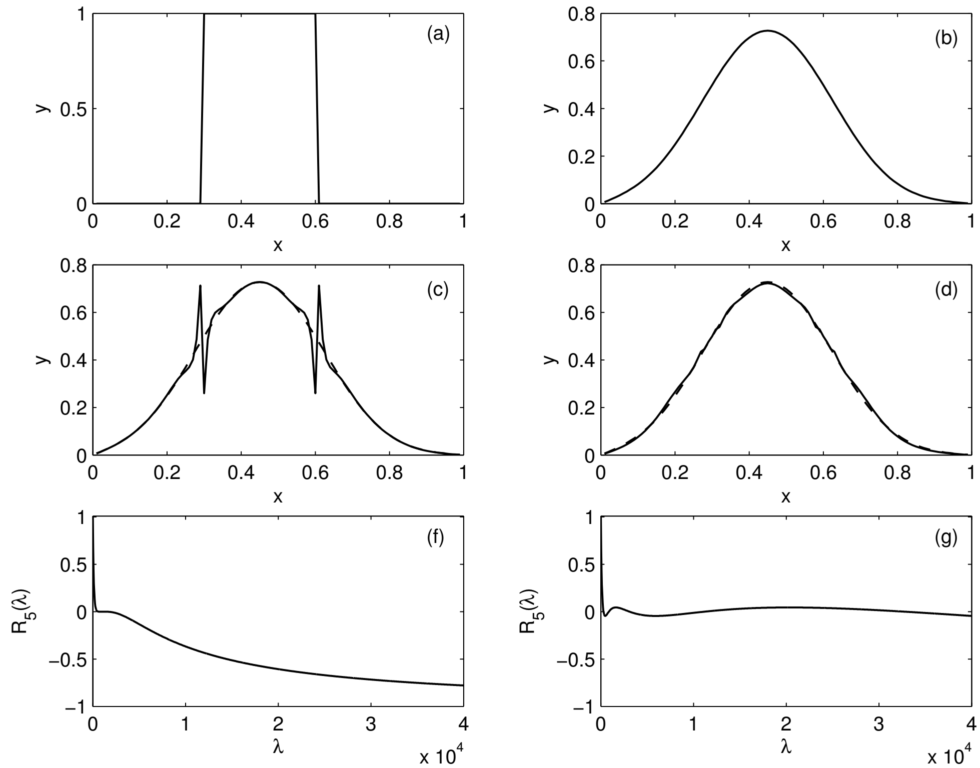

FIG. 5.1. *Initial value of the heat equation (5.2) (a). Exact solution of the equation (5.2) (b). The solution of the heat equation (1.5) by Crank-Nicolson method with $m = 3$ constant steps $\tau = \Delta x/m$ (c) and solution (5.2) by the method (2.2) with the same sum of steps $\tau = \sum_{i=1}^{m} h_i = \Delta x$ (d). Stability function of the Crank-Nicolson schema after $m = 3$ steps $\tau = \Delta x/m$ (f). Optimal Zolotarev stability function for $\omega = 0.05$ and $\tau = \Delta x$ (g).*

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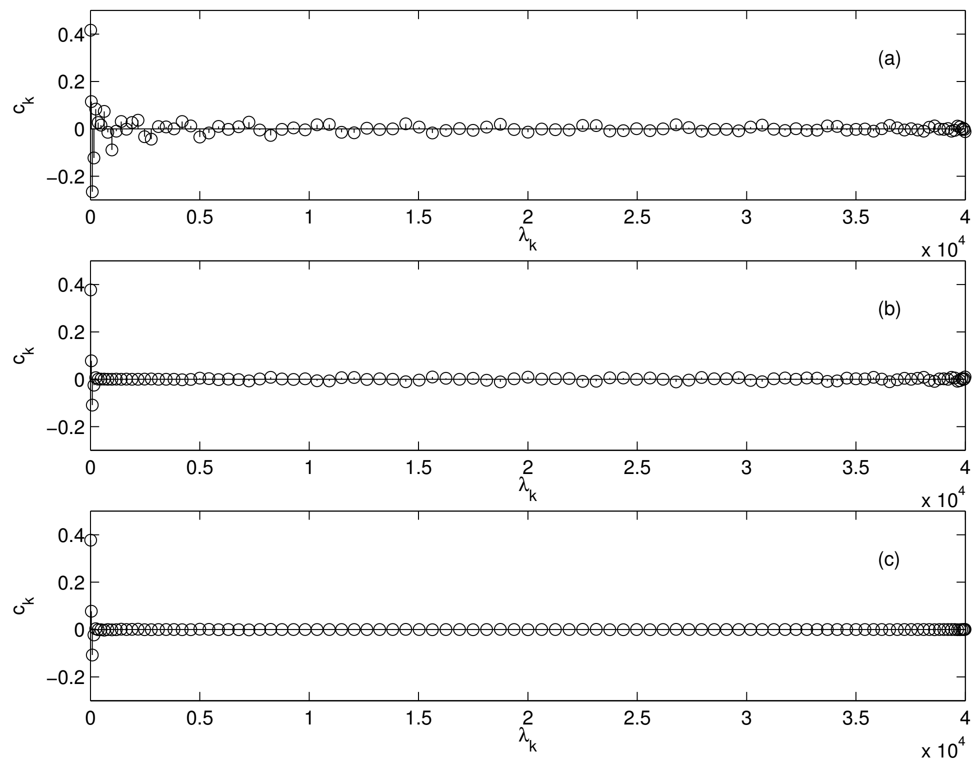

FIG. 5.2. *Distribution of coefficients c_k of initial value (5.2) (a). Distribution of coefficients c_k after $m = 3$ steps by Crank-Nicolson schema with constant steps $\tau = \Delta x/m$ (b) and variable steps (c).*