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COMPARATIVE ANALYSIS BY MEANS OF FINITE DIFFERENCES AND DM METHODS FOR LINEARIZED PROBLEM OF GYROTRONS

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Abstract. The problem of Schrödinger equation with complex boundary conditions for modelling a motion of electrons in gyrotrons is considered. Numerical results obtained by using Fourier, Finite Differences (FD) and Degenerate Matrices (DM) methods are compared in the simplest case. For DM methods they are analysed also in more general cases, when FD can not be applied because of fast oscillations of the solution.

Key words: gyrotron, Schrödinger equation, complex boundary conditions, Fourier method, finite differences, degenerate matrices method

1. Formulation of the problem

When modelling the motion of electrons in gyrotrons, it is necessary to solve the following initial-boundary value problem:

$$\begin{cases} i\dfrac{\partial u}{\partial t} = \dfrac{\partial^2 u}{\partial x^2} + \delta(x)u, \quad x \in (0, L),\ t > 0, \\ u|_{t=0} = u_0(x), \qquad\qquad \text{(initial values)}, \\ u|_{x=0} = 0, \quad \frac{\partial u}{\partial x}\big|_{x=L} = -i\gamma u\big|_{x=L}, \ \text{(boundary conditions)}, \end{cases} \tag{1.1}$$

where $u = u(t, x)$ is an unknown complex function, $\delta(x)$ and $u_0(x)$ are given functions, $\gamma > 0$ is a given constant, $i = \sqrt{-1}$.

Quasi-stationary solutions in the case $\delta(x) = \delta_0 = const$ were considered in [1, 5]. They are given by:

$$u(t, x) = g(x) \exp\big(it(\alpha - \delta_0)\big), \tag{1.2}$$

where $\alpha = \alpha_1 + i\alpha_2$ are complex eigenvalues and $g(x)$ are the corresponding eigenfunctions. Denoting $\alpha = \lambda^2, z = \lambda L$ we obtain the equation

$$z \cos z = -i\gamma L \sin z \tag{1.3}$$

for finding z. Each complex root $z = z_1 + iz_2$ of (1.3) generates a solution in the form (1.2) with

$$\mathrm{Re}\alpha = \alpha_1 = \frac{z_1^2 - z_2^2}{L^2}, \quad \mathrm{Im}\alpha = \alpha_2 = \frac{2z_1z_2}{L^2}, \quad g(x) = \sin\Big(\frac{zx}{L}\Big). \tag{1.4}$$

Using the *argument principle* for analytical complex functions it is possible to prove that all roots of equation (1.3), except $z = 0$, are disposed only in domains

$$\{\,\mathrm{Re}z > 0, \ \ \mathrm{Im}z > 0\,\}, \ \ \{\,\mathrm{Re}z < 0, \ \ \mathrm{Im}z < 0\,\},$$

symmetrically with respect to $z = 0$ [7]. Therefore the roots can be calculated only in the first quadrant of z-plane. We use the software package "*Maple*" for $|z|$ not large and asymptotic formulas in the case of large $|z|$. These asymptotic formulas can be found by the method of indeterminate coefficients. The method is often used to solve equations with entire analytic functions. For roots z_n, $n \to \infty$, they are given as follows:

$$z_n = s_n + \frac{a_1}{s_n} + \frac{a_2}{s_n^3} + \frac{a_3}{s_n^5} + \frac{a_4}{s_n^7} + O\Big(\frac{1}{s_n^9}\Big), \ \ s_n = \pi\Big(n + \frac{1}{2}\Big),$$

$$a_1 = i\tau, \ \ a_2 = \tau^2\Big(1 + \frac{i\tau}{3}\Big), \ \ a_3 = \frac{4\tau^4}{3} + \frac{i\tau^3(\tau^2 - 10)}{5},$$

$$a_4 = \tau^4\Big(\frac{47}{36}\tau^2 - 3\Big) + \frac{i\tau^5}{120}(17\tau^2 - 440), \ \ \tau = \gamma L.$$

Let $\lambda_k = \dfrac{z^{(k)}}{L}$, where $(z^{(k)}), k = 1, 2, \dots,$ be the sequence of roots of (1.3) numbered according to the increase of $\mathrm{Re}(z^{(k)})$. Then the solution of problem (1.1) can be expended into the following convergent infinite Fourier series:

$$u(t, x) = \sum_{k=1}^{\infty} c_k g_k(x) \exp\big(i(\lambda_k^2 - \delta_0)t\big), \tag{1.5}$$

$$g_k(x) = \sin(\lambda_k x), \quad c_k = \frac{\int_0^L g_k(s) u_0(s)\, ds}{\int_0^L g_k^2(s)\, ds}.$$

Moreover, numerical results obtained by (1.5) are accurate enough only for very large number of the summands in (1.5), especially if t is not large. Therefore, in the following sections we will consider other methods for numerical solving of the problem (1.1).

2. Application of the finite difference method

We consider the uniform space grid in the x-direction with the interior grid points

$$x_j = jh, \quad j = \overline{1, N-1}, \quad x_0 = 0, x_N = L,$$

and the time grid with the grid points $t_n = n\tau, \quad n = 1, 2, \ldots$, here h, τ are the steps of the grids. We replace the continuous solution $u = u(t, x)$ of the problem (1.1) by the discrete grid function $y = y(t, x)$ with values $y(t_n, x_j) = y_j^n$.

An approximation of the problem (1.1) is based on the following finite difference scheme:

$$\begin{cases} i\dfrac{y_j^{n+1} - y_j^n}{\tau} = \sigma\Lambda y_j^{n+1} + (1-\sigma)\Lambda y_j^n, \quad j = \overline{1, N-1}, \\ y_0^{n+1} = 0, \quad l y_N^{n+1} = -i\gamma y_N^{n+1}, \\ y_j^0 = u^0(x_j), \quad j = \overline{0, N}, \end{cases} \tag{2.1}$$

where $\sigma \in [0, 1]$ is a parameter of the scheme. Λy_j denotes a central difference expression of the second order approximation for the derivative $\dfrac{\partial^2 u}{\partial x^2}$ at the grid point x_j:

$$\Lambda y_j = \frac{y_{j+1} - 2y_j + y_{j-1}}{h^2} + \delta_0 y_j,$$

$l y_N$ denotes a difference expression of the first order approximation for the derivative $\dfrac{\partial u}{\partial x}$ in one of the following forms:

a) using the two points difference for the first order approximation

$$l y_N = \frac{y_N - y_{N-1}}{h}\,; \tag{2.2}$$

b) using the three points difference for the second order approximation

$$l y_N = \frac{1.5 y_N - 2 y_{N-1} + 0.5 y_{N-2}}{h}\,. \tag{2.3}$$

The approximation order (AO) of the difference equations (2.1) with respect to time and space coordinates is equal to two if $\sigma = 0.5$, and equal to one with respect to time if $\sigma \neq 0.5$. Approximation order of boundary conditions is 1 (formula (2.2)) and 2 (formula (2.3)).

The discrete quasi-stationary solution has the following form:

$$y_j^n = g_j \exp(in\tau\alpha)\,, \tag{2.4}$$

where the discrete eigenfunctions $g_j^{(k)}$ are given by [1]:

$$g_j^{(k)} = \sin(q^{(k)} x_j), \;\; k = 1, 2, \ldots, N-1.$$

Here $q^{(k)}$ are roots of one of the transcendent equations:

1) Approximation (2.2)

$$\sin(qL) = C_1 \sin\big(q(L-h)\big)\,, \tag{2.5}$$

2) Approximation (2.3)

$$\sin(qL) = C_2\Big(2\sin\big(q(L-h)\big) - 0.5\sin\big(q(L-2h)\big)\Big), \tag{2.6}$$

$$C_1 = \frac{1}{1+i\gamma h}, \quad C_2 = \frac{1}{1.5+i\gamma h}\,.$$

The parameter α in (2.4) can be obtained from expressions:

$$\alpha = \ln\frac{1-\tau\alpha_*/(i+\sigma\tau\alpha_*)}{i\tau}, \quad \alpha_* = \frac{2\big(1-cos(qh)\big)}{h^2} - \delta_0\,.$$

The approximate values $\alpha_*^{(k)}$ are complex, i.e., $\alpha_*^{(k)} = A_k + iB_k$:

$$A_k = \frac{2\big(1-\cos(a_k h)\mathrm{ch}(b_k h)\big)}{h^2} - \delta_0, \quad B_k = \frac{2\sin(a_k h)\mathrm{sh}(b_k h)}{h^2}\,,$$

where $q^{(k)} = a_k + ib_k$. Using the argument principle we can prove that all complex roots of (2.5) or (2.6) for $\mathrm{Re}q > 0$ or $a_k > 0$ are in the first quadrant of the complex q-plane, and $B_k \geq 0$.

The stability conditions for finite–difference schemes (2.1) – (2.2), and (2.1)–(2.3) follow from [6]:

$$\sigma \geq 0.5, \quad B_k \geq 0\,.$$

The solution of finite-difference scheme (2.1)–(2.2) can be obtained also in the discrete form of Fourier series:

$$y_j^n = h\sum_{k=1}^{N-1} c_k \sin(q^{(k)}x_j)\exp(i\alpha^{(k)}n\tau), \tag{2.7}$$

where

$$c_k = \sum_{s=1}^{N-1}\frac{1}{d_k}\sin(q^{(k)}x_s)u_0(x_s), \quad d_k = \frac{1}{2}\Big(L - \frac{h\sin(q^{(k)}L)\cos\big(q^{(k)}(L-h)\big)}{sin(q^{(k)}h)}\Big)\,.$$

In this case the discrete eigenfunctions (2.4) are orthogonal:

$$(g^{(k)}, g^{(m)}) = h\sum_{j=1}^{N-1} g_j^{(k)} g_j^{(m)} = 0, \quad k \neq m.$$

3. Application of the Degenerate Matrix method

In this section we will consider another scheme for solving problem (1.1), which can be used also in the case when $\delta(x)$ is not equal to a constant. The DM method [3, 4] is based on using such differentiation matrices $\mathbf{A}$ for derivatives with respect to x which ensure that the approximation of the unknown function u is nonsaturated. Choosing the partitions $x_k,\ k = 0, 1, \dots, n+1$, on the interval $(0, L)$ we form the $(n+2) \times (n+2)$ matrix $\mathbf{A}$ with elements

$$a_{mk} = \begin{cases} \dfrac{w'(x_m)}{(x_m - x_k)w'(x_k)}, & \text{if } m \neq k, \\ \dfrac{w''(x_k)}{2w'(x_k)}, & \text{if } m = k\,, \end{cases} \tag{3.1}$$

where $w(x) = \prod\limits_{j=0}^{n+1}(x - x_j)$.

Remark 1. We usually choose the nodes s_k as zeroes of classical orthogonal polynomials on the standard interval $[-1, 1]$. Then the mapping $x_k = \frac{L}{2}\big(s_k + 1\big)$ gives the required partition of $(0, L)$, and the nonsaturatedness of approximations is ensured.

Contracting equation (1.1) on the nodes x_k, $k = 0, 1, \dots, n+1$, and applying the matrix $\mathbf{A}$ we obtain the following equation

$$i\frac{d\vec{u}}{dt} = (\mathbf{A}^2 + \mathbf{D})\vec{u}, \tag{3.2}$$

where $\vec{u}$ and $\mathbf{D}$ are the column-vector and the diagonal matrix, respectively, with corresponding components $u(x_k)$ and diagonal elements $\delta(x_k)$, $k = 0, 1, \dots, n+1$. Matrix equation (3.2) holds only at the interior points $x_1, x_2, \dots, x_n$ of the interval $(0, L)$. Therefore, we must take off its first and last rows. Then we exclude values $u(x_0)$ and $u(x_{n+1})$ in the first and last columns from the remaining equations using the discretized boundary conditions

$$u(x_0) = 0, \quad \sum_{k=0}^{n+1} a_{n+1,k}u(x_k) = -i\gamma u(x_{n+1}),$$

which are obtained after discretization of boundary conditions (1.1). This yields the system of n homogeneous linear differential equations

$$\frac{d\vec{u}}{dt} = \mathbf{S}\vec{u} \tag{3.3}$$

with initial values obtained by discretization of initial value in (1.1). Here (3.3) has constant coefficient matrix $\mathbf{S}$ with elements $s_{m,k},\ m, k = 1, 2, \dots, n$:

$$s_{mk} = -i\left(a^{(2)}_{mk} + \mu a^{(2)}_{m,n+1}a_{n+1,k} + d_{mk}\right), \tag{3.4}$$

where $a^{(2)}_{mk}$ are the elements of the matrix $\mathbf{A}^2$, $a_{n+1,k}$ are the elements of the last row of $\mathbf{A}$,

$$\mu = \frac{i\gamma - a_{n+1,n+1}}{\gamma^2 + a_{n+1,n+1}^2}, \quad d_{mk} = \begin{cases} 0, & \text{if} \quad m \neq k, \\ \delta(x_k), & \text{if} \quad m = k\,. \end{cases} \tag{3.5}$$

Finally, we solve system (3.3) exactly finding eigenvalues and eigenvectors for the matrix **S** and using discretized initial values.

Comments

$\mathbf{1^0}$. Now we prove that for finding eigenvalues λ and eigenfunctions u, which are defined by the following problem:

$$\begin{cases} u'' + \delta(x)u = -\lambda u, \\ u(0) = 0, \quad u'(L) = -i\gamma u(L), \end{cases} \tag{3.6}$$

it is appropriate to use matrices for derivatives with nodes $s_k = 1, 2, \ldots, N$ as zeroes of one of the classical orthogonal Jacobi polynomials $P_N^{(\alpha,\beta)}(s)$ supplemented with $s_0 = -1$ and $s_{N+1} = 1$.

Let L be the eigenvalue $x_k = \frac{L}{2}\big(s_k + 1\big), k = 0, 1, \ldots, N+1$. Let λ be the eigenvalue and $u(x)$ is the eigenfunction of (3.6) corresponding to given λ . We denote $v(s) = u\big(\frac{L}{2}(s+1)\big)$ and consider the following Fourier series for $s \in [-1, 1]$:

$$v(s) = \sum_{k=0}^{\infty} c_k P_k^{(\alpha,\beta)}(s), \quad c_k = \frac{1}{\parallel P_k^{(\alpha,\beta)} \parallel^2} \int_{-1}^{1} \rho(s) v(s) P_k^{(\alpha,\beta)}(s)\, ds\,, \tag{3.7}$$

where $\rho(s) = (1-s)^\alpha (1+s)^\beta$ is the weight function. Series (3.7) converges very rapidly because $v(s)$ is analytical. Therefore,

$$v(s) = \sum_{k=0}^{N} c_k P_k^{(\alpha,\beta)}(s) + R_N(s), \quad R_N(s) = O\big(\exp(-\nu N)\big)\,, \tag{3.8}$$

when $N \to +\infty$ with some constant $\nu > 0$. Replacing the integral in (3.7) by the Gauss-Lobatto quadrature formula, substituting it into (3.8) and using the classical Christoffel-Darboux formula for Jacobi polynomials it is possible to prove that [2]

$$v(s) = \sum_{k=0}^{N+1} \frac{p_{N+2}(s) v(s_k)}{(s - s_k) p'_{N+2}(s_k)} + \hat{R}_N(s), \quad \hat{R}_N(s) = O\big(\exp(-\nu N)\big), \tag{3.9}$$

where $p_{N+2}(s) = (1-s^2) P_N^{(\alpha,\beta)}(s)$, and the remainder in (3.9) has the same asymptotic estimate as in (3.8). This follows from the asymptotic behaviour of a difference between the integral in (3.7) and its quadrature formula in the case when $v(s)$ is an analytical function on $[-1, 1]$. Therefore, (3.9) gives also the nonsaturated approximation of $v(s)$. Returning to the variable x and using matrices for derivatives according to the scheme given at the beginning of the section, we obtain the equation

$$\Big(\mathbf{S}_N + \big(\lambda + O(\exp(-\nu N))\big)\mathbf{E}_N\Big)\vec{u}_N = 0\,. \tag{3.10}$$

All elements of the matrix $\mathbf{S}_N$ can be computed by analogy with (3.4) and (3.5). Therefore, the eigensystem for the matrix $\mathbf{S}_N$ is close to the one for the matrix

$$\mathbf{S}_N + O\big(\exp(-\nu N)\big)\mathbf{E}_N, \quad \text{if} \quad N \to +\infty\,.$$

$\mathbf{2^0}$. The computing scheme described above can be used not only for (1.1), but also for solving different linear problems of heat or wave equations.

$\mathbf{3^0}$. A possibility to compute the matrix $\mathbf{S}$ in (3.3) efficiently and to calculate its eigenvalues gives very simple criterion of the stability of the DM-methods for linear problems. They are stable if all n eigenvalues of $\mathbf{S}$ have negative real parts. For example, the DM-method for (1.1) with uniformly distributed nodes is unstable even for $n \geq 5$. The choice of nodes as zeroes of classical orthogonal polynomials leads to stable schemes for very large n. For example, the method with nodes as zeroes of Chebyshev polynomials of the second kind is stable at least for $n \leq 240$, for Legendre polynomials – at least for $n \leq 120$.

4. Numerical results

Table 1. Values of $|u(x,t)|$ for $x = L = 15$, $\gamma = 2$ and $\delta(x) = 0$.

t	F	FD	DM
0.1	0.05087	0.05082	0.05058
0.2	0.06217	0.06224	0.06209
0.3	0.06871	0.06862	0.06868
0.4	0.07289	0,07286	0.07277
0.5	0.07574	0.07593	0.07572
0.6	0.07806	0.07827	0.07799
0.7	0.08041	0.08013	0.08019
0.8	0.08103	0.08164	0.08105
0.9	0.08214	0.08291	0.08226
1.0	0.08310	0.08398	0.08303
10	0.09468	0.09526	0.09466
20	0.08996	0.08994	0.08996
30	0.10289	0.10299	0.10288
40	0.09560	0.09561	0.09560
50	0.09127	0.09127	0.09127

In Table 1 we present absolute values of the numerical solutions on the boundary $x = L$ of problem (1.1) with $\delta(x) = 0$ and simple initial conditions $u_0(x) = \sin\frac{\pi x}{L}$. We set parameters $\gamma = 2$ and $L = 15$. Such choice is very interesting for applications. In column (F) of Table 1 we give results obtained by the classical Fourier method (1.5) with $N = 2000$. In column (FD) we present the results obtained by Finite difference method (2.7) with space step $h = 0.02$ and time step $\tau = 0.01$, and in the last column (DM) the results obtained by the DM-method with 240 grid points

Table 2. Values of $|u(x,t)|$ obtained by the DM method with the Chebyshev and Legendre nodes for $x = L = 15, \gamma = 2$ and $\delta(x) = \tanh(7x - 3.5L)$.

	$n = 60$			$n = 120$			$n = 240$	
t	Cheb.1	Leg.	Cheb.2	Cheb.1	Leg.	Cheb.2	Cheb.1	Cheb.2
0.1	0.0515	0.0498	0.0481	0.0511	0.0515	0.0514	0.0505	0.0506
0.2	0.0622	0.0632	0.0636	0.0628	0.0624	0.0613	0.0621	0.0621
0.3	0.0689	0.0698	0.0699	0.0685	0.0687	0.0683	0.0682	0.0685
0.4	0.0703	0.0710	0.0716	0.0729	0.0715	0.0718	0.0719	0.0718
0.5	0.0737	0.0734	0,0729	0.0745	0.0755	0.0746	0.0748	0.0745
0.6	0.0769	0.0768	0.0761	0.0762	0.0760	0.0751	0.0761	0.0759
0.7	0.0866	0.0858	0.0861	0.0847	0.0850	0.0848	0.0844	0.0843
0.8	0.0799	0.0801	0.0793	0.0789	0.0790	0.0787	0.0788	0.0788
0.9	0.0743	0.0757	0.0753	0.0761	0.0767	0.0760	0.0761	0.0760
1.0	0.0963	0.0949	0.0938	0.0939	0.0942	0.0942	0.0945	0.0944
10	0.1417	0.1417	0.1416	0.1422	0.1422	0.1422	0.1422	0.1422
20	0.1586	0.1586	0.1585	0.1577	0.1577	0.1577	0.1577	0.1577
30	0.1561	0.1561	0.1561	0.1549	0.1549	0.1549	0.1549	0.1549
40	0.1350	0.1350	0.1350	0.1339	0.1339	0.1339	0.1338	0.1338
50	0.0671	0.0671	0.0671	0.0684	0.0684	0.0684	0.0685	0.0685

distributed as zeroes of Chebyshev polynomials of the second kind are given. Numerical results were obtained by means of mathematical systems Maple-5 (Fourier series and Finite differences) and Mathematica 2.2 (the DM-method).

As we see, Finite differences and the DM-methods give the same order of accuracy, but such accuracy was achieved by the DM-method using approximately three times less grid points than by Finites differences. Moreover, the DM-method was very fast in calculations. It is due to the usage of the eigensystem of matrix **S** in (3.3) which allows us to solve (3.3) exactly. Therefore, we can easily calculate the numerical solution of (1.1) for any t without using discrete time integration. So, all results in column (DM) were obtained in 47 seconds on a computer with Celeron 400 processor and 256 mb RAM.

In Table 2 we present numerical results obtained by the DM-method with

$$\delta(x) = \tanh(7x - 3.5L), \quad \gamma = 2, \quad L = 15$$

and for different sets of n grid points ($n = 60, 120, 240$) distributed as zeroes of Chebyshev polynomials of the first and second kind and as zeroes of Legendre polynomials. We note that for $\delta(x) \neq const$, the method of Finite differences (2.7) has failed.

It is seen from Table 2, that all distributions of grid points with fixed n give the same accuracy which rises by increasing n. The corresponding graph of $|u(L,t|$ for $n = 240$ and nodes distributed as zeroes of Chebyshev polynomial of the second kind is shown in Fig.1, and the graphs of $|u(x,t)|$ at various time moments are shown in Fig.2.

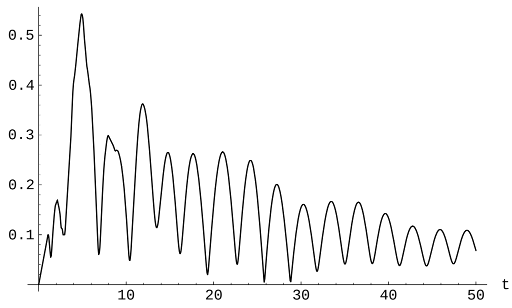

Figure 1. The graph of $|u(L,t)|$ for $\delta(x) = \tanh(7x - 3.5L)$.

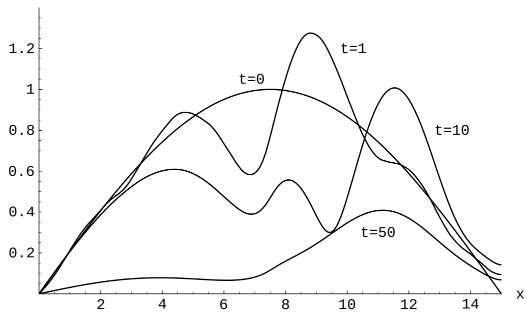

Figure 2. Evolution in time of $|u(x,t)|$ for $\delta(x) = \tanh(7x - 3.5L)$.

Thus we conclude that the DM method can be used efficiently to solve the problem (1.1) also for $\delta(x) \neq const$.

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Baigtinių skirtumų ir DM metodo lyginamoji analizė linearizuotam girotrono uždaviniui

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Nagrinėjamas kraštinis uždavinys Šredingerio lygčiai, aprašantis elektronų judėjimą girotrone. Darbe lyginami ir analizuojami Furje, baigtinių skirtumų ir degeneruotų matricų (DM) metodais gauti skaitiniai rezultatai. Aptartas metodo taikymas greitų osciliacijų atveju.