Analysis of splitting schemes for 2D and 3D Schrödinger problems

Aleksas Mirinavičius

Department of Mathematical Modelling, Vilnius Gediminas Technical University

Saulėtekio al. 11, LT-10223 Vilnius

E-mail: amirinavicius@gmail.com

Abstract. New splitting finite difference schemes for 2D and 3D linear Schrödinger problems are investigated. The stability and convergence analysis is done in the discrete L_2 norm. It is proved that the 2D scheme is unconditionally stable and conservative in the case of zero boundary condition. The splitting scheme is generalized for 3D problems. It is proved that in this case the scheme is only ρ-stable and consequently discrete conservation laws are no longer valid. Results of numerical experiments are presented.

Keywords: finite difference method, Schrödinger problem, ADI scheme, stability, convergence.

Introduction

Schrödinger problems are solved in variety of areas including nonlinear optics, laser physics and quantum mechanics. Thus fast numerical algorithms with good approximation properties are of practical importance.

We consider the following two and three dimensional $(d = 2, 3)$ linear Schrödinger problem

$$-i\frac{\partial u}{\partial t} = \sum_{s=1}^{d} \frac{\partial^2 u}{\partial x_s^2}, \quad (x_1, \ldots, x_d, t) \in \Omega \times (0, T], \tag{1}$$

$$u(x_1, \ldots, x_d, 0)|_{\bar{\Omega}} = u_0(x_1, \ldots, x_d), \tag{2}$$

$$u(x_1, \ldots, x_d, t)|_{\partial\Omega \times (0,T]} = \mu(x_1, \ldots, x_d, t), \tag{3}$$

in rectangular domain $\Omega = (a_1, b_1) \times \cdots \times (a_d, b_d)$. Hereafter spatial variables x_1, x_2 and x_3 will be denoted as x, y and z respectively.

1 Scheme for 2D Schrödinger problem

Finite difference splitting scheme under consideration is described in [1]. Domain $\bar{\Omega}$ is covered by discrete grid

$$\bar{\Omega}_h = \big\{ (x_j, y_k)\colon x_j = a_1 + jh, \ y_k = a_2 + kh, \ j = 0, \ldots, N_x, \ k = 0, \ldots, N_y \big\}.$$

One time step of the discrete scheme is implemented in two sub-steps: only tridiagonal systems of linear equations are solved:

$$-i\left(\mathcal{L}_x - i\frac{\tau}{2}\partial_x^2\right)\widehat{U}_{jk}^n = \mathcal{L}_y\partial_x^2 U_{jk}^n + \mathcal{L}_x\partial_y^2 U_{jk}^n, \quad (x_j, y_k) \in \Omega_h, \tag{4}$$

$$\widehat{U}_{jk}^n = \left(\mathcal{L}_y - i\frac{\tau}{2}\partial_y^2\right)\partial_t\mu_{jk}^n, \quad j = 0, N_x, \ k = 1, \ldots, N_y - 1, \tag{5}$$

$$\left(\mathcal{L}_y - i\frac{\tau}{2}\partial_y^2\right)\partial_t U_{jk}^n = \widehat{U}_{jk}^n, \quad (x_j, y_k) \in \Omega_h, \tag{6}$$

where the discrete operators are defined by the following formulas

$$\partial_t U_{jk}^n = \frac{U_{jk}^{n+1} - U_{jk}^n}{\tau}, \qquad \partial_x U_{jk}^n = \frac{U_{j+1,k}^n - U_{jk}^n}{h},$$

$$\mathcal{L}_y U_{jk}^n = \frac{1}{12}\left(U_{j,k-1}^n + 10U_{jk}^n + U_{j,k+1}^n\right).$$

Here $\mathcal{L}_y$ is the averaging operator. Equation (5) defines artificial boundary conditions for $\widehat{U}_{jk}^n$.

1.1 Stability, convergence and conservativity

We define the following discrete norms for grid functions W satisfying boundary conditions $W|_{\partial\Omega_h} = 0$:

$$\|W\| = \sqrt{\sum_{j=1}^{N_x-1}\sum_{k=1}^{N_y-1}|W_{jk}|^2 h^2}, \qquad \|W\|_x = \sqrt{\sum_{j=0}^{N_x-1}\sum_{k=1}^{N_y-1}|W_{jk}|^2 h^2},$$

$$\|W\|_y = \sqrt{\sum_{j=1}^{N_x-1}\sum_{k=0}^{N_y-1}|W_{jk}|^2 h^2}, \qquad \|W\|_E^2 = \|\partial_x W\|_x^2 + \|\partial_y W\|_y^2,$$

$$\|W\|_{L_\infty} = \max_{j=1,\ldots,N_x-1}\max_{k=1,\ldots,N_y-1}|W_{jk}|.$$

Eigenproblem for operators ∂_x^2 and $\mathcal{L}_x$

$$\partial_x^2 V_p = -\lambda_p V_p, \qquad \mathcal{L}_x V_p = \gamma_p V_p.$$

It is well known that for both eigenproblems in domain $(0,1)^2$ the orthonormal eigenvectors are defined as $V_p(x) = \sqrt{2}\sin p\pi x$.

Theorem 1. *Scheme* (4)–(6) *is unconditionally stable.*

Proof. We write the solution of problem (4)–(6) with $\mu \equiv 0$ as Fourier series:

$$U^n = \sum_{p=1}^{N_x-1}\sum_{q=1}^{N_y-1} c_{pq}^n V_p V_q. \tag{7}$$

We put (7) into (4), (6) and obtain coefficients:

$$c_{pq}^{n+1} = \frac{\gamma_p \gamma_q - \frac{\tau^2}{4}\lambda_p\lambda_q - i\frac{\tau}{2}(\lambda_p\gamma_q + \gamma_p\lambda_q)}{\gamma_p\gamma_q - \frac{\tau^2}{4}\lambda_p\lambda_q + i\frac{\tau}{2}(\lambda_p\gamma_q + \gamma_p\lambda_q)}c_{pq}^n = \alpha_{pq}^n c_{pq}^n.$$

By noting that the numerator of factor α_{pq}^n is complex conjugate of its denominator, we can easily conclude, that $|\alpha_{pq}^n| = 1$ and consequently $|c_{pq}^{n+1}| = |c_{pq}^n|$.

Next we derive discrete conservation laws for solution of the scheme (4)–(6) in the case of zero boundary condition $\mu \equiv 0$. It is well-known that the following norms can be calculated by using the Fourier coefficients:

$$\left\|U^n\right\|^2 = \sum_{p=1}^{N_x-1}\sum_{q=1}^{N_y-1}\left|c_{pq}^n\right|^2, \qquad \left\|U^n\right\|_E^2 = \sum_{p=1}^{N_x-1}\sum_{q=1}^{N_y-1}(\lambda_p + \lambda_q)\left|c_{pq}^n\right|^2. \qquad (8)$$

Since $|c_{pq}^{n+1}| = |c_{pq}^n|$, then it follows from (8) that splitting scheme satisfies discrete analogues of charge and energy conservation laws:

$$Q_h^n = \left\|U^n\right\|^2 = \|u_0\|^2, \qquad E_h^n = \left\|U^n\right\|_E^2 = \|u_0\|_E^2.$$

The following convergence theorem is valid. A proof of it is similar to 3D case analysis presented in the further section.

Theorem 2. *Suppose, that exact solution $u(x,y,t)$ of problem (1)–(3) is sufficiently smooth. Then solution of linear alternating direction implicit discrete scheme (4)–(6) converges to $u(x,y,t)$ and the following estimate is valid*

$$\max_{n=1,\dots,N_t}\left\|u^n - U^n\right\| \leqslant C\left(\tau^2 + h^4\right).$$

Example. We use Example 2 given in [1]. 2D Schrödinger problem (1)–(3) is solved in the rectangular domain $\Omega = (-2.5, 2.5) \times (-2.5, 2.5)$ with initial and boundary conditions obtained from the exact particular solution

$$u(x,y,t) = \frac{i}{i-4t}\exp\left[-i\left((x-1)^2 + (y-1)^2 + ik(x-1) + ik^2t\right)/(i-4t)\right],$$

where $k = 2.5$. Results of computational experiments are presented in Table 1, they show the second-order convergence in time and the fourth-order convergence in space in both L_2 and L_∞ norms.

Table 1. Absolute errors and convergence order ($t = 0.75$).

h	τ	$\|u^n - U^n\|$	$\|u^n - U^n\|_{L_\infty}$	Order	
				$\|\cdot\|$	$\|\cdot\|_{L_\infty}$
0.2	0.001	$9.52 \cdot 10^{-3}$	$4.78 \cdot 10^{-3}$		
0.1	0.001/4	$5.79 \cdot 10^{-4}$	$3.05 \cdot 10^{-4}$	4.04	3.97
0.05	0.001/16	$3.60 \cdot 10^{-5}$	$1.89 \cdot 10^{-5}$	4.01	4.01
0.025	0.001/64	$2.24 \cdot 10^{-6}$	$1.19 \cdot 10^{-6}$	4.00	3.99

2 Scheme for 3D Schrödinger problem

Square grid $\bar{\Omega}_h = \left\{ (x_j, y_k, z_l) \right\}$ is used for discretization of domain $\bar{\Omega}$.

We propose the following 3D alternating direction implicit (ADI) scheme:

$$-i\left(\mathcal{L}_x - \frac{i\tau}{2}\partial_x^2\right)\widehat{U}_{jkl}^n = \mathcal{L}_y\mathcal{L}_z\partial_x^2 U_{jkl}^n + \mathcal{L}_x\mathcal{L}_z\partial_y^2 U_{jkl}^n + \mathcal{L}_x\mathcal{L}_y\partial_z^2 U_{jkl}^n, \tag{9}$$

$$\left(\mathcal{L}_y - \frac{i\tau}{2}\partial_y^2\right)\widehat{\widehat{U}}_{jkl}^n = \widehat{U}_{jkl}^n, \tag{10}$$

$$\left(\mathcal{L}_z - \frac{i\tau}{2}\partial_z^2\right)\partial_t U_{jkl}^n = \widehat{\widehat{U}}_{jkl}^n, \tag{11}$$

with boundary conditions for $\widehat{U}^n$ and $\widehat{\widehat{U}}^n$

$$\widehat{U}_{jkl}^n = \left(\mathcal{L}_y - \frac{i\tau}{2}\partial_y^2\right)\left(\mathcal{L}_z - \frac{i\tau}{2}\partial_z^2\right)\partial_t\mu_{jkl}^n,$$

$$j = 0, N_x, \ k = 1, \ldots, N_y - 1, \ l = 1, \ldots, N_z - 1, \tag{12}$$

$$\widehat{\widehat{U}}_{jkl}^n = \left(\mathcal{L}_z - \frac{i\tau}{2}\partial_z^2\right)\partial_t\mu_{jkl}^n, \quad k = 0, N_y, \ j = 1, \ldots, N_x - 1, \ l = 1, \ldots, N_z - 1. \tag{13}$$

2.1 Stability with respect to the initial condition

The following estimates of eigenvalues of operators ∂_x^2 and $\mathcal{L}_x$ will be needed: $8 \leqslant \lambda_j \leqslant \frac{4}{h^2}$, $\frac{2}{3} \leqslant \gamma_j \leqslant 1$.

Similarly to 2D case we express the discrete solution as a sum

$$U^n = \sum_{p=1}^{N_x-1}\sum_{q=1}^{N_y-1}\sum_{r=1}^{N_z-1} c_{pqr}^n V_p V_q V_r, \tag{14}$$

where coefficients

$$c_{pqr}^{n+1} = \left(1 + \frac{\tau(\gamma_q\gamma_r\lambda_p + \gamma_p\gamma_r\lambda_q + \gamma_p\gamma_q\lambda_r)}{i(\gamma_p + \frac{i\tau}{2}\lambda_p)(\gamma_q + \frac{i\tau}{2}\lambda_q)(\gamma_r + \frac{i\tau}{2}\lambda_r)}\right)c_{pqr}^n = \alpha_{pqr}^n c_{pqr}^n. \tag{15}$$

Since $\lambda_j > 0$, $\gamma_j > 0$, it can be verified that $|\alpha_{pqr}^n| > 1$, so scheme is unconditionally unstable. Thus we can consider the ρ-stability of this scheme, only.

The following estimate can be easily derived:

$$\left|\alpha_{pqr}^n\right| \leqslant 1 + \tau\left(\frac{\lambda_p}{\gamma_p} + \frac{\lambda_q}{\gamma_q} + \frac{\lambda_r}{\gamma_r}\right) \leqslant 1 + \frac{18\tau}{h^2}. \tag{16}$$

2.2 Convergence

The error $Z_{jkl}^n = u_{jkl}^n - U_{jkl}^n$ satisfies the problem

$$-i\left(\mathcal{L}_x - \frac{i\tau}{2}\partial_x^2\right)\left(\mathcal{L}_y - \frac{i\tau}{2}\partial_y^2\right)\left(\mathcal{L}_z - \frac{i\tau}{2}\partial_z^2\right)\partial_t Z_{jkl}^n$$

$$= \mathcal{L}_y\mathcal{L}_z\partial_x^2 Z_{jkl}^n + \mathcal{L}_x\mathcal{L}_z\partial_y^2 Z_{jkl}^n + \mathcal{L}_x\mathcal{L}_y\partial_z^2 Z_{jkl}^n + R_{jkl}^n, \tag{17}$$

$$Z_{jkl}^0 = 0, \qquad Z_{jkl}^n|_{\partial \Omega_h} = 0, \tag{18}$$

where R_{jkl}^n is the approximation error. We write Z^n and R^n as sums:

$$Z^n = \sum_{p,q,r} z_{pqr}^n V_p V_q V_r, \qquad R^n = \sum_{p,q,r} r_{pqr}^n V_p V_q V_r. \tag{19}$$

Substituting (19) into (17) after simple computations we get

$$z_{pqr}^{n+1} = \alpha_{pqr}^n z_{pqr}^n + \tau \beta_{pqr}^n r_{pqr}^n, \tag{20}$$

where $\beta_{pqr}^n = \frac{i}{(\gamma_p + \frac{i\tau}{2}\lambda_p)(\gamma_q + \frac{i\tau}{2}\lambda_q)(\gamma_r + \frac{i\tau}{2}\lambda_r)}$.

Let us assume that $|\alpha_{pqr}^n| \leqslant \delta$. Since $\gamma_j \geqslant 2/3$, we get the estimate $|\beta_{pqr}| \leqslant 27/8$.

By using (20), we can express Z^{n+1} as sum of two discrete functions, then use the triangle inequality and finally by using the discrete Parseval's identity we deduce the stability estimate

$$\|Z^{n+1}\| \leqslant \delta\|Z^n\| + \frac{27}{8}\tau\|R^n\|. \tag{21}$$

By using (21) and since $\|R^n\| \leqslant C_a(\tau^2 + h^4)$ we get the following estimate

$$\|Z^n\| \leqslant \frac{27}{8}C_a\tau\left(\tau^2 + h^4\right)\frac{\delta^n - 1}{\delta - 1}. \tag{22}$$

If we choose $\tau = Ch^{2+\eta}$ and use inequality (16), then we obtain the estimate

$$\left|\alpha_{pqr}^n\right| \leqslant 1 + Ch^\eta = 1 + \tilde{C}\tau^{1/(2+\eta)} = \delta,$$

which is acceptable for the stability with respect to the initial condition. But by extending inequality (22) we get

$$\|Z^n\| = \mathcal{O}\left(h^{2(3+\eta)} \exp\left(n^{1-1/(2+\eta)}\right)\right),$$

thus controlling the error growth and getting convergence of the discrete solution can be problematic.

Example 1. We solve equation (1) with $d = 3$ in domain $(0,1) \times (0,1) \times (0,1)$ with initial and boundary conditions (2)–(3) prescribed from the exact solution:

$$u(x, y, z, t) = \sin(\pi x)\sin(\pi y)\sin(\pi z)\exp\left(-3i\pi^2 t\right). \tag{23}$$

Table 2. Absolute errors and convergence order ($t = 0.75$).

N_x	N_t	$\|u^n - U^n\|$	$\|u^n - U^n\|_{L_\infty}$	Order
VC6				
5	313	$5.18 \cdot 10^{-3}$	$1.26 \cdot 10^{-2}$	
10	1252	$3.20 \cdot 10^{-4}$	$9.05 \cdot 10^{-4}$	4.02
20	5008	$2.40 \cdot 10^{-5}$	$8.77 \cdot 10^{-5}$	3.74
icc				
5	313	$5.18 \cdot 10^{-3}$	$1.26 \cdot 10^{-2}$	
10	1252	$3.20 \cdot 10^{-4}$	$9.05 \cdot 10^{-4}$	4.02
20	5008	$3.14 \cdot 10^{-5}$	$1.17 \cdot 10^{-4}$	3.35

A code implementing ADI scheme for 3D problem was compiled by using two different compilers (VC6, icc). Results of computations are presented in Table 2. We note significant differences in results for different compilers which may be due to the lack of classical stability estimates with respect to the right hand side.

References

[1] Z. Gao and S. Xie. Fourth-order alternating direction implicit compact finite difference schemes for two-dimensional Schrödinger equations. *Appl. Numer. Math.*, **61**:593–614, 2011.

REZIUMĖ

Skaidymo schemų dvimačiams ir trimačiams Šrėdingerio uždaviniams analizė
A. Mirinavičius

Tiriamos naujos skaidymo baigtinių skirtumų schemos dvimačiams ir trimačiams tiesiniams Šrėdingerio uždaviniams. Stabilumo ir konvergavimo analizė atlikta diskrečioje L_2 normoje. Įrodyta, kad dvimatė schema yra nesąlygiškai stabili ir konservatyvi nulinės kraštinės sąlygos atveju. Skaidymo schema apibendrinta trimačiams uždaviniams. Įrodyta, kad šiuo atveju schema yra tik ρ-stabili ir todėl diskretieji tvermės dėsniai jau nebegalioja. Pateikti skaitinių eksperimentų rezultatai.

Raktiniai žodžiai: baigtinių skirtumų metodas, Šrėdingerio uždavinys, kintamųjų krypčių neišreikštinė schema, stabilumas, konvergavimas.