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ROTHE-MARUYAMA DIFFERENCE SCHEME FOR THE STOCHASTIC SCHRÖDINGER EQUATION

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Abstract: In this study, the initial value stochastic Schrödinger type problem in an abstract Hilbert space with the self-adjoint operator is investigated.

Rothe-Maruyama method for the numerical solution of this problem is presented. Theorem on the convergence of this difference scheme is established. A numerical example is given.

AMS Subject Classification: 60H30, 35J25, 65H10
Key Words: Rothe-Maruyama differrence scheme; modified Gauss elimination method; stochastic Schrödinger equation

1. Introduction

In the literature, stochastic and deterministic type Schrödinger equations have been extensively studied by many researchers (see [2], [3], [6], [11] and the references given therein). Although, in any Hilbert space, numerical approximation of abstract stochastic Schrödinger equation, using Rothe-Maruyama difference scheme has not been studied yet. In this article, the initial value problem for the stochastic Schrödinger equation

$$idu(t) + Au(t)dt = f(t)dw_t, \ 0 < t < T, \ u(0) = 0 \tag{1}$$

in a Hilbert space H with a self-adjoint positive definite operator A is considered. For the approximate solution of (1), first order of accuracy Rothe-Maruyama difference scheme is constructed. The results are supported by nu-

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merical implementation. Throughout the paper:

(i) w_t is a standard Wiener process given on the probability space (Ω, F, P).

(ii) $f(z)$ is an element of the space $M_w^2([0,T], H_1)$ for any $z \in [0,T]$, where H_1 is a subspace of H.

Here, $M_w^2([0,T], H)$ denote the space of $H-$valued measurable processes which satisfy :

(a) $\phi(t)$ is F_t measurable, a.e. in t,

(b) $E\int\limits_0^T \|\phi(t)\|_H^2 \, dt < \infty$.

Strong, mild and weak solutions of stochastic differential equations are studied by many researchers, as an example see [5], [10]. In the present paper, following [1] and [4], we study the initial value problem (1) in a Hilbert space.

Our main interest in this study is to construct and investigate the single-step Rothe-Maruyama difference scheme for the numerical solution problem (1). On the segment $[0,T]$ we consider the uniform grid space

$$[0,T]_\tau = \{t_k = k\tau, k = 0, 1, ..., N, N\tau = T\} \tag{2}$$

with step size $\tau > 0$ and N is an arbitrary but fixed positive integer.

Note that for the self-adjoint operator A in a Hilbert space H, linear operator e^{itA} is bounded and it is a strongly continuous semigroup (see [8], [9]). Also,

$$\left\|e^{itA}\right\|_{H \to H} \leq 1 \tag{3}$$

and

$$u(t) = -i \int\limits_0^t e^{i(t-s)A} f(s) dw_s \tag{4}$$

is a unique mild solution of the problem (1) under the assumptions $(i) - (ii)$.

2. Rothe-Maruyama Difference Scheme

First, applying the semigroup property of e^{itA} and single step difference scheme for solution of problem (1) and replacing $e^{i\tau A}$ by $R = (I - i\tau A)^{-1}$, we can construct the corresponding Rothe-Maruyama difference scheme (see [1])

$$\begin{cases} i(u_k - u_{k-1}) + \tau A u_k = f(t_{k-1})\Delta w_k, \\ \Delta w_k = w_k - w_{k-1}, 1 \leq k \leq N,\ u_0 = 0 \end{cases} \tag{5}$$

for the numerical solution of problem (1). By induction, we can write

$$u_k = -i \sum_{j=1}^{k} R^{k-j+1} f(t_{j-1})\Delta w_j \tag{6}$$

for the solution of the Rothe-Maruyama difference scheme (5). Now we show that Rothe-Maruyama difference scheme (5) for the solution of problem (1) has a convergence of order 1/2. It is possible under stronger assumption than (ii) for $f(t)$: case without Wiener process. Assume that

$$\max_{0\leq t\leq T} \|A^2 f(t)\|_H + \max_{0\leq t\leq T} \|Af'(t)\|_H \leq M_4. \tag{7}$$

Moreover, for this we need some related estimates which is stated in the following lemma.

Lemma 1. *Let A be a self-adjoint positive definite operator, then the following estimates hold:*

$$\|A^\alpha R^k\|_{H\to H} \leq \frac{M_1}{(\sqrt{k}\tau)^\alpha},\ 1 \leq k \leq N,\ 0 \leq \alpha \leq 1, \tag{8}$$

$$\|A^{-\beta}(R^k - e^{ik\tau A})\|_{H\to H} \leq M_2(\sqrt{k}\tau)^\beta,\ 1 \leq k \leq N,\ 1 \leq \beta \leq 2. \tag{9}$$

Here the positive constants M_1 and M_2 do not depend on k and τ but depend on α and β, respectively.

Proof. For $0 \leq \alpha \leq 1$ except the case $\alpha = k = 1$ using the spectral representations of self-adjoint operators we have

$$\|A^\alpha R^k\|_{H\to H} \leq \sup_{-\infty<\mu<\infty} \frac{|\mu^\alpha|}{(1+\tau^2\mu^2)^{k/2}}.$$

Let $g(\mu) = \frac{\mu^\alpha}{(1+\tau^2\mu^2)^{k/2}}$. Then, $g(\mu)$ attains its supremum at $g'(\mu^*) = 0$, that is for $(\mu^*)^2 = \frac{\alpha}{(k-\alpha)\tau^2}$. The supremum of $g(\mu)$ is

$$g(\mu^*) = (\frac{\alpha}{(k-\alpha)\tau^2})^{\alpha/2}(\frac{1}{1+\frac{\alpha}{k-\alpha}})^{k/2} = \frac{\alpha^{\alpha/2}}{(\sqrt{k}\tau)^\alpha}(\frac{k-\alpha}{k})^{(k-\alpha)/2}$$

$$\leq \frac{\alpha^{\alpha/2}}{(\sqrt{k}\tau)^\alpha} \leq \frac{M_1}{(\sqrt{k}\tau)^\alpha}.$$

Now let us consider the case $\alpha = k = 1$. Using the spectral representation of self-adjoint operators, we get

$$\|AR\|_{H\to H} \leq \sup_{\infty<\mu<\infty} \frac{|\mu|}{|1-i\tau\mu|} \leq \frac{1}{\tau}.$$

Hence the estimate (8) holds. Now let $R(s) = (I - i\tau sA)^{-1}$. Then

$$\|A^{-\beta}(R^k(s) - e^{ik\tau A})\|_{H\to H}$$

$$= \|A^{-\beta}\int_0^1 \frac{d}{ds}(R^k(s)e^{ik\tau(1-s)A})ds\|_{H\to H}$$

$$= \|A^{-\beta}\int_0^1 ik\tau AR^{k+1}(s)e^{ik\tau(1-s)A}(i\tau sA)ds\|_{H\to H}$$

$$\leq k\tau^2\int_0^1 \|A^{-\beta+2}R^{k+1}(s)\|_{H\to H}\|e^{ik\tau(1-s)A}\|_{H\to H}sds$$

$$\leq k\tau^2\int_0^1 \frac{M_1}{(\sqrt{k+1}\tau s)^{2-\beta}}sds \leq M_1(\sqrt{k}\tau)^\beta.$$

Hence the estimate (9) holds for some positive constant M_1 depends on β, but not depends on k and τ. □

Theorem 2. *Let A be a self-adjoint positive definite operator and $A \geq \delta I(\delta > 0)$. Then, the Rothe-Maruyama difference scheme (5) for the solution of problem (1) has a convergence of order 1/2. That is, the convergence estimate*

$$\max_{0\leq k\leq N} \left(E\|u(t_k) - u_k\|_H^2\right)^{1/2} \leq M\tau^{1/2} \tag{10}$$

holds. Here the positive constant M does not depend on τ.

Proof. By (6), we have the formula

$$u(t_k) - u_k = T_{1k} + T_{2k} + T_{3k}, \tag{11}$$

where

$$T_{1k} = -i\sum_{j=1}^{k}[e^{i(k-j)\tau A} - R^{k-j}]\int_{t_{j-1}}^{t_j} e^{i(t_j-s)A}f(s)dw_s], \tag{12}$$

$$T_{2k} = -i\sum_{j=1}^{k} R^{k-j}[\int_{t_{j-1}}^{t_j} e^{i(t_j-s)A}f(s)dw_s - e^{i\tau A}f(t_{j-1})\Delta w_j], \tag{13}$$

$$T_{3k} = -i\sum_{j=1}^{k} R^{k-j}[e^{i\tau A} - R]f(t_{j-1})\Delta w_j. \tag{14}$$

We estimate these three terms separetely. First, let us obtain an estimate for T_{1k}. Using the triangle inequality, inequality (9), Ito isometry and estimate (7), we have

$$E\|T_{1k}\|_H^2$$

$$\leq \sum_{j=1}^{k} \|A^{-1}[e^{i(k-j)\tau A} - R^{k-j}]\|_{H\to H}^2 \int_{t_j-1}^{t_j} \|Ae^{i(t_j-s)A}f(s)\|_H^2 ds$$

$$\leq \sum_{j=1}^{k} M_2^2((k-j)\tau^2)\int_{t_{j-1}}^{t_j} \|Af(t)\|_H^2 ds$$

$$\leq \sum_{j=1}^{k} M_2^2 T\tau \int_{t_{j-1}}^{t_j} \|Af(t)\|_H^2 ds \leq M_2^2 T^2 \tau \left(\max_{0\leq t\leq T} \|Af(t)\|_H\right)^2.$$

Hence,

$$\max_{0\leq k\leq N} \left(E\|T_{2k}\|_H^2\right)^{1/2} \leq M_2 T \tau^{1/2}.$$

Now let us estimate T_{2k}.

$$E\|T_{2k}\|_H^2$$

$$= E\left\|\sum_{j=1}^{k} R^{k-j}\int_{t_j-1}^{t_j} [e^{i(t_j-s)A}f(s)dw_s - e^{i\tau A}f(t_{j-1})\Delta w_j]\right\|_H^2$$

$$\leq \sum_{j=1}^{k} \|R^{k-j}\|_{H\to H}^2 E \left\| \int_{t_j-1}^{t_j} (e^{i(t_j-s)A} f(s) - e^{i\tau A} f(t_{j-1})) dw_s \right\|_H^2$$

$$\leq \sum_{j=1}^{k} E \left\| \int_{t_j-1}^{t_j} \int_{t_j-1}^{s} \frac{d}{dx} (e^{i(t_j-x)A} f(x)) dx dw_s \right\|_H^2$$

$$\leq \sum_{j=1}^{k} E \left(\int_{t_j-1}^{t_j} \int_{t_j-1}^{s} \| -iAe^{i(t_j-x)} Af(x) + e^{i(t_j-x)} Af'(x)\|_H dx dw_s \right)^2$$

$$\leq M_4^2 \sum_{j=1}^{k} E \left(\int_{t_j-1}^{t_j} \int_{t_j-1}^{s} dx dw_s \right)^2$$

$$\leq M_4^2 \sum_{j=1}^{k} \int_{t_j-1}^{t_j} \left(\int_{t_j-1}^{s} dx \right)^2 ds \leq M_4^2 \sum_{j=1}^{k} \tau^3 \leq M_4^2 \tau.$$

Let us estimate T_{3k}. For $k \neq j$

$$E\|T_{3k}\|_H^2 = E \left\| -i \sum_{j=1}^{k} R^{k-j} [e^{i\tau A} - R] f(t_{j-1}) \Delta w_j \right\|^2$$

$$\leq \sum_{j=1}^{k} \|AR^{k-j}\|_H^2 \left\|A^{-2}[e^{i\tau A} - R]\right\|_H^2 \|Af(t_{j-1})\|_H^2 j$$

$$\leq \sum_{j=1}^{k} \frac{M_1^2}{j\tau^2} M_2^2 \tau^4 M_4^2 j \leq M_1^2 M_2^2 M_4^2 T\tau.$$

For $k = j$, using the Taylor expansion formula for exponential function and R, easily seen that $\max\limits_{0\leq k\leq N} \left(E\|T_{3k}\|_H^2\right)^{1/2} \leq M\tau^{1/2}$. Therefore,

$$\max_{0\leq k\leq N} \left(E\|T_{3k}\|_H^2\right)^{1/2} \leq M\tau^{1/2}.$$

Hence the result follows from the estimates of T_{1k}, T_{2k}, T_{3k}. □

3. Numerical Results

In this section, the numerical experiments of the initial value problem

$$\begin{cases} idu(t,x) - u_{xx}(t,x)dt = ie^{it\pi^2}\sin(\pi x)dw_t, \\ 0 < t, x < 1, \quad u(0,x) = 0, \quad 0 \le x \le 1, \\ u(t,0) = u(t,1) = 0, \qquad 0 \le t \le 1, \end{cases} \tag{15}$$

for the stochastic Schrödinger equation using Rothe-Maruyama difference scheme are presented. It is clear that this problem satisfies the assumptions of Theorem 2. The exact solution of this problem is

$$u\,(t,x) = \ e^{it\pi^2}\,(\sin\pi x)\,w_t.$$

Here $w_t = \sqrt{t}\xi$, $\xi \in N(0,1)$. For the approximate solution of problem (15), the set $[0,1]_\tau \times [0,1]_h$ of a family of grid points depending on the small parameters τ and h

$$\begin{aligned} [0,1]_\tau \times [0,1]_h &= \{(t_k, x_n) : t_k = k\tau,\ 0 \le k \le N,\ \ N\tau = 1, \\ x_n &= nh,\ \ 0 \le n \le M, Mh = 1\} \end{aligned}$$

is defined. We suggest the following Rothe-Maruyama difference scheme for the approximate solution of problem (15)

$$\begin{cases} i(u_n^k - u_n^{k-1}) - \dfrac{\left(u_{n+1}^k - 2u_n^k + \pi^2 u_{n-1}^k\right)\tau}{h^2} = f(t_k, x_n)\Delta w_k, \\ 1 \le k \le N, \quad 1 \le n \le M-1, \quad \Delta w_k = w_k - w_{k-1}, \\ u_n^0 = 0,\ 1 \le n \le M-1, \quad u_0^k = 0,\ u_M^k = 0,\ 0 \le k \le N. \end{cases} \tag{16}$$

So we have $(N+1) \times (N+1)$ system of linear equations which can be written in the matrix form as:

$$\begin{cases} AU_{n+1} + B\,U_n + CU_{n-1} = D\varphi_n, \quad 1 \le n \le M-1, \\ U_0 = 0,\ U_M = 0, \end{cases} \tag{17}$$

where

$$\varphi_n = \begin{bmatrix} \varphi_n^0 \\ \varphi_n^1 \\ \cdots \\ \varphi_n^N \end{bmatrix}_{(N+1)\times 1}, \qquad \varphi_n^k = \begin{cases} 0, & k = 0, \\ f(t_k, x_n), & 1 \le k \le N, \end{cases}$$

$A(i,i+1) = a$, $B(i,i+1) = c$, $C(i,i+1) = d$ for any $1 \leq i \leq N$, $B(i,i) = b$ for any $1 \leq i \leq N+1$, $B(N+1,1) = 1$ and the other entries for the matrices A, B and C are all zero. The matrix D is an identity matrix of order $N+1$ and

$$U_s = \left[U_s^0, U_s^1, ..., U_s^{N-1}, U_s^N\right]^t, \quad s = \ n-1, n, n+1.$$

In the above matrices entries are

$$a = -\frac{\tau}{h^2}, \ b = -i, \ c = i + \frac{2\tau}{h^2}, \ d = -\frac{\tau}{h^2}.$$

Thus, we have the first order difference equation with respect to n with matrix coefficients. To solve this difference equation we have applied the same modified Gauss elimination method for the difference equation with respect to n with matrix coefficients as in [7]. For the comparison of the numerical solution of the difference equation and the analytical solution of the differential equation, the error terms are computed by the following formulation:

$$E_M^N = \max_{1 \leq k \leq N} \frac{1}{N_{sim}} \sum_{j=1}^{N_{sim}} \left(\sum_{n=1}^{M-1} \left[u(t_k, x_n) - u_n^k\right]^2 h \right)^{1/2}.$$

The numerical solutions of the problem (15) are recorded for various values of N and M based on the numerical scheme (16), where $u(t_k, x_n)$ represents the exact solution and u_n^k represents the numerical solution at (t_k, x_n). The result are shown in the Table 1 for $N = M = 5$, 10, 20, 40. In all of these numerical experiments the number of simulations N_{sim} is kept constant at 1000. Hence, each numerical problem has been solved based on 1000 different sample paths for the process of standard Brownian motion w_t.

Table 1. Comparison of the errors for the exact solution of the differential equation (15) and the numerical solution of the Rothe-Maruyama difference scheme (16).

$N = M = 5$	$N = M = 10$	$N = M = 20$	$N = M = 40$
0.37923	0.2557	0.13629	0.06927

From Table 1 it is seen that, using the Monte Carlo simulation, the Rothe-Maruyama difference (16) converges to the solution of stochastic Schrödinger equation (15).

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