ROTHE-MARUYAMA DIFFERENCE SCHEME FOR
THE STOCHASTIC SCHRÖDINGER EQUATION

Ali Sirma
Halic University
Beyoglu, Istanbul – 34445, TURKEY

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.

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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

\[ i du(t) + Au(t)dt = f(t)dw_t, \quad 0 < t < T, \quad u(0) = 0 \]  

(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-
Numerical implementation. Throughout the paper:

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

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

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

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

(b) \( E \int_0^T \| \phi(t) \|^2_H \, dt < \infty \).

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

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

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,

\[ \| e^{itA} \|_{H \to H} \leq 1 \]  

(3)

and

\[ u(t) = -i \int_0^t e^{i(t-s)A} f(s) dw_s \]  

(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])

\[
\begin{cases}
  i(u_k - u_{k-1}) + \tau Au_k = f(t_{k-1})\Delta w_k, \\
  \Delta w_k = w_k - w_{k-1}, 1 \leq k \leq N, u_0 = 0
\end{cases}
\]

(5)

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

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

(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

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

(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:

\[
\|A^\alpha R^k\|_{H \rightarrow H} \leq \frac{M_1}{(\sqrt{k\tau})^\alpha}, \quad 1 \leq k \leq N, \quad 0 \leq \alpha \leq 1,
\]

(8)

\[
\|A^{-\beta}(R^k - e^{i\tau A})\|_{H \rightarrow H} \leq M_2(\sqrt{k\tau})^\beta, \quad 1 \leq k \leq N, \quad 1 \leq \beta \leq 2.
\]

(9)

Here the positive constants $M_1$ and $M_2$ do not depend on $k$ and $\tau$ but depend on $\alpha$ and $\beta$, respectively.

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

\[
\|A^\alpha R^k\|_{H \rightarrow H} \leq \sup_{-\infty < \mu < \infty} \frac{|\mu^\alpha|}{(1 + \tau^2 \mu^2)^{k/2}}.
\]}
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 \( (\mu^*)^2 = \frac{\alpha}{(k-\alpha)\tau^2} \). The supremum of \( g(\mu) \) is

\[
g(\mu^*) = \left( \frac{\alpha}{(k-\alpha)\tau^2} \right)^{\alpha/2} \left( \frac{1}{1 + \frac{\alpha}{\kappa - \alpha}} \right)^{k/2} = \frac{\alpha^{\alpha/2}}{(\sqrt{k} \tau)^\alpha} \left( \frac{k - \alpha}{k} \right)^{(k-\alpha)/2}
\]

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

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

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

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

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

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

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

Hence the estimate (9) holds for some positive constant \( M_1 \) depends on \( \beta \), but not depends on \( k \) and \( \tau \). 

**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

\[
\max_{0 \leq k \leq N} (E\|u(t_k) - u_k\|_H^2)^{1/2} \leq M\tau^{1/2}
\]

holds. Here the positive constant \( M \) does not depend on \( \tau \). 

**Proof.** By (6), we have the formula

\[ u(t_k) - u_k = T_{1k} + T_{2k} + T_{3k}, \]

where

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

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

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

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

\[ E\|T_{1k}\|_H^2 \leq \sum_{j=1}^{k} \left\| A^{-1}[e^{i(k-j)\tau A} - R^{k-j}] \right\|_{H \rightarrow H}^2 \int_{t_{j-1}}^{t_j} \left\| A e^{i(t_j-s)A} f(s) \right\|_H^2 ds \]

\[ \leq \sum_{j=1}^{k} M_2^2 ((k-j)\tau^2) \int_{t_{j-1}}^{t_j} \left\| A f(t) \right\|_H^2 ds \]

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

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 \( T_{2k} \).

\[ E\|T_{2k}\|_H^2 \]

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

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

\[
\leq \sum_{j=1}^{k} E \left( \int_{t_j-1}^{t_j} \int_{t_j-1}^{s} \left\| -iAe^{i(t_j-x)} Af(x) + e^{i(t_j-x)} Af'(x) \right\|_{H dx dw} \right)^2
\]

\[
\leq M_4^2 \sum_{j=1}^{k} \left( \int_{t_j-1}^{t_j} \int_{t_j-1}^{s} dx dw \right)^2
\]

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

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

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

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

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

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

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

Hence the result follows from the estimates of $T_{1k}, T_{2k}, T_{3k}$. \qed
3. Numerical Results

In this section, the numerical experiments of the initial value problem
\[
\begin{cases}
  idu(t, x) - u_{xx}(t, x) dt = i e^{i t \pi^2} \sin(\pi x) dw_t, \\
  0 < t, x < 1, \quad u(0, x) = 0, \quad 0 \leq x \leq 1, \\
  u(t, 0) = u(t, 1) = 0, \quad 0 \leq t \leq 1,
\end{cases}
\]
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
\[
u(t, x) = e^{i t \pi^2} (\sin \pi x) w_t.
\]

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 \( \tau \) and \( h \)
\[
[0, 1]_\tau \times [0, 1]_h = \{(t_k, x_n) : t_k = k \tau, \quad 0 \leq k \leq N, \quad N \tau = 1, \\
x_n = nh, \quad 0 \leq n \leq M, \quad Mh = 1\}
\]
is defined. We suggest the following Rothe-Maruyama difference scheme for the approximate solution of problem (15)
\[
\begin{cases}
  i(u_n^k - u_n^{k-1}) - \frac{(u_{n+1}^k - 2u_n^k + \pi^2 u_{n-1}^k)}{h^2} \tau = f(t_k, x_n) \Delta w_k, \\
  1 \leq k \leq N, \quad 1 \leq n \leq M - 1, \quad \Delta w_k = w_k - w_{k-1}, \\
  u_0^0 = 0, \quad 1 \leq n \leq M - 1, \quad u_0^k = 0, \quad u_M^k = 0, \quad 0 \leq k \leq N.
\end{cases}
\]
So we have \((N + 1) \times (N + 1)\) system of linear equations which can be written in the matrix form as:
\[
\begin{cases}
  AU_{n+1} + BU_n + CU_{n-1} = D \varphi_n, \quad 1 \leq n \leq M - 1, \\
  U_0 = 0, \quad U_M = 0,
\end{cases}
\]
where
\[
\varphi_n = \begin{bmatrix}
  \varphi_n^0 \\
  \varphi_n^1 \\
  \vdots \\
  \varphi_n^N
\end{bmatrix}_{(N+1) \times 1}, \quad \varphi_n^k = \begin{cases}
  0, & k = 0, \\
  f(t_k, x_n), & 1 \leq k \leq N,
\end{cases}
\]
\[ A(i, i + 1) = a, \quad B(i, i + 1) = c, \quad C(i, i + 1) = d \]
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

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

In the above matrices entries are

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

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:

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

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 \(u^k_n\) 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).

| \(N = M\) | 0.37923 | 0.2557 | 0.13629 | 0.06927 |
|---|---|---|---|---|
| 5 | 10 | 20 | 40 |

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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References

[1] A. Ashyralyev, On modified Crank-Nicholson difference schemes for stochastic parabolic equation, *Numer. Funct. Anal. Optim.*, 29, No 3-4 (2008), 268-282.

[2] A. Ashyralyev, A. Sirma, Nonlocal boundary value problems for the Schrödinger equation, *Comput. Math. Appl.*, 55 (2008), 392-407.

[3] A. Kharab, H. Eleuch, Analytical solution of the position dependent mass Schrödinger equation with a hyperbolic tangent potential, *International Journal of Applied Mathematics*, 32, No 2 (2019), 357-367; doi:10.12732/ijam.v32i2.14.

[4] A. Ashyralyev, M.E. San, An approximation of semigroups method for stochastic parabolic equations, *Abstr. Appl. Anal.*, 2012 (2012), 1-24; doi:10.1155/2012/684248.

[5] C. Privot, M. Röchner, *A Concise Course on Stochastic Partial Differential Equations*, Springer-Verlag, Berlin (2007).

[6] L. Bouten, M. Guta, H. Maassen, Stochastic Schrödinger equations, *J. Phys. A. Math. Gen.*, 37 (2004), 3189-3209.

[7] C. Ashyralyyev, Stability of Rothe difference scheme for the reverse parabolic problem with integral boundary condition, *Math. Meth. Appl. Sci.*, 43 (2020), 5369–5379.

[8] H.O. Fattorini, *Second Order Linear Differential Equations in Banach Space*, Notas de Matematica, North-Holland (1985).

[9] A. Ashyralyev, H.O. Fattorini, On uniform difference-schemes for 2nd-order singular perturbation problems in Banach spaces, *SIAM J. Math. Anal.*, 23, No 1 (1992), 29–54.

[10] G. Da Prato, J. Zabczyk, *Stochastic Equations in Infinite Dimensions*, Encyclopedia of Mathematics and its Applications Book 152, Cambridge University Press (2014).
[11] A. Ashyralyev, D. Agirseven, On the stable difference schemes for the Schrödinger equation with time delay, *Computational Methods in Applied Mathematics*, 20, No 1 (2020), 27-38.