Numerical Exponential Stability of a Time-Dependent Stochastic Schrödinger Equation

Cutberto Romero-Meléndez[1*], David Castillo-Fernández[2]

[1] Department of Basic Sciences, Autonomous Metropolitan University, Mexico.
[2] Engineering Department, La Salle University, México.

*Corresponding author. Tel.: +52 5534359640; email: cutberto@azc.uam.mx
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Abstract: In this work, we will define two new types of exponential asymptotic stability for the Euler-Maruyama numerical scheme in the stochastic controlled Schrödinger equation dependent on time, corresponding to a stochastic quantum two-level system, namely, almost sure exponential robust stability and asymptotic stability. These types of stability are variants of Mao and Mora definitions for the stability of numerical schemes, in the control case. Through the techniques used by Tsoi, we demonstrate the almost sure exponential robust stability and the asymptotic stability of the Euler-Maruyama numerical scheme for the stochastic controlled Schrödinger equation.

Key words: Asymptotic stability, Euler-Maruyama numerical scheme, exponential robust stability, time-dependent stochastic controlled Schrödinger equation.

1. Introduction

Many applications on control of quantum systems have led to questions about the stochastic stability and robustness of solutions. If we require to select the optimal control so that the stochastic quantum system steers an initial state to a target with probability one, minimizing the cost, requiring some asymptotic stability properties for the resulting system, it is important to have several stability results that allow achieving the desired task. We can use stability results to select controls assuring asymptotic stability properties. Also, studying the stability of the numerical schemes for stochastic controlled Schrödinger equations and computing approximations, it's important to analyze the choice of step size Δt_k, in order to extend the stability properties to the exact solution of the corresponding stochastic controlled Schrödinger equation, by very large time. There are different types of exponential stochastic stability and we look for the most suitable four our optimal control problem.

The stability and robustness analysis of numerical computations in the stochastic controlled Schrödinger equation is motivated, at first, by the insensitivity of the numerical solution found via Euler-Maruyama numerical scheme, with respect to the ensemble of parameters related with the Nuclear Magnetic Resonance (NMR) phenomenon. For this purpose, in this paper we will considerate asymptotic and robust analysis to study the stability of solutions of Euler-Maruyama numerical scheme for the time-dependent stochastic Schrödinger equation.

2. Preliminaries

We consider the following stochastic controlled quantum system: a two-level open quantum system interacting on the one hand with a constant and longitudinal static electromagnetic field with magnitude $B_0 = 1$ in the direction of the Z axis and the other hand, with two randomly time varying electromagnetic fields, one of them with amplitude $u_1(t)$ along the X axis and the other, with amplitude $u_2(t)$ along the Y axis. This two-level quantum system is governed by the time-dependent Schrödinger equation for a pure state (we use natural units, $\hbar$ =1):

$$\frac{d}{dt}\psi(t) = -iH\big(u(t)\big)\psi(t), \tag{1}$$

where $\psi = (\psi_1, \psi_2): [0, T] \rightarrow \mathbb{C}^2$ is a quantum state, $u: [0, T] \rightarrow \mathbb{R}$, $u(\mathrm{t}) = (u_1(t), u_2(t))$ are stochastic controls and the energy of the system is represented by the Hamiltonian operator $H(t)$. By splitting real and imaginary parts of ψ and considering $x: = (\psi_{\mathbb{R}}, \psi_{\Im})^t$, we obtain, as in [1], the following equivalent stochastic differential system:

$$dx(t) = S_3 x(t)\, dt + (S_2 u_2(t) + S_1 u_1(t))x(t)\, dW, \tag{2}$$

With initial state $x\left(\frac{\pi}{\sqrt{2}}\right) = (0,0,0,1)$, where S_i is the real representation of the Pauli matrix, for $i = 1,2,3$, $W(t)$ is a standard Wiener real process, defined over a probabilistic real valued space $(\Omega, B, \{B_t\}, P)$ and $\{B_t\}_{t>0}$ is a sub-σ-algebra defined by the usual conditions. Let $\|\ \|$ be the Euclidean norm in $\mathbb{R}^n$ and let's consider the trace as the norm in $\mathbb{R}^{nm}$. In the context of the optimal control, equation (2) represent a stochastic differential system whose analytic solution cannot be found, so numerical solution is needed. So, in [1], we use the Euler-Maruyama method.

The Euler-Maruyama method is obtained by truncating the Itô's formula of the stochastic Taylor series after the first terms. This method computes approximations $x_{k+1} \approx x_k(k\Delta t)$, selecting a grid of [0, T] : $0 < t_0 < \cdots < t_N = T$ and defining $\Delta t_{k+1} = t_{k+1} - t_k$ and $\Delta W_{k+1} = W(t_{k+1}) - W(t_k)$:

$$x_{k+1} = x_k + S_3 x_k \Delta t_{k+1} + \big(S_1 u_1(t) + S_2 u_2(t)\big) x_k \Delta W_{k+1} \tag{3}$$

Now, in order to addressing the concepts of stochastic stability in our discussion and according to Lyapunov theory, it is important to introduce a Lyapunov function $V(t,x) \in C^{1,2}(\mathbb{R}^+ \times \mathbb{R}^n; \mathbb{R}^+)$, which allows to guarantee the stability of the solution of the stochastic differential equation

$$dx(t) = b(t,x)dt + \sigma(t,x)dW \tag{4}$$

The aforementioned function $V(t,x)$ must satisfy, according to Itô's formula, the expression:

$$dV(t,x) = LV(t,x)dt + V_x(t,x)\sigma(t,x)dW(t) \tag{5}$$

where $L: \mathbb{R}^+ \times \mathbb{R}^n \rightarrow \mathbb{R}$ is the diffusion operator acting on $V(t,x)$ and defined by

$$LV(t,x) = V_t(t,x) + (V_x(t,x), b(t,x)) + \frac{1}{2}\, trace\, [\sigma(t,x)^t V_{xx}(t,x)\sigma(t,x)] \tag{6}$$

It is also convenient to introduce the operator $Q: \mathbb{R}^+ \times \mathbb{R}^n \rightarrow \mathbb{R}$, which acts on $V(t,x)$ as follows:

$$QV(t,x) = \ trace\ [\sigma(t,x)^t V_x(t,x)^t V_x(t,x)\sigma(t,x)\ ] \tag{7}$$

We will establish the following result, called the *exponential martingale inequality*, which is a straightforward application of the Itô formula and that is a fundamental tool in the formulation of our results. Its demonstration can be consulted in [2]

Lemma 2.1 Let α, β, be any positive numbers. Let $x(t)$ be solution of the stochastic differential equation (4). If there exists a function $V(t,x)\in C^{1,2}(\mathbb{R}^+ \times \mathbb{R}^n; \mathbb{R}^+)$ satisfying equation (5) for a diffusion operator $LV(t,x)$, then

$$\mathrm{P}\left[\sup_{0\le t\le T}[\int_0^T (\sigma(t,x)^t, V_x(t,x))\, dW(s) - \frac{\alpha}{2}\int_0^T trace\ [\sigma(t,x)^t V_x(t,x)^t V_x(t,x)\sigma(t,x)]\, ds] > \ \beta\right] \le e^{-\alpha\beta} \tag{8}$$

3. Long-Time Asymptotic Behavior

In this section, we will introduce the definitions of almost sure exponential robust stability and asymptotic stability of the trivial solution of the numerical scheme defined by equation (3), associated to the stochastic controlled Schrödinger equation (2).

Definition 3.1 Let $\Delta t > 0$ and $\{\lambda_k\}$ a positive continuous and increasing sequence. The numerical scheme defined by equation (3) is called almost surely exponentially and robustly stable, if there exists a constant $r > 0$ such that

$$\limsup_{k\to\infty} \frac{1}{\log \lambda_k(\Delta t)} \log \| x_k \|^p < -r \qquad \text{a.s.}$$

Definition 3.2 Let $p\in(0,1]$ be arbitrary, $\Delta t > 0$ and $f: \mathbb{R}\to\mathbb{R}$ a continuous and increasing function. The numerical scheme defined by equation (3) is called asymptotically stable if there exist a constant $l > 0$ such that

$$\limsup_{k\to\infty} \frac{\log f(x_k)}{k} < -l$$

Next, we will establish the first of the results of this paper, through the techniques used by [3] and [4], in exponential asymptotic stability, adapted to the case where the diffusion term contains a control $u(t)$, as in equation (3).

Theorem 3.3 Let $p\in(0,1]$ be arbitrary. Assume that the conditions of lemma 2.1 are satisfied and let $\{x_k\}_k$ a Markov process. If there exists a function $V(t,x)\in C^{1,2}(\mathbb{R}^+ \times \mathbb{R}^n; \mathbb{R}^+)$, a positive continuous and increasing sequence $\{\lambda_k(t)\}_k$, $\lambda_k: \mathbb{R} \to \mathbb{R}^+$, with $\lambda_k(t) \ge 1$, a continuous and non-negative function $g: \mathbb{R}\to\mathbb{R}$, such that

a) $LV(t,x) < -g(t)V(t,x), \ \ \forall\, t \in \mathbb{R}^+$

b) $\| x_k \|^p \ \lambda_k(t) \ < \ V(t,x), \ \forall\, t \in \mathbb{R}^+, \ \forall\, k \in \mathbb{N}$

Then, the numerical scheme defined by equation (3) is almost surely exponentially and robustly stable.

Proof. Let $z_1(t)$, $z_2(t)$ be the following processes:

$$z_1(t) = \sum_{k=0}^{\infty} x_k\, 1_{[k\Delta t,(k+1)\Delta t]}(t), \ \ z_2(t) = \sum_{k=0}^{\infty} x_{k+1}\, 1_{[k\Delta t,(k+1)\Delta t]}(t)$$

where x_k satisfies equation (3). Using equation (5) and Itô's formula we have

$$dV(z_2(t),t) = V_t(z_2(t),t)\,dt + V_x(z_2(t),t)dz_2 + \frac{1}{2}\,trace\,[\sigma(t,x)^t V_{xx}(t,x)\sigma(t,x)] \tag{9}$$

Now, in combination with the following expression:

$$d\log V(z_2(t),t) = \frac{1}{V(z_2(t),t)}\left[dV(z_2(t),t) - \frac{1}{2}\frac{1}{V(z_2(t),t)}\,dV(z_2(t),t)^2\right]$$

We have

$$\begin{aligned}\log V(z_2(t),t) &= \log V(x_k,k) + \int_0^{t_{k+1}} \frac{1}{V(z_1(s),s)}\left[LV(z_1(s),s) - \frac{1}{2}\frac{QV(z_1(s),s)}{V(z_1(s),s)}\right] ds \\ &+ \int_0^{t_{k+1}} \frac{1}{V(z_1(s),s)} \sum_{k=1}^{n}\sum_{k=1}^{n} [((S_2u_2(t_{k+1}) \\ &+ S_1u_1(t_{k+1}))x_k 1_{[k\Delta s,(k+1)\Delta s]}(s)]\,\frac{\partial V(z_1(s),s)}{ð\,z_1(s)}\,dW_s\end{aligned} \tag{10}$$

Let's use lemma 2.1, considering $T = t_{k+1}$, $\beta = 2\log C$, $\alpha = 1$ and

$$\sigma(t,x) = ((S_2u_2(t_{k+1}) + S_1u_1(t_{k+1}))x_k 1_{[k\Delta t,(k+1)\Delta t]}(t),$$

To get

$$\mathrm{P}\left[\begin{array}{l}\sup\limits_{0\le t\le T}[\int_0^{t_{k+1}} ((S_2u_2(t_{k+1}) + S_1u_1(t_{k+1}))x_k 1_{[k\Delta t,(k+1)\Delta t]}(t)V_x(t,x)\,dW(s) \\ -\frac{1}{2}\int_0^{T}[((S_2u_2(t_{k+1}) + S_1u_1(t_{k+1}))x_k 1_{[k\Delta t,(k+1)\Delta t]}(t)]^2\,[V_x(t,x)]^2\,ds] > 2\log C\end{array}\right] \le C^{-2}$$

Now, as usual, the Borel-Cantelli lemma allows to deduce the existence of a random integer k_0 such that, for all $k \ge k_0$

$$\begin{aligned}&\int_0^{t_{k+1}} ((S_2u_2(t_{k+1}) + S_1u_1(t_{k+1}))x_k 1_{[k\Delta t,(k+1)\Delta t]}(t)V_x(t,x)dW(s) \\ &\qquad -\frac{1}{2}\int_0^{T}[((S_2u_2(t_{k+1}) + S_1u_1(t_{k+1}))x_k 1_{[k\Delta t,(k+1)\Delta t]}(t)]^2\,[V_x(t,x)]^2 ds] \le 2\,log\,C\end{aligned}$$

So, using equation (10), we have

$$\begin{aligned}&\int_0^{t_{k+1}} \frac{1}{V(z_1(s),s)} \sum_{k=1}^{n}\sum_{k=1}^{n} [((S_2u_2(t_{k+1}) + S_1u_1(t_{k+1}))x_k 1_{[k\Delta t,(k+1)\Delta t]}(s)]\,\frac{\partial V(z_1(s),s)}{ð\,z_1(s)}\,dW_s \\ &\qquad -\frac{1}{2}\int_0^{t_{k+1}} \frac{1}{V^2(z_1(s),s)}\;QV(z_1(s),s)\,ds \\ &\qquad \le 2log\,C\end{aligned} \tag{11}$$

And, by using hypotheses (a) and (b), and inequality (11), this turns out

$$\log V(z_2(t),t) \leq \log V(x_0,0) - \int_0^{t_{k+1}} g(t)\,dt + 2log\,C \tag{12}$$

Then, from (b), there hold

$$\frac{1}{\log \lambda_k(\Delta t)}\log \| x_k \|^p \leq \frac{\log V(x_0,0)}{\log \lambda_k(\Delta t)} - \frac{\int_0^{t_{k+1}} g(t)\,dt}{\log \lambda_k(\Delta t)} + \frac{2\,log\,C}{\log \lambda_k(\Delta t)}$$

Finally, because sequence $\{\lambda_k(t)\}_k$ is increasing and $g(t)$ is non-negative, there exists $r > 0$, such that

$$\limsup_{k\to\infty} \frac{1}{\log \lambda_k(\Delta t)} \log \| x_k \|^p < -r \qquad \text{a.s.}$$

Obtaining the conclusion.

The last result presented here is the following theorem.

Theorem 3.4 Let $p\in[0,1]$ be arbitrary. Let $f:\mathbb{R}\to\mathbb{R}$ be a function continuous increasing, $\Delta t > 0$ and suppose that there exists a function $V(t,x)\in C^{1,2}(\mathbb{R}^+ \times \mathbb{R}^n;\mathbb{R}^+)$ and a constant $r > 0$, such that

a) $f(x_k) \leq V(t,x),\ \ \forall\, t \in \mathbb{R}^+,\ \forall\, k \in \mathbb{N}$
b) $LV(t,x) < -r\,V(t,x),\ \ \forall\, t \in \mathbb{R}^+$

Then, the numerical scheme defined by equation (3) is asymptotically stable.

Proof. Let $V(t,x)\in C^{1,2}(\mathbb{R}^+ \times \mathbb{R}^n;\mathbb{R}^+)$ and $f:\mathbb{R}\to\mathbb{R}$ be the functions mentioned in the hypothesis. We can follow the argumentation exposed in the proof of Theorem 3.3, so, by equation (12) and hypothesis (b), we have

$$\frac{1}{k}\log \mathrm{V}(\mathrm{z}_2(t),t) \leq \frac{1}{k}[\log V(x_0,0) - rt_{k+1} + 2log\,C\,] \tag{13}$$

From which, using hypothesis (a),

$$\frac{1}{k}\log f(x_k) \leq \left[\frac{\log V(x_0,0)}{k} - r\frac{t_{k+1}}{k} + \frac{2log\,C}{k}\right] \tag{14}$$

Taking $k \to \infty$, the first and the third term in right hand of equation (14) tend to 0 and, because $t_{k+1} \leq k+1$, there exist $l > 0$ such that the conclusion is satisfied:

$$\limsup_{k\to\infty} \frac{1}{k} \log f(x_k) < -l$$

4. An Application in Stochastic Optimal Control for NMR

In this section, we will apply Theorem 3.3 and Theorem 3.4 to the model of stochastic controlled Schrödinger equation (2).

We consider again, the model describing a spin ½-particle in an electromagnetic field, fluctuating in the X and Y directions by white noise. The optimal control problem for this quantum stochastic systems is the following:

To find controls $u_1(t), u_2(t)$ which steers the initial condition $x(0) = (1,0,0,0)$ of stochastic system given by equation (2), to the final state $x\left(\frac{\pi}{\sqrt{2}}\right) = (0,0,0,1)$ and minimize the cost functional Bolza type following:

$$\min \longrightarrow J(u_1, u_1) = E\left[< x^t\left(\frac{\pi}{\sqrt{2}}\right)|O|\, x\left(\frac{\pi}{\sqrt{2}}\right) > + \int_0^{\frac{\pi}{\sqrt{2}}} \left(u_1^2(t) + u_2^2(t)\right) dt\right]$$

where $E[f]$ denotes the conditional expectation with respect to f and O is the symmetric, negative defined matrix $O = x^t\left(\frac{\pi}{\sqrt{2}}\right) x\left(\frac{\pi}{\sqrt{2}}\right)$, called the observable operator.

Reference [1] shows the application of maximum principle, stochastic maximum principle and second order maximum principle to determine the form of the optimal control in this case. The corresponding adjoint equations for the co-state λ and state equations for x, constitute an associated two-point boundary value problem which can't be analytically solved. Through the Euler-Maruyama scheme, we have numerically obtained the optimal controls $u_1(t)$, $u_2(t)$ and state trajectory $x = (x_1, x_1, x_1, x_1)$. Fig. 1 shows a computer simulation of the optimal stochastic trajectory steering initial state $x(0) = (1,0,0,0)$ (the North Pole on Bloch sphere) to final state $x\left(\frac{\pi}{\sqrt{2}}\right) = (0,0,0,1)$ (the South Pole on Bloch sphere), for this control problem, using Euler-Maruyama scheme given by equation (3), obtained in [1]. Now, we have interested in almost sure exponential robust stability and asymptotic stability of the Euler-Maruyama scheme for this optimal control problem.

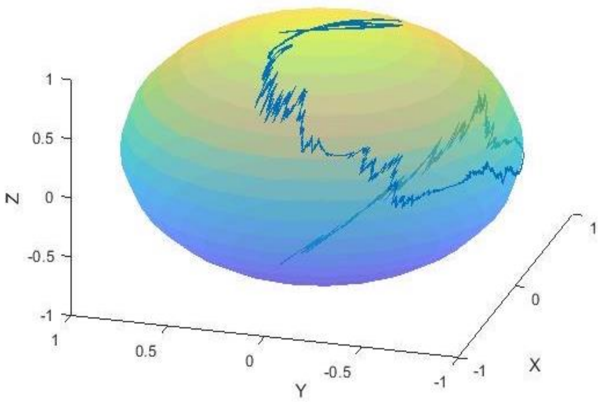

Fig. 1. The optimal stochastic trajectory on the Bloch sphere of the solution $x = (x_1, x_1, x_1, x_1)$ to trivial solution of the numerical scheme in the stochastic controlled Schrödinger equation.

Let consider for $k \in \mathbb{N}$ and $u_1(t) \neq 0, u_2(t) \neq 0$, controls obtained in [1], namely,

$$u_1(t) = -\frac{1}{2}\,\Lambda(\mathrm{t}) S_1 x(t), \quad u_2(t) = -\frac{1}{2}\,\Lambda(\mathrm{t}) S_2 x(t),$$

where $\Lambda(t)$ is the adjoint state to $x(t)$, the Lyapunov function

$$V(t,x) = [u_1(t) + u_2(t)]^{-2} \parallel x_k(t) \parallel^2 1_{[k\Delta\mathrm{t},(k+1)\Delta\mathrm{t}]}(t) \tag{15}$$

And la function $g: \mathbb{R} \to \mathbb{R}$ given by

$$g(t) = -2(u_1(t) + u_2(t) + 1)\big(u'_1(t) + u'_2(t)\big)$$

We obtain the corresponding diffusion operator

$$LV(t,x) = \Big\{\| x_k \|^2 \Big[-2[u_1(t) + u_2(t)]^{-2}\big[\big(u_1(t) + u_2(t)\big)\big(u'_1(t) + u'_2(t)\big) + 1\big]\Big] + 1\Big\}\ 1_{[k\Delta t,(k+1)\Delta t]}(t)$$

Then

$$LV(t,x) < V(t,x) - 2(u_1(t) + u_2(t) + 1)[u'_1(t) + u'_2(t)] + 1 < g(t)V(t,x) + 1$$

So, applying Theorem 3.3, we conclude that Euler-Maruyama numerical scheme, defined by equation (3), is almost surely exponentially and robustly stable, for all sufficiently small step sizes Δt_k.

Similarly, we apply Theorem 3.4, using again equation (15) to define the Lyapunov function $V(t,x)$, considering $f(x) = x$ in Theorem 3.3 and setting $p = 1$, to deduce that Euler-Maruyama numerical scheme defined by equation (3) is asymptotically stable

5. Conclusion

In this paper, we have presented definitions of almost sure exponential robust stability and asymptotic stability for the Euler-Maruyama numerical scheme in the stochastic controlled Schrödinger equation to a stochastic quantum two-level system. These types of stability are variants of Mao and Mora definitions in [5] and [6], respectively. Through techniques used in [3] and [5], adapted to controlled systems, we have demonstrated the almost sure exponential robust stability and asymptotic stability of the numerical solution, for the step-size Δt small and for long-time, found by numerical integration of coupled stochastic differential equations, describing a stochastic quantum two-level system in NMR. We have presented a simulation obtained in [1], using Euler-Maruyama scheme, of the optimal stochastic trajectory, which is solution of the optimal control problem posed.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Author Contributions

Both authors contributed equally and significantly in writing this paper. Both authors had reviewed and approved the final version of the paper.

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Cutberto Romero-Meléndez received the degree in mathematical physics from National Polytechnic Institute at Mexico, the master degree in mathematics from the Metropolitan Autonomous University, at Mexico and the Ph.D. degree Trés Honorable in mathematics from the Bourgogne University, at Dijon, France, in 1985, 1989 and 2004, respectively. He is currently a full professor in the Department of Basic Sciences of the Metropolitan Autonomous University, at Mexico. His research interests include geometric control theory, optimal and nonlinear control theory, control of quantum mechanical systems, complexity on motion planning and path planning.

Dr. Romero belongs to the Mathematical Mexican Society, he is the general chairman of the Organizing Committee of the Multidisciplinary Congress of Sciences Applied in Latin America and he received an Academic Teaching Award in Engineering in 1994.

David Castillo-Fernández received the degree in mathematical physics from the Higher School of Physics and Mathematics from the National Polytechnic Institute at Mexico and the master degree in mathematics science from the Research and Advanced Studies Center of Mexico. He is PhD candidate in physics and mathematics from the Higher School of Physics and Mathematics.

He is a subject teacher in the Engineering Department of the La Salle University, at Mexico, City. His research interests include stability of stochastic differential equations, stochastic Navier-Stokes equations and stochastic differential equations with Poisson jumps.