Improving the Stability of Numerical Simulations of Quantum Dynamical Systems using Stochastic Differential Equations Techniques

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Abstract

Quantum dynamical systems typically deal with huge numbers of degrees of freedom, particularly functional integrals, which makes them very difficult to simulate using deterministic methods. Modeling such systems with stochastic differential equations (SDEs) is an attractive alternative to Markov chain Monte-Carlo, but there remain stability problems. An example of a multi-dimensional complex SDE arises from an anharmonic oscillator with a one-mode Bose-Einstein condensate (BEC) Hamiltonian given in [1], for which the numerical solution becomes unreliable after approximatively $t = 0.3$ for all tested numerical methods. Splitting of drift methods as introduced in [3] have been tried on this problem and seemed to improve the stability of the results, but not to the desired extent (see [1]).

To improve the results, new numerical splitting methods have recently been developed. However, it seems that the choice of the numerical scheme alone might not guarantee the reliability of the results. The use of carefully chosen stochastic gauges as in [1] improves the accuracy of the simulation greatly by taking into account some aspects of the dynamics of the system. Non-vanishing boundary terms from partial integration can be problematic and have to be taken care of, for example considering them as constraints and using projected SDEs techniques [2].

1. Simulation of Bose-Einstein condensates

Consider the case of an anharmonic oscillator with one-mode BEC Hamiltonian treated in [1]. From the master equation

$$\frac{\partial \hat{\rho}}{\partial t} = -\frac{i}{\hbar}\left[\hat{H}, \hat{\rho}\right], \tag{1}$$

where $\hat{H}$ is the Hamiltonian and $\hat{\rho}$ the density matrix, a Fokker-Planck (FP) equation can be derived and from it an Itô SDE of the form

$$dX_t = a(X_t)\,dt + b(X_t)\,dW_t, \tag{2}$$

which can be solved numerically using standard SDE techniques (where $X_t \in \mathbb{R}^n, a : \mathbb{R}^n \to \mathbb{R}^n, b : \mathbb{R}^n \to \mathbb{R}^{n\times m}$ and W_t is a m-dimensional Brownian motion). However, a stable integrator is needed to solve (2). For instance, explicit methods produce divergent numerical solutions, whereas semi-implicit schemes or splitting schemes give a reliable solution for the integration time interval $[0, 0.3]$ at least, see Figure 1.

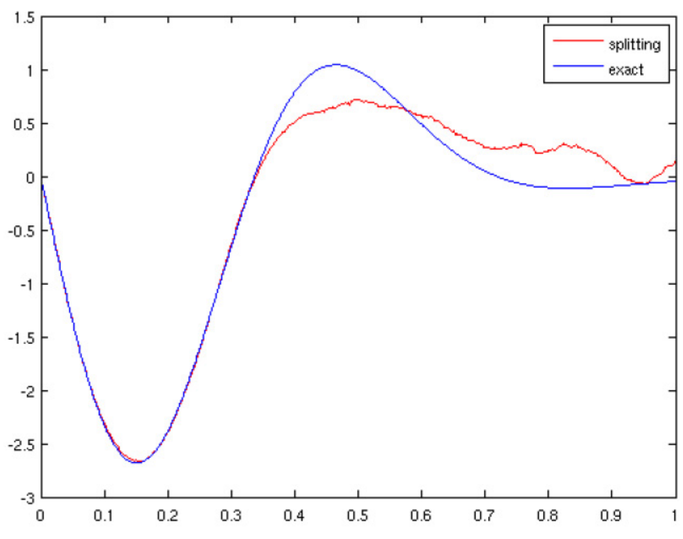

Figure 1: *exact and numerical solution of the Y-observable from [1] with a drift-splitting scheme*

It can be seen that after $t = 0.3$, the numerical solution diverges, and this for all tested methods, time steps and number of sample paths. In order to improve those results, several approaches were tried. The first one was to develop a specific method, resulting in a scheme using a splitting of both drift and diffusion coefficient, which will be treated in section 2.

2. A drift and diffusion coefficient splitting scheme

Using the same techniques as in [3], we can derive an order 2.0 method using splittings of both the drift and diffusion coefficient:

$$a(x) = A(x) + B(x),\ b(x) = C(x) + D(x),$$

where A and C are 'nice' functions and

$$\frac{\partial^2}{\partial x_i \partial x_j} C(x) = 0, \quad \forall i, j,$$

which is not too harsh a condition since linear C are convenient to use. Using the notation $f_t := f(X_t)$, the obtained scheme is then for $\alpha = 1, \ldots, n$

$$\begin{aligned} X^\alpha_{t+h} = X^\alpha_t &+ \frac{h}{2}\left(A^\alpha_{t+h} + B^\alpha(Y_e) + a^\alpha_t\right) + \sum_{\beta,\epsilon,\gamma}\left(\partial_\epsilon b^{\alpha\beta}_t\right) b^{\epsilon\gamma}_t \Xi^{\gamma\beta} \\ &+ \frac{1}{2}\sum_\beta \left(C^{\alpha\beta}_{t+h} + D^{\alpha\beta}\left(\overline{Y}\right) + b^{\alpha\beta}_t\right)\xi^\beta_1 \\ &+ \frac{1}{2}\sum_\beta \left(b^{\alpha\beta}\left(Y_+\right) + b^{\alpha\beta}\left(Y_-\right) - 2b^{\alpha\beta}_t\right)\xi^\beta_1 \\ &- \frac{1}{2}\sum_{\beta,\epsilon,\gamma}\left(\partial_\epsilon C^{\alpha\beta}_t\right) b^{\epsilon\gamma}_t \xi^\gamma_1 \xi^\beta_1, \end{aligned} \tag{3}$$

where

$$\begin{aligned} Y_e &= x_t + a_t h + b_t \xi_1, \quad Y_\pm = x_t \pm b_t \xi_0, \\ \overline{Y} &= x_t + a_t h \end{aligned}$$

and $\xi^\alpha_0, \xi^\alpha_1 \sim N(0, h)$ (thus modeling $W^\alpha_{t+h} - W^\alpha_t$), while $\Xi^{\alpha\beta}$ is an approximation to $\int_t^{t+h} W^\alpha_s\, dW^\beta_s$.
The method (3) can be shown to have an order of 2.0. In all tested cases, it behaves similarly to the scheme defined in [3] and thus does not reduce the numerical error significantly, unfortunately.

3. Changing the SDE

It is worth mentioning that the gauges introduced in [1] do reduce the error by several orders of magnitude. The form of the SDE can indeed have a huge impact on its numerical solution, and thus some effort was invested into finding an appropriate one. The density matrix here is

$$\hat{\rho} = \int P(\alpha, \beta, \theta, t)\hat{\Lambda} e^{-g}\, d\alpha\, d\beta\, d\theta \tag{4}$$

with $\alpha, \beta \in \mathbb{C}$, $\theta \in \mathbb{R}$ and kernel

$$\begin{aligned} \hat{\Lambda} &= e^{i\theta}\|\alpha\rangle\langle\beta\| + e^{-i\theta}\|\beta\rangle\langle\alpha\| \\ e^g &= 2e^{\mathsf{Re}(\alpha\cdot\overline{\beta})}\cos(\theta + \mathsf{Im}(\alpha\cdot\overline{\beta})) \end{aligned}$$

From the master equation (1) and

$$\hat{H} = \frac{\hbar}{2}(\hat{a}^\dagger\hat{a})^2,$$

where $\hat{a}^\dagger, \hat{a}$ are the creation and annihilation operator of the boson field, we can derive (writing $d\mu := d\alpha\, d\beta\, d\theta$)

$$\begin{aligned} \dot{\hat{\rho}} &\overset{(4)}{=} \int \frac{\partial P}{\partial t}\hat{\Lambda} e^{-g}\, d\mu \\ &\overset{(1)}{=} \frac{i}{\hbar}\int P[\hat{\Lambda}, \hat{H}] e^{-g}\, d\mu, \end{aligned}$$

where the Poisson bracket $[\hat{\Lambda}, \hat{H}]$ is

$$[\hat{\Lambda}, \hat{H}] = \frac{1}{2}\left[\left(\overline{\alpha}\frac{\partial}{\partial\overline{\alpha}}\right)^2 + \left(\overline{\beta}\frac{\partial}{\partial\overline{\beta}}\right)^2 - \left(\alpha\frac{\partial}{\partial\alpha}\right)^2 - \left(\beta\frac{\partial}{\partial\beta}\right)^2\right]\hat{\Lambda}$$

Using partial integration and assuming that the boundary terms vanish, we get a FP equation of the form

$$\frac{\partial P}{\partial t} = \sum_i A_i \frac{\partial P}{\partial x_i} + \sum_{i,j} D_{ij}\frac{\partial^2 P}{\partial x_i \partial x_j} \tag{5}$$

where we wrote $x_1 = \mathsf{Re}(\alpha), x_2 = \mathsf{Im}(\alpha), x_3 = \mathsf{Re}(\beta), x_4 = \mathsf{Im}(\beta), x_5 = \theta$. We can obtain the SDE of interest by writing $A_i = -a_i$, $D_{ij} = -\frac{1}{2}(bb^\top)_{ij}$. Note that partial derivatives with respect to θ do not occur without using gauges, which are identities that can be added freely to the equation, one of them being

$$C^2\left(\frac{\partial^2}{\partial\theta^2} + 1\right)\hat{\Lambda} = 0. \tag{6}$$

The gauge used in [1] is depending on a free parameter μ (and vanishes when $\mu = 0$). As can be seen in Figure 2, the numerical solution is exploding without the gauges, whereas the choice $\mu = 0.001$ gives the best result.

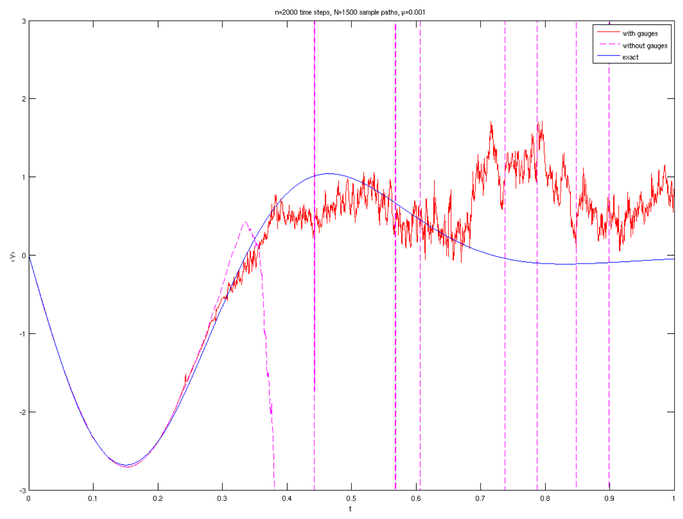

Figure 2: *exact and numerical solution of the Y-observable from [1] with a linear drift-splitting scheme, with or without gauges*

Without changing the coordinates in the way presented in [1], we found that the obtained FP equation is ultrahyperbolic, which makes the passage to a SDE system problematic.

4. Conclusion and future work

It is thought that the lack of reliability after $t = 0.3$ lies in the fact that the chosen SDE do not model the process accurately after some time. It is quite possible that the appearance of non-vanishing boundary terms (meaning that we cannot derive the FP equation directly, although we might be able to do it using identities like (6)) requires us to modify the SDE with time. An other option would be to impose some constraints on the system, which can be done numerically by using a projection technique as introduced in [2]. However, it is as yet unclear wether these tricks might be enough to overcome the problem of ultrahyperbolicity of the FP equation. In any case we would need more information about the boundary terms and the constraints. More effort will be directed toward working with stochastic differential-algebraic equations with several constraints using projected SDE techniques.

References

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