Improving the stability of numerical simulations of quantum dynamical systems using stochastic differential equations techniques

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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 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 Figure 1 and [1]).

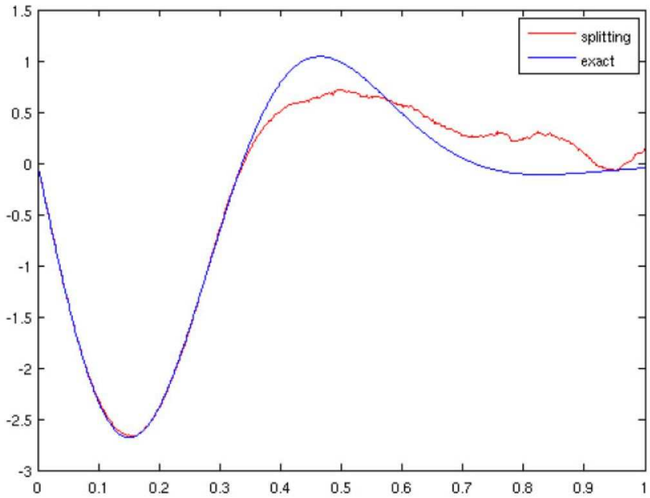

Figure 1: exact and numerical solution of the Y-observable from [1] with a drift-splitting scheme

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]. The results using various techniques will be discussed.

References

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