Completely Positive Trace Preserving Methods for the Lindblad Equation

Michael Riesch, Alek Pikl, and Christian Jirauschek
Department of Electrical and Computer Engineering
Technical University of Munich
Arcisstraße 21, 80333 Munich, Germany
Email: michael.riesch@tum.de

***Abstract*—The Lindblad master equation is a valuable tool in quantum mechanics, which describes the dynamics of open systems. In the scope of our research, it is combined with the one-dimensional Maxwell's equations to form the generalized Maxwell-Bloch equations. Since analytical solutions are not available in the general case, numerical methods have to be employed to solve the Lindblad equation. In this work, we focus on methods that are completely positive trace preserving (CPTP), i.e., that guarantee to preserve the properties of the density matrix. We review existing approaches and compare the most promising candidates in terms of computational performance.**

I. Introduction

In quantum mechanics, the Lindblad master equation

$$\partial_t \hat{\rho} = -\mathrm{i}\hbar^{-1}[\hat{H}, \hat{\rho}] + \mathcal{D}(\hat{\rho}) \tag{1}$$

is a valuable tool that describes the dynamics of open systems [1], which are represented by the density matrix $\hat{\rho}$. Here, $\hat{H}$ is the Hamiltonian of the system, $[\cdot, \cdot]$ denotes the commutator, and $\hbar$ is the reduced Planck constant. The dissipation term $\mathcal{D}$ stems from the interaction of the system with the environment. Since the Lindblad equation belongs to the basic concepts of quantum mechanics, it plays a significant role in the fields of quantum optics, condensed matter, atomic physics, quantum information, decoherence, and quantum biology [2]. In the scope of our research, it is used to model optoelectronic devices such as the quantum cascade laser (QCL) [3], where, together with the one-dimensional Maxwell's equations, it forms the generalized Maxwell-Bloch equations [4].

Similar to the majority of physical problems, the Lindblad equation cannot be solved analytically for most cases. Therefore, we need to resort to numerical methods. In previous work, we compared methods that treat the generalized Maxwell-Bloch equations [5], [6] beyond the rotating wave approximation (RWA), and demonstrated their efficient implementation on modern parallel architecture [7]. However, as already pointed out in [8], solving the Lindblad equation numerically remains to be a computational bottleneck. In [9], we reviewed approaches to solve this problem. This discussion was carried out in terms of computational complexity. In the work at hand, we implement promising methods for the Lindblad equation and compare their actual performance.

This work was supported by the German Research Foundation (DFG) within the Heisenberg program (JI 115/4-2).

II. Numerical Methods for the Lindblad Equation

From the numerical point of view, Eq. (1) is no more than a system of coupled ordinary differential equations (ODEs). Therefore, standard text book methods are frequently employed to solve the Lindblad equation in related literature. While those methods are computationally efficient, the problem is that they may not preserve the properties of the density matrix. For example, Bidégaray et al. [8] showed that the Crank-Nicolson scheme applied to the Lindblad equation may violate the positive semidefiniteness of the density matrix. In recent work [9], we found that the same holds for the predictor-corrector approach suggested in [10], and the Runge-Kutta method (used in e.g., [11]). In the following, we focus on numerical methods that guarantee the preservation of the density matrix properties – namely, trace, Hermiticity, and positivity).

Those methods can be divided into two groups [9]. Methods of the first group solve the Lindblad equation exactly for one time step and are, by definition, CPTP. Typically, they can be related to Krylov subspace methods and polynomial expansion schemes [12], [13]. From this group, we found the algorithm presented in [14] very promising. This algorithm efficiently calculates the action of a matrix exponential on a vector. Therefore, the density matrix elements must be rearranged as vector. Since the matrix is Hermitian, it is sufficient to store the real and imaginary values of one half of the off-diagonal elements. In the following, we refer to this arrangement as real-valued representation (RVR).

The other group of methods uses approximations, but nevertheless preserves the properties from time step to time step. For example, the operator splitting technique can be employed to determine solutions to the commutator part and the dissipation part in Eq. (1), respectively, and combine the separate solutions to an approximate solution of the complete Lindblad equation. In [8], the authors introduce a further approximation for the matrix exponential based on the Cayley transform (in the following referred to as "Cayley approximation"). Here, the density matrix remains in the regular representation. In [15], on the other hand, the matrix exponential assumes a form that can be solved using the generalized Rodrigues' formula. This is due to the coherence vector representation (CVR), in which the density matrix was arranged.

978-1-7281-6086-3/20/$31.00 ©2020 IEEE

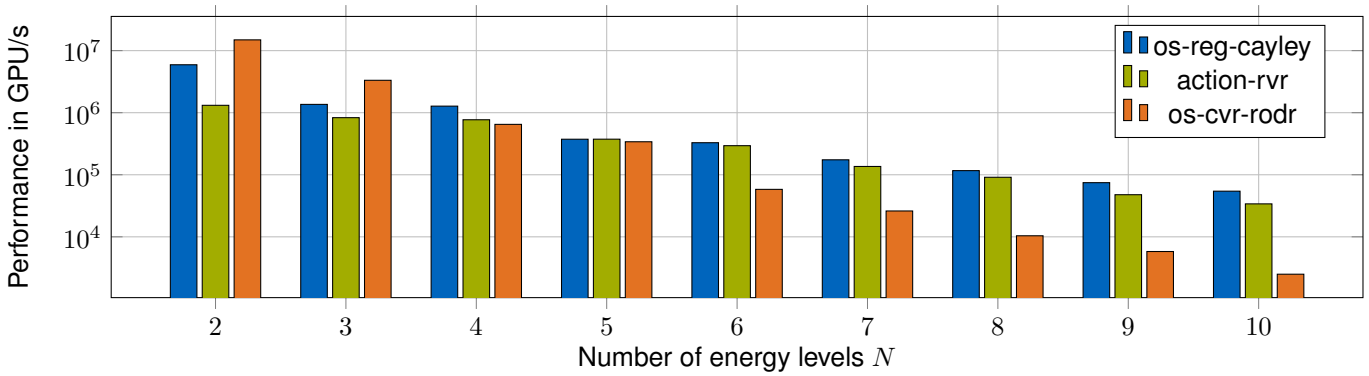

Fig. 1. Single-thread performance of the three methods that solve the Lindblad equation numerically. The metric grid point updates per second (GPU/s) is used as figure of merit. It is calculated as $P = N_x N_t / t_{\text{exec}}$, where N_x, N_t denote the number of spatial and temporal grid points, respectively, and t_{exec} is the measured execution time.

III. Implementation and Performance Comparison

We implemented three candidates within the framework of our open-source software mbsolve [16]. Those candidates are the operator splitting approach that uses the Cayley approximation [8] (in regular representation, os-reg-cayley), the action approach in real-valued representation [14] (action-rvr), and the operator splitting approach in coherence vector representation that uses the Rodrigues' formula (os-cvr-rodr). The matrix operations were delegated to the Eigen library. As test case, we generalized the six-level anharmonic ladder setup from [17] and varied the number of energy levels N between two and ten. Thereby, we assessed the scaling of the performance with respect to N. We compiled mbsolve using the GNU C++ compiler 9.2.0 and performed the performance measurements on a Intel Xeon E5-2697 v3 CPU. Here, we used only one thread. The single-thread performance measurement results in Fig. 1 demonstrate that the os-reg-cayley features the best overall performance. However, this comes at the cost of accuracy, since operator splitting and the Cayley approximation produce numerical errors. The os-cvr-rodr approach shows the best performance for systems with two or three levels, but for larger N there is a sudden decrease in performance. The numerical error is smaller, since only operator splitting is employed. Finally, the action-rvr method performs reasonably well and features robust scaling with respect to N. Here, the numerical error is minimal.

IV. Conclusion

We implemented three methods for solving the Lindblad equation numerically and compared their performance. While the method presented in [8] shows the best overall performance, the candidate from [15] is well-suited for two-level and three-level systems. Finally, the approach based on the work in [14] is a promising alternative with reasonable performance and improved accuracy.

References

[1] H.-P. Breuer and F. Petruccione, *The Theory of Open Quantum Systems*. Oxford University Press, Oxford, 2002.

[2] D. Manzano, "A short introduction to the Lindblad master equation," *AIP Adv.*, vol. 10, no. 2, p. 025106, Feb. 2020.

[3] C. Jirauschek and T. Kubis, "Modeling techniques for quantum cascade lasers," *Appl. Phys. Rev.*, vol. 1, p. 011307, Feb. 2014.

[4] C. Jirauschek, M. Riesch, and P. Tzenov, "Optoelectronic device simulations based on macroscopic Maxwell–Bloch equations," *Adv. Theor. Simul.*, vol. 2, no. 8, p. 1900018, Aug. 2019.

[5] M. Riesch, N. Tchipev, H.-J. Bungartz, and C. Jirauschek, "Performance evaluation of numerical methods for the Maxwell-Liouville equations," in *Numerical Simulation of Optoelectronic Devices (NUSOD), 2017 International Conference on*, Jul. 2017, pp. 223–224.

[6] M. Riesch, N. Tchipev, S. Senninger, H.-J. Bungartz, and C. Jirauschek, "Performance evaluation of numerical methods for the Maxwell–Liouville–von Neumann equations," *Opt. Quant. Electron.*, vol. 50, no. 2, p. 112, Feb. 2018.

[7] M. Riesch, N. Tchipev, H.-J. Bungartz, and C. Jirauschek, "Numerical simulation of the quantum cascade laser dynamics on parallel architectures," in *Proceedings of the Platform for Advanced Scientific Computing Conference*, Jun. 2019, pp. 5:1–5:8.

[8] B. Bidégaray, A. Bourgeade, and D. Reignier, "Introducing physical relaxation terms in Bloch equations," *J. Comput. Phys.*, vol. 170, no. 2, pp. 603–613, Jun. 2001.

[9] M. Riesch and C. Jirauschek, "Analyzing the positivity preservation of numerical methods for the Liouville-von Neumann equation," *J. Comput. Phys.*, vol. 390, pp. 290–296, Feb. 2019.

[10] R. W. Ziolkowski, J. M. Arnold, and D. M. Gogny, "Ultrafast pulse interactions with two-level atoms," *Phys. Rev. A*, vol. 52, no. 4, pp. 3082–3094, Oct. 1995.

[11] W. Cartar, J. Mørk, and S. Hughes, "Self-consistent Maxwell-Bloch model of quantum-dot photonic-crystal-cavity lasers," *Phys. Rev. A*, vol. 96, no. 2, p. 023859, Aug. 2017.

[12] M. Berman, R. Kosloff, and H. Tal-Ezer, "Solution of the time-dependent Liouville-von Neumann equation: dissipative evolution," *J. Phys. A: Math. Gen.*, vol. 25, no. 5, pp. 1283–1307, Mar. 1992.

[13] R. Kosloff, "Propagation methods for quantum molecular dynamics," *Annu. Rev. Phys. Chem.*, vol. 45, no. 1, pp. 145–178, Oct. 1994.

[14] A. H. Al-Mohy and N. J. Higham, "Computing the action of the matrix exponential, with an application to exponential integrators," *SIAM J. Sci. Comput.*, vol. 33, no. 2, pp. 488–511, Mar. 2011.

[15] M. Riesch and C. Jirauschek, "Numerical method for the Maxwell-Liouville-von Neumann equations using efficient matrix exponential computations," *https://arxiv.org/abs/1710.09799*, Oct. 2017.

[16] ——, "mbsolve: An open-source solver tool for the Maxwell-Bloch equations," https://github.com/mriesch-tum/mbsolve, Jul. 2017.

[17] R. Marskar and U. Österberg, "Multilevel Maxwell-Bloch simulations in inhomogeneously broadened media," *Opt. Express*, vol. 19, no. 18, pp. 16 784–16 796, Aug. 2011.