プログラム名： 量子人工脳を量子ネットワークでつなぐ高度知識社会基盤の実現
PM 名： 山本喜久
プロジェクト名：量子シミュレーション

委 託 研 究 開 発

実 施 状 況 報 告 書（成果）

平成 29 年度

研究開発課題名：

現代コンピュータに実装できる量子多体系の新計算手法の開発(理論研究)

研究開発機関名：

国立研究開発法人理化学研究所

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Ⅰ　当該年度における計画と成果

１．当該年度の担当研究開発課題の目標と計画

The broad objective for QuTiP in 2017 was to continue to extend the range of quantum system dynamics that can be efficiently solved using the toolkit, and increasing the applicability of these tools by supporting different models. We also planned to generally improve the efficiency of core processing modules, and to look at improving the accessibility and usability of the toolkit for our global network of users.

Specifically we planned:

1.) To add support for time-dependent Hamiltonians in the hierarchy equations of motion (HEOM) solver and the Bloch-Redfield (BR) solver.

2.) A new implementation of the Monte-Carlo and stochastic solvers.

3.) Increase the functionality and improve usability of the quantum information processing (QIP) modules.

4.) Utilize OpenMP parallel processing tools introduced in 2016 to reduce processing time in core functions.

２．当該年度の担当研究開発課題の進捗状況と成果

2-1 進捗状況

Our plan has been progressing well, as indicated by a major new release of QuTiP, version 4.2.　This milestone was reached in July 2017, and includes, as a major new feature, an efficient time-dependent Bloch-Redfield (BR) solver.

Additional features added to QuTiP in 2017 include support for time-dependent dynamics generators, low-level changes which enable easier use on Windows machines, and new Cythonised Monte-Carlo and Stochastic solvers. As planned in last year's report, we have made many improvements in the functionality and output presentation of the QIP module as well.

A preliminary development release of a time-dependent HEOM method, as mentioned in last year's plan, has been made available to the public, but requires further testing and improvement.

2-2 成果

1) A major achievement was the implementation of an efficient time-dependent Bloch-Redfield (BR) solver. The BR solver has a large numerical overhead, and thus required many low-level improvements to work efficiently. Hence, many of matrix

operation efficiencies that have been recently introduced in QuTiP were primarily to support this solver. This is a very substantial progression for QuTiP.

2) Support for time-dependent dynamics generators, for both system and control (Hamiltonian) operators has been added and included in the 4.2 release.

3) On the technical side, a major improvement was made by switching from C to C++ compiled components, which allows users with MS Windows operating systems to use QuTiP with the latest version of Python. This also significantly reduced issues with installation of QuTiP on MS Windows, which broadened its accessibility, particularly for students.

4) The new Monte-Carlo and Stochastic solvers, based on Cython compiled core components, are currently being reviewed and tested. These will remove the dependence on Fortran components, which were inaccessible to users with MS Windows operating systems.

5) Processing efficiencies have been realized in the methods for calculating analytic coefficients in coherent states, function-based time-dependent Lindblad master equation and Schrödinger equation solvers, and time-dependent solver output to NumPy arrays.

2-3 新たな課題など

In addition to the ongoing projects and developments discussed above, we have started on some major new projects which we plan to complete in 2018:
1.) A new module for solving quantum systems exploiting permutational symmetries.
2.) A new scattering module to compute temporal photon scattering in an arbitrarily-specified quantum optical systems, following the theoretical framework developed in K.A. Fischer, et.al. (2017), "Scattering of Coherent Pulses from Quantum-Optical Systems" (arXiv: 1710.02875).
3) Support for GPU parallelization.

２．アウトリーチ活動報告

QuTiP has been used and cited in more than 370 papers, including 130 in 2017--2018 alone. It is used by various commercial endeavors in the “quantum technology” field, including IBM and Google.

We have been promoting QuTiP at international conferences, including presentations at CQIS (NII, Tokyo), and PyCon 2017 (Tokyo).