pyTTN: A tree tensor network based open-source toolbox for open and closed system quantum dynamics simulations and its application in quantum algorithms

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We present the Python Tree Tensor Network package (pyTTN) for the evaluation of dynamical properties of closed and open quantum systems that makes use of Tree Tensor Network (TTN) based representations of wavefunctions [1], and also demonstrate its integration in quantum algorithms. This package includes several features allowing for easy setup of zero- and finite-temperature calculations for general Hamiltonians using single and multi-set TTN ansätze with an adaptive bond dimension through the use of subspace expansion techniques. pyTTN provides several tools for setting up efficient simulation of open quantum system dynamics, including the use of the TTN ansatz to represent the auxiliary density operator space for the simulation of the Hierarchical Equation of Motion (HEOM) method and generalised pseudo-mode methods. We present a set of applications of the package, including photo-excitation and exciton dynamics in molecules, as well as open quantum systems, including the spin-boson model, a set of extended dissipative spin models, and an Anderson impurity model. We also present an Anderson impurity solver integrating tensor network methods with quantum computing [2], thereby exploiting the efficiency of tensor networks for preparing ground states on classical computers and taking advantage of quantum processors for the evaluation of the time evolution, which can become intractable on classical computers.

This work was supported by the Engineering and Physical Sciences Research Council [grant EP/Y005090/1], Innovate UK - UKRI through grant 1468/10074167, and the UK Government Department of Science, Innovation and Technology through the UK National Quantum Technologies Programme. UK National Quantum Technologies Programme.

[1] J. Chem. Phys. 163 (2025) 202501

[2] APL Quantum 2 (2025) 016121