Accepted Manuscript

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PII: DOI: Reference:	S0010-4655(17)30420-4 https://doi.org/10.1016/j.cpc.2017.12.015 COMPHY 6398
To appear in:	Computer Physics Communications
	7 March 2017 13 November 2017 18 December 2017



Please cite this article as: D. Jaschke, M.L. Wall, L.D. Carr, Open source Matrix Product States: Opening ways to simulate entangled many-body quantum systems in one dimension, *Computer Physics Communications* (2017), https://doi.org/10.1016/j.cpc.2017.12.015

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Open source Matrix Product States: Opening ways to simulate entangled many-body quantum systems in one dimension

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Abstract

Numerical simulations are a powerful tool to study quantum systems beyond exactly solvable systems lacking an analytic expression. For one-dimensional entangled quantum systems, tensor network methods, amongst them Matrix Product States (MPSs), have attracted interest from different fields of quantum physics ranging from solid state systems to quantum simulators and quantum computing. Our open source MPS code provides the community with a toolset to analyze the statics and dynamics of one-dimensional quantum systems. Here, we present our open source library, Open Source Matrix Product States (OSMPS), of MPS methods implemented in Python and Fortran2003. The library includes tools for ground state calculation and excited states via the variational ansatz. We also support ground states for infinite systems with translational invariance. Dynamics are simulated with different algorithms, including three algorithms with support for long-range interactions. Convenient features include built-in support for fermionic systems and number conservation with rotational $\mathcal{U}(1)$ and discrete \mathbb{Z}_2 symmetries for finite systems, as well as data parallelism with MPI. We explain the principles and techniques used in this library along with examples of how to efficiently use the general interfaces to analyze the Ising and Bose-Hubbard models. This description includes the preparation of simulations as well as dispatching and post-processing of them.

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Preprint submitted to Computer Physics Communications

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