

Abstract Submitted
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The Multilayer Multiconfiguration Time-Dependent Hartree Theory¹ HAOBIN WANG, New Mexico State University — The multilayer multi-configuration time-dependent Hartree (ML-MCTDH) theory is a powerful tool for carrying out wave packet propagation. This rigorous, variational quantum approach is based on an efficient representation of the functional via several dynamically contracted layers, and thus applicable to systems with many degrees of freedom. The presentation gives an overview on the general derivation of the theory, the scaling of the method for model problems, and examples of application to electron transfer processes in the condensed phase. Generalizations of the theory to treat identical fermion/boson systems will also be presented.

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