Towards a systematic convergence of Multi-Layer (ML) Multi-Configuration Time-Dependent Hartree nuclear wavefunctions: The ML-spawning algorithm

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The Multi-Layer (ML) variant of the Multi-Configuration Time-Dependent Hartree (MCTDH) method is a powerful tool for the efficient computation of nuclear quantum dynamics in high-dimensional systems.[1,2] By providing an optimal choice of layered effective degrees of freedom in form of the so-called ML tree, one is able to reduce the computational cost to an amenable number of configurations.[3] Nevertheless, the fact that one must also make a series of ad hoc decisions often based on intuition or experience at the outset — such as the number of configurations per node and the branching of the ML tree — directly affect the efficiency of the computation and make its use less straight-forward than the standard MCTDH method. Therefore, herein we detail a new algorithm for adaptively expanding the size of every node on-the-fly (i.e. spawning) and a derived criterion for the selection of an efficient tree's branching.[4]

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