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Multi-Layer Operators: a new way to represent the Hamiltonian for ML-MCTDH

Abstract:

Traditionally, MCTDH and ML-MCTDH have relied on Hamilton operators in sum-of-products (SOP) form to provide a fast evaluation of the equations of motion. But representing a general potential energy surface (PES) in SOP form can lead to an expansion with many terms (especially if a highly accurate representation is desired), which leads to high computational resource usage in (ML-)MCTDH. In this talk, an alternative representation of the Hamilton operator as a "multi-layer operator" (MLOp) is presented, which constructs the operator hierarchically from one- or low-dimensional operators. It is shown that the ML-MCTDH equations of motion with a Hamiltonian in MLOp form can be evaluated efficiently. A method for representing a PES in MLOp format, multi-layer Potfit, is discussed. It can provide very accurate PES representations at rather moderate resource usage for ML-MCTDH.