Quantum dynamical treatment of systems with many degrees of freedom using time-dependent multiconfiguration methods

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The accurate theoretical treatment and simulation of quantum dynamical processes in many-body systems is a central issue in chemical and condensed matter physics. In this talk, the multilayer multiconfiguration time-dependent Hartree (ML-MCTDH) method [1] is discussed as an example of an approach that allows an accurate description of quantum dynamics in systems with many degrees of freedom. The ML-MCTDH method is a variational basis-set approach, which uses a multiconfiguration expansion of the wavefunction employing a multilayer representation and time-dependent basis functions. It extends the original MCTDH method [2] to significantly larger and more complex systems. Employing the second quantization representation of Fock space, the ML-MCTDH method has recently been extended to allow the treatment of indistinguishable particles [3,4]. The performance of the ML-MCTDH method is illustrated by several application to models of charge and energy transport in molecular systems in the condensed phase [4,5,6,7].

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