Attosecond electron dynamics via tensor network state methods in strongly correlated molecular systems

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Quantum many-body systems out of equilibrium pose some of the most intriguing questions in physics and chemistry. Unfortunately, numerically keeping track of time evolution of states under Hamiltonian dynamics constitutes a severe challenge for all known methods. Prominently, tensor network methods are marred by an entanglement blowup, which allows simulating systems following global quenches only to constant time. We present a novel scheme that allows to significantly extend the simulation time for interacting fermionic or equivalent spin systems. We show that if the manifold containing both tensor network states and fermionic mode transformations is chosen, significantly longer times can be achieved. First, we overview general tensor network state techniques, which can be used for the treatment of strongly correlated molecular systems, and connect them to concepts already used in many-body quantum physics. Recent developments on the externally corrected coupled cluster density matrix renormalization group (DMRG-TCCSD) method, fermionic orbital optimization, and time-dependent variational principle (TDVP) will be discussed in more detail. In fact, these are key ingredients of novel algorithms to study dynamics of the electron systems via tensor product approximation. Finally, new results will be shown for extended periodic systems, transition metal complexes, and Wigner crystals.

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