Grassmann time-evolving matrix product operators for quantum impurity models

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The time-evolving matrix product operators (TEMPO) method, which makes full use of the Feynman-Vernon influence functional, is the state-of-the-art tensor network method for bosonic impurity problems. However, for fermionic impurity problems the Grassmann path integral prohibits application of this method. We develop Grassmann time-evolving matrix product operators, a full fermionic analog of TEMPO, that can directly manipulates Grassmann path integrals with similar numerical cost as the bosonic counterpart. We further propose a zipup algorithm to compute expectation values on the fly without explicitly building a single large augmented density tensor, which boosts our efficiency on top of the vanilla TEMPO. Our method has a favorable complexity scaling over existing tensor network methods, and we demonstrate its performance on the non-equilibrium dynamics of the single impurity Anderson models. Our method solves the long standing problem of turning Grassmann path integrals into efficient numerical algorithms, which could significantly change the application landscape of tensor network based impurity solvers, and could also be applied for broader problems in open quantum physics and condensed matter physics.