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Matrix-product-state method with local basis optimization for nonequilibrium electron-phonon systems[1] FABIAN HEIDRICH-MEISNER, LMU Munich, Germany, CHRISTOPH BROCKT, University of Hanover, Germany, FLORIAN DORFNER, LMU Munich, Germany, LEV VIDMAR, Penn State University, USA, ERIC JECKELMANN, University of Hanover, Germany — We present a method for simulating the time evolution of quasi-one-dimensional correlated systems with strongly fluctuating bosonic degrees of freedom (e.g., phonons) using matrix product states [1]. For this purpose we combine the time-evolving block decimation (TEBD) algorithm with a local basis optimization (LBO) approach. We discuss the performance of our approach in comparison to TEBD with a bare boson basis, exact diagonalization, and diagonalization in a limited functional space. TEBD with LBO can reduce the computational cost by orders of magnitude when boson fluctuations are large and thus it allows one to investigate problems that are out of reach of other approaches. First, we test our method on the non-equilibrium dynamics of a Holstein polaron [2] and show that it allows us to study the regime of strong electron-phonon coupling. Second, the method is applied to the scattering of an electronic wave packet off a region with electron-phonon coupling. Our study reveals a rich physics including transient self-trapping and dissipation.
[1] C. Brockt, F. Dorfner, L. Vidmar, F. Heidrich-Meisner, and E. Jeckelmann, arXiv:1508.00694
[2] F. Dorfner, L. Vidmar, C. Brockt, E. Jeckelmann, F. Heidrich-Meisner, Phys. Rev. B 91, 104302 (2015)

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