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A Numerical Study of Many-Body Localization using LOBPCG¹ GREGORY D. MEYER, University of California, Berkeley, ROEL VAN BEEU-MEN, CHAO YANG, Lawrence Berkeley National Laboratory, NORMAN Y. YAO, University of California, Berkeley — Many-body localization (MBL) has generated excitement in the past decade as a fundamentally out-of-equilibrium state of quantum matter. Numerical studies have been a crucial tool for exploring MBL. For example, computing the so-called level statistics of eigenenergies by exactly diagonalizing the Hamiltonian is a common way of identifying localization. However, such exact diagonalization of an exponentially large Hamiltonian is tremendously challenging. Iterative solvers like Lanczos help with this problem by reducing memory and computation costs, but to find interior eigenvalues they must operate on a transformed matrix which is costly to compute. To avoid these costs, we apply the LOBPCG eigensolver to only the matrices H and H^2 , reducing memory costs significantly. In this scenario we are able to run all computations without ever explicitly storing the Hamiltonian in memory (matrix-free), allowing the solver to run on a single compute node for system sizes up to L = 28 spins. By using MPI for inter-node communication, we are able to push even further. Our new solver has the potential to yield insight into new MBL systems, including localization in two dimensions.

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