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Numerical studies of strongly correlated systems: beating the exponential growth in computation time

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In simulating strongly correlated systems, where approximate approaches based on small parameters are unreliable, the key problem is the exponential growth in computation time with system size, inverse temperature, or accuracy. For example, in exact diagonalization methods, the size of the vector describing the wavefunction has a length which is exponential in the number of sites. Progress in simulation methods has often involved removing this exponential for a certain class of problems. In quantum Monte Carlo, for example, for unfrustrated, half-filled Hubbard or Heisenberg models, the lack of a fermion sign problem eliminates the exponential, and large systems can be studied with high accuracy. In contrast, for most frustrated or doped systems, the expectation value of the sign falls exponentially and thus the computation time grows exponentially with the system size. The density matrix renormalization group eliminates the exponential for 1D systems. In this approach, the low entanglement of many-body ground states is exploited in a systematically improvable matrix product description of the wavefunction. For 2D systems, one is again faced with an exponential growth, but in a weaker form: an exponential of the width only, not the length. This weaker exponential has made DMRG the current method of choice for many 2D systems with a sign problem. Recently, the first approaches which appear to eliminate the exponential much more broadly have appeared, based on tensor networks such as projected entangled pair states (PEPS), which are closely related to DMRG. These methods also exploit the relatively low entanglement of ground states of realistic Hamiltonians. The computation time of these approaches, while non-exponential, is still quite high. Nevertheless, practical calculations with these methods are now becoming as good as DMRG and other approaches for 2D systems, and the methods are improving at a rapid rate.