Solving the nonequilibrium Dyson equation with quantics tensor trains

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Nonequilibrium correlated electron systems exhibit a wide variety of physical phenomena across different time scales. Numerical studies of these phenomena require accurate descriptions of short- to long-time dynamics. The nonequilibrium Green's function (NEGF) method [1] is a powerful tool for treating electron correlations and time-evolution on an equal footing. However, in nonequilibrium systems, the Green's function depends on two distinct time variables. This leads to a significant increase in memory usage, especially in long-time simulations and large lattice systems.

To address this challenge, various memory compression techniques have been proposed for the NEGF method [2,3,4]. Among them, a tensor network approach known as the quantics tensor train (QTT) has attracted attention for its ability to significantly compress the data size of Green's functions [5]. Although a prototype implementation of the QTT-based NEGF method (QTT-NEGF method) has been developed, its benchmarks have been limited to short-time simulations because of technical difficulties, such as the slow convergence of self-consistent calculations [6].

In this talk, we present advanced implementations of the QTT-NEGF method. We first developed a variational linear equation solver for the Dyson equation [7]. This allowed us to demonstrate nonequilibrium simulations up to a scale of $\mathcal{O}(100)$ inverse hopping times for a large two-dimensional lattice system with more than 4000 sites. However, this solver does not exploit the causality of the Green's function and requires a global update of the Green's function in the whole time domain, making it difficult to efficiently obtain accurate converged solutions in the long-time domain. Therefore, we developed a causality-based divide-and-conquer algorithm, where the calculation of the Green's function is limited to the newly added time domain [8]. Our algorithm allows for extending the simulated time domain without a significant increase in the cost of storing the Green's function. Furthermore, we recently developed a QTT-based dynamic mode decomposition for predicting an effective initial guess for the self-consistent calculation [9]. By combining this with the divide-and-conquer algorithm, we demonstrate that the number of self-consistent iterations is effectively reduced.

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