A highly parallelizable Quantum Monte Carlo approach to the nonequilibrium steady state of open quantum systems

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Many-body open quantum systems have attracted increasing attention in recent years due to the improvement in several experimental areas. The nonequilibrium steady state (NESS) can be characterized by quantum correlations which cannot be neglected when approaching criticality. Hence, the necessary computational cost scales exponentially with the system size. The theoretical description of open many-body systems represents a major challenge and inspite of numerous improvements the numerical modeling can be handled only for small system sizes.

In this contribution, we will discuss our recent progress in the development of a projector Monte Carlo approach which is designed for high-level parallelism allowing to run efficiently on large computational resources. The algorithm stochastically samples the time evolution of the density matrix – as dictated by the Liouville-von-Neumann equation – towards the NESS.

For closed, Hamiltonian systems, various quantum Monte Carlo approaches have been the election tool to stochastically sample system properties. Modeling the ground state properties at zero temperature in particular, is made possible by stochastically sampling the time evolution of the imaginary-time Schrödinger equation, with a class of methods generally known as projector Monte Carlo [1]. The Liouvillian dynamics towards the steady state shares with the imaginary-time Schrödinger equation the fact that, in the long-time limit, the eigenstate with the smallest-real-part-eigenvalue will dominate. In the Liouvillian case, this corresponds to the NESS. It is therefore natural to attempt an extension of projector Monte Carlo techniques to the simulation of the NESS properties.

Recently, a new projector Monte Carlo approach – called Full Configuration Interaction Quantum Monte Carlo (FCIQMC) – has been developed for quantum chemistry simulations, and was found to alleviate significantly the sign problem [2]. We present a proof of principle of the possibility to apply FCIQMC to the real-time evolution of the Liouville-von-Neumann equation towards the NESS.

We study in particular the properties of the NESS of simple nonlinear arrays, where the FCIQMC results can be compared with exact numerical results obtained using quantum trajectories. We assess the accuracy and extent of the method, testing the parallel performance on large computational clusters. FCIQMC holds promise as a computationally effective tool to address open quantum system independently of their dimensionality.

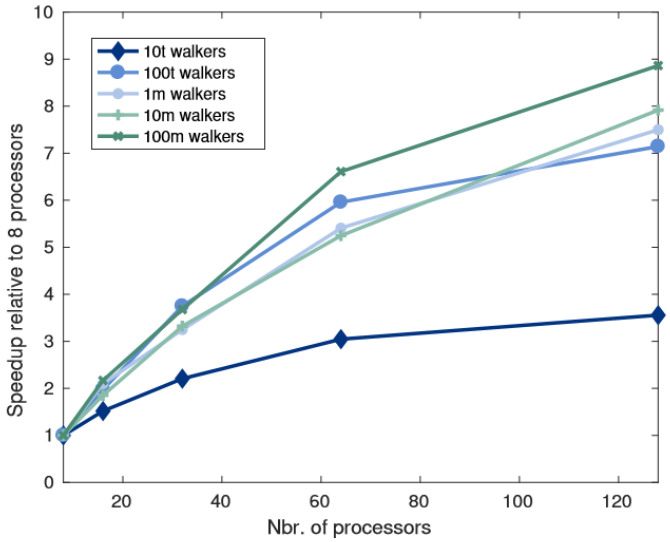

Figure 1. The speed-up as the number of parallel threads is increased from 8 to 128. The scaling improves with increasing walker population. The studied system is the 2 dimensional $J_1 - J_2$ Heisenberg-model with 16 sites.

[1] C. J. Umrigar, J. Chem. Phys. **143**, 164105 (2015).

[2] G. H. Booth, et al., J. Chem. Phys. **131**, 054106 (2009); F. R. Petruzielo, et al., Phys. Rev. Lett. **109**, 230201 (2012); J. S. Spencer, et al., J. Chem. Phys. **136**, 054110 (2012).