Hybrid Kernel Polynomial Method

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The evaluation of spectral quantities and correlation functions of large entangled systems is a core problem in computational physics today. As technology progresses, classical computers struggle to keep pace with the growing size of the quantum systems to be described. Quantum computers appear to be the solution to keep advancing in the field of quantum simulations.
However, currently available machines are still prone to errors and noise when dealing with long, dense, wide, and ultra-connected algorithms. So far, what appears to be the primary benefit of using them is the creation of random (pseudo-) circuits (as in Google's recent Sycamore processor experiment).
Decades of scientific research on quantum simulation techniques have resulted in sophisticated classical algorithms. A well-known example is the kernel polynomial method (KPM) [1], which is used to obtain the density of states (DOS), local-DOS and correlation functions through their Chebyshev expansion. The bottleneck of the algorithm resides in the computation of the Chebyshev moments, namely $Tr[H^n A]$ for different n, where A is an observable and H the Hamiltonian of the system. Our goal is to use quantum computers to solve this last step.

We are building a hybrid algorithm that uses a set of random states to perform a stochastic evaluation of trace to calculate the moments of the expansion. The powers of the Hamiltonian are implemented as derivatives of the time-evolution operator, in the manner of Ref.[2]. The trace is evaluated using a DQC1-like circuit, with a random state in place of the identity state, which cannot be directly built on a digital quantum computer. We are currently applying Richter's technique to create a random state [3], which we checked to be extremely performing in the simulation of Haar distribution and with the Trotterisation in high-dimensional Hilbert spaces. We are using the XXZ model as testing Hamiltonian, but the algorithm can be generalized to a broader class of systems.

References

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