Integrating tensor networks with quantum computing for simulations of strongly correlated materials

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The accurate numerical simulation of materials from first principles inherently relies on an efficient description of the electronic correlation underpinning many observable properties. Especially in regimes of strong correlation, dynamical mean-field theory (DMFT) has emerged as one of the main workhorses for the accurate extraction of system properties that cannot be captured efficiently by higher level theories. However, the scalability of this approach often remains limited due to inabilities of classical techniques to capture the emergence of strong entanglement within the underlying many-body problems. In this talk, we discuss novel routes towards overcoming such barriers by integrating quantum algorithms into the DMFT pipeline which aid the computation of dynamical properties such as Green's functions. We outline a hybrid quantum-classical approach [1] aiming to bring together the strengths of classical tensor network approaches and quantum algorithms to enable scalable simulations of strongly correlated materials.
Within our hybrid scheme, schematically depicted in Fig. 1, we leverage the representational power of tensor networks as a classical description of the Hamiltonian's ground state, which typically exhibits low to medium degrees of entanglement. We then extract the dynamical properties required for DMFT simulations by applying a quantum algorithm to perform a real-time evolution of the state [2] naturally increasing the entanglement and limiting the applicability of classical wavefunction methods.
In addition to the suitability of the tensor network to represent targeted Fermionic ground state, the success of the hybrid approach particularly hinges on the ability to prepare Fermionic tensor network states as shallow quantum circuits. In this talk, we show how general-purpose compilation approaches [3] can be adapted to reach necessary fidelities for the preparation of Anderson impurity model ground states. This paves the way for scaling the hybrid approach to practically relevant scenarios and eventually enable simulations that are out of reach of classical techniques.

References

[1] F. Jamet, et. al., arXiv:2304.06587
[2] F. Jamet, et. al., arXiv:2205.00094
[3] M. S. Rudolph, et. al., Quantum Sci. Technol. 9 015012 (2024)

Figures

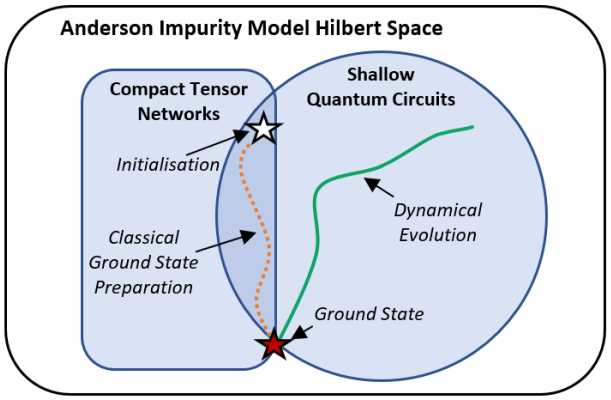

Figure 1: Schematic overview hybrid approach to compute dynamical quantities for Anderson impurity models.