

Quantum computing algorithms for Green's functions in materials science

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Quantum embedding approaches for materials simulations, such as the dynamical mean-field theory (DMFT), provide corrections to first-principles calculations for strongly correlated electrons, which are poorly described at lower levels of theory. These embedding methods are computationally demanding on classical computing architectures, and hence remain restricted to small systems, limiting the scope of their applicability. Quantum computers have the potential to overcome this limitation. In this talk we present different methods to compute the Green's functions on quantum computers for materials science simulations, which are based either on the Lehman representation (arXiv:1910.04735, Nature Comp. Sci. 1. 410 (2021)), or on a continued fraction representation using the Krylov basis. We consider two methods to construct the Krylov states. The first is based on the Krylov variational quantum algorithm (KVQA, arXiv:2105.13298), while the second method uses the quantum subspace expansion for Green's functions (QSEG, arXiv:2205.00094).