

Creation of sparse Hamiltonians optimal for quantum computing using classical-quantum hybrid schemes

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We have developed a procedure that allows us to perform embedding calculations using a classical-quantum hybrid scheme. The impurity Hamiltonian is immediately parametrized to recover the self-energy of a realistic system in the limit of high frequencies or short time. The effective interactions parametrizing the fictitious impurity Hamiltonian are local to the embedded regions thus providing a sparse Hamiltonian resulting in a low circuit depth that is excellent for quantum computing. We show that this impurity Hamiltonian can lead to excellent total energies and self-energies that approximate the quantities of the initial realistic system very well. Moreover, we show that as long as the effective impurity Hamiltonian parametrization is designed to recover the self-energy of the initial realistic system for high frequencies, we can expect a good total energy and self-energy.