Ground and excited state calculations of auxiliary-field Quantum Monte Carlo in solids*

Fengjie Ma, Wirawan Purwanto, Shiwei Zhang, and Henry Krakauer
Department of Physics, College of William and Mary, Williamsburg, VA 23187.

We present recent developments of auxiliary-field Quantum Monte Carlo (AFQMC) calculations for ground and excited state[1] in solids. Two approaches are discussed. In the first, a systematic downfolding method is developed for extended systems, which allows many-body calculations to operate on a simpler and systematically improvable Hamiltonian, while retaining material-specific properties. As a by-product, pseudopotential errors are essentially eliminated using a frozen-core treatment[2]. Dramatic savings of computational cost and excellent accuracy are achieved for a range of solids with AFQMC[3]. With this method, we determine the spin gap in NiO, a challenging material with strong electron correlation effects. In the second approach, we have implemented the recently developed multiple-projector pseudopotentials[4] into planewave based AFQMC (pw-AFQMC), which improves transferability and leads to much smaller planewave cutoff, hence less computational cost, in the pw-AFQMC calculations.

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