

Auxiliary-field quantum Monte Carlo calculations in solids[†]

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We present two recent developments in ab initio auxiliary-field quantum Monte Carlo (AFQMC) calculations of solid systems: down-folded Hamiltonians and the treatment of excited states. In the first, we derive simplified many-body Hamiltonians using truncated basis sets of Kohn-Sham orbitals obtained from the best possible density-functional calculations. AFQMC calculations are then performed on the down-folded Hamiltonians. The approach allows many-body calculations to treat a much simpler Hamiltonian while retaining material-specific properties. The Hamiltonians are systematically improvable and allow one to dial, in principle, between the simplest model and the full Hamiltonian. Test applications to typical semiconductors (Si and diamond), an ionic insulator (NaCl), and metallic systems (Na and Al) are presented. As a by-product of this approach, pseudopotential-free QMC calculations can be performed for solids².

In the second development, we formulate a many-body approach for quasi-particle band structure calculations in solids using AFQMC. An orbital orthogonalization constraint is introduced³ to prevent collapse of the stochastic Slater determinants in the imaginary-time propagation. Detailed band structures can be calculated. Results for standard semiconductors are in good agreement with experiments. For the challenging ZnO wurtzite structure, we obtain a fundamental band gap of 3.26(16) eV, consistent with experiments.

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- [2] W. Purwanto, S. Zhang, and H. Krakauer, in preparation.
- [3] F. Ma, S. Zhang, H. Krakauer, arXiv:1211.4635