An auxiliary-field quantum Monte Carlo study of the chromium dimer†

Wirawan Purwanto, Shiwei Zhang, and Henry Krakauer

Department of Physics, College of Wiliam and Mary
Williamsburg, Virginia, USA

The chromium dimer (Cr_2) has become a challenging test case for many-body electronic structure methods because of its strong correlations and complicated nature of the binding. The ground state is highly multiconfigurational; in addition, accurate treatment of the dynamic correlation is essential to describe its weak binding. The quest for a scalable many-body method that is capable of treating this system properly is still ongoing despite many years of efforts. We will present results from an ongoing study of Cr_2 molecule using the auxiliary-field quantum Monte Carlo (AFQMC) method. We use the phaseless AFQMC (ph-AFQMC) method[1] to calculate the ground-state properties of Cr_2 using large, realistic basis sets. In parallel, we perform unconstrained (exact) AFQMC calculations for smaller basis sets to systematically improve the ph-AFQMC results. The calculated spectroscopic properties of the Cr_2 molecule are in good agreement with the experimental results.

† This research work is supported by DOE and NSF. Computing is provided by NCSA Blue Waters, CPD, and W&M SciClone.

[1] Zhang and Krakauer, Phys. Rev. Lett. **90**, 136401 (2003)