Slater determinant and pfaffian expansions for wave functions in electronic structure QMC

Michal Bajdich, Shuming Hu, and Lubos Mitas

CHIPS, Department of Physics, North Carolina State University
Raleigh, NC, USA

We investigate several types of expansions in Slater determinants and pfaffians [1] for trial wave functions in fixed-node quantum Monte Carlo. The long expansions in determinants are analyzed in order to identify the terms with the largest contributions towards decreasing the fixed-node errors. We demonstrate a mapping of the CI wave functions with single and double excitations onto pfaffians with reduced expansion size. We test this approach on the cases of atomic and molecular systems and we discuss the amounts of recovered correlation energy relative to the expansion size. Finally, following upon our previous study [1], we explore the use of multiple determinants and pfaffians for the accurate description of the wave functions of simple solids.

[1] M. Bajdich *et al.* Phys. Rev. Lett. **96**, 130201 (2006); Phys. Rev. B **77**, 115112 (2008).