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Slater determinant and pfaffian expansions for wave functions in electronic structure quantum Monte Carlo MICHAL BAJDICH, LUBOS MITAS, CHiPS, Department of Physics, North Carolina State University — We investigate several types of expansions in Slater determinants and pfaffians 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 further investigate the efficient mapping of these terms onto pfaffian expansions. We apply this technique to test the cases of molecular and atomic 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).

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