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Approach toward Linear Scaling QMC[1] BRYAN CLARK, Physics Department, University of Illinois Urbana-Champaign (UIUC), DAVID CEPERLEY, Physics Department, NCSA at UIUC, ERIC DE STURLER, Department of Mathematics, Virginia Tech, Computer Science Department at UIUC — Quantum Monte Carlo simulations of fermions are currently done for relatively small system sizes, e.g., fewer than one thousand fermions. The most time-consuming part of the code for larger systems depends critically on the speed with which the ratio of a wavefunction for two different configurations can be evaluated. Most of the time goes into calculating the ratio of two determinants; this scales naively as $O(n^3)$ operations. Work by Williamson, et al. (2) have improved the procedure for evaluating the elements of the Slater matrix, so it can be done in linear time. Our work involves developing methods to evaluate the ratio of these Slater determinants quickly. We compare a number of methods including work involving iterative techniques, sparse approximate inverses, and faster matrix updating.

(2) A. J. Williamson, R.Q. Hood and J.C. Grossman, Phys. Rev. Lett. 87, 246406 (2001)

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