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Systematic reduction of sign errors in many-body calculations of atoms and molecules P.R.C. KENT, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 , M. BAJDICH, M.L. TIAGO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, R.Q. HOOD, Lawrence Livermore National Laboratory, Livermore, CA 94550, F.A. REBOREDO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 — We apply the self-healing diffusion Monte Carlo algorithm (SHDMC) [Phys. Rev. B **79** 195117 (2009), ibid. **80** 125110 (2009)] to the calculation of ground states of atoms and molecules. By comparing with configuration interaction results we show the method yields systematic convergence towards the exact ground state wave function and reduction of the fixed-node DMC sign error. We present results for atoms and light molecules, obtaining, e.g. the binding of N_2 to chemical accuracy. Moreover, we demonstrate that the algorithm is robust enough to be used for the systems as large as the fullerene C_{20} starting from a set of random coefficients. SHDMC thus constitutes a practical method for systematically reducing the Fermion sign problem in electronic structure calculations. Research sponsored by the ORNL LDRD program (MB), U.S. DOE BES Divisions of Materials Sciences & Engineering (FAR, MLT) and Scientific User Facilities (PRCK). LLNL research was performed under U.S. DOE contract DE-AC52-07NA27344 (RQH).

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