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Optimization of quantum Monte Carlo wave functions by energy minimization[1] JULIEN TOULOUSE, CYRUS UMRIGAR, Theory Center and LASSP, Cornell University, Ithaca, New York, USA. — We present a simple, robust and highly efficient method for optimizing all parameters of many-body wave functions by energy minimization in quantum Monte Carlo calculations. Using a strong zero-variance principle, the optimal parameters are determined by diagonalizing the Hamiltonian matrix in the space spanned by the wave function and its derivatives [1-2]. We discuss the connection with previously-proposed energy minimization methods, namely the modified Newton method [3] and the perturbative energy fluctuation potential method [4]. Application of the method to electronic atomic and molecular systems show that it systematically reduces the diffusion Monte Carlo fixed-node error. [1] J. Toulouse and C. J. Umrigar, submitted to J. Chem. Phys. [2] C. J. Umrigar, J. Toulouse, C. Filippi, S. Sorella, and R. G. Hennig, cond-mat/0611094. [3] C. J. Umrigar and C. Filippi, Phys. Rev. Lett. 94, 150201 (2005). [4] A. Scemama and C. Filippi, Phys. Rev. B 73, 241101 (2006).

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