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Energy optimization of quantum Monte Carlo wave functions¹ C.J. UMRIGAR, J. TOULOUSE, Cornell University — In recent years many methods have been proposed for energy optimizing quantum Monte Carlo wave functions. Of these, the three highly efficient methods are: 1) The generalized eigenvalue method of Nightingale and Melik-Alaverdian, which was proposed by them for linear parameters only but extended by us to nonlinear parameters. 2) The effective fluctuation potential (EFP) method of Fahy, Filippi and coworkers, and the recent perturbative EFP of Schautz, Scemama and Filippi. We show that the latter can be more simply derived as first-order perturbation theory in a nonorthogonal basis. 3) The modified Newton method of Umrigar and Filippi and of Sorella. We show that the three methods are related to each other and point out that a control parameter can be employed in each of them to make them totally stable. We use these methods to optimize all the parameters in the Jastrow and the determinantal parts of the wave function and point out that different issues arise in optimizing the Jastrow and the determinantal parameters. By systematically increasing the number of determinants we find that seemingly similar systems, such as C_2 and Si_2 have vastly different fixed-node errors for single-determinant wave functions.

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