Improving the scalings of Quantum Monte Carlo methods, with multi-determinant expansions.

Roland Assaraf, Claudia Filippi and Saverio Moroni.

Department of Chemistry, Université P. et M. Curie
Paris, France

We present recent developments of quantum Monte Carlo methods in real space, to compute efficientlly many energy derivatives and observables, with a multi-determinant Jastrow-Slater wave function. The computational scaling as a function of the number N_e+1 of determinants is reduced to $O(N_e)$ for an entire set of derivatives down from $O(N_e)^1$ or $O(NN_e)^2$ per derivative, where N is the number of electrons. As a function of N, the computational cost, $O(N^{0-2})$ per derivative, extends what is obtained with the less transparent algorithmic differentiation technique for one single determinant.

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