Computing efficiently energy derivatives in quantum Monte Carlo with multi-determinant expansions.

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We present recent advances for computing with quantum Monte Carlo methods energy derivatives and properties (interatomic forces and so on), 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 $O(N_e)$ per derivative [1], down from $O(NN_e)$ [2] where N is the number of electrons. Our formulas use simple matrix algebra, and recover the efficiency of the less transparent algorithmic differentiation technique for one single determinant ($N_e = 0$). We also show that the scaling can be further reduced from $O(N_e)$ per derivative to $O(N_e)$ for the entire set of derivatives[3]. In practice the extra cost of an expansion ($N_e > 0$) on the numerical scaling is only $O(N_e)$ per Monte Carlo step, independently of the number of derivatives.

[1] C. Filippi, R. Assaraf and S. Moroni, J. Chem. Phys. **144**, 194105 (2016).

[2] K. Clark, M. A. Morales, J. McMinis, J. Kim, and G. E. Scuseria, J. Chem. Phys. **135**, 244105 (2011).

[3] In preparation.